Scientific Computing with PCs

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Preface

This book tells "what to", "why to" and "when to" use personal computers (PCs) for carrying out scientific computing tasks. There are many books that purport to tell users how to operate particular software packages or to set up and maintain their personal computer hardware. These "how to" volumes have their proper role and utility. Our goal is different: we aim to present ideas about the management decisions involved in using PCs for scientific and technical computing.

The audience for this book is any scientist, engineer, statistician, economist, or similar worker who is considering using a personal computer for all or part of his or her technical work. The ideas we present can be used at the individual or group level. Being ideas about the management of resources, they are kept simple to the extent that readers will think "I know that." We stress, however, that it is the day-to-day practice of management ideas that counts; theoretical knowledge is like a smoke alarm without a battery.

There are three themes to this book:

- Deciding what is or is not reasonable to attempt in the way of scientific computing with a PC;
- Learning about and finding software to carry out our tasks with a minimum of fuss;
- Choosing the tools to match the task to keep costs low.

By PC we will mean any computer system that is managed, used and maintained by a single person. The typical examples are the relatives and descendants of the original IBM PC and the Apple Macintosh, but other machines and workstations have similar properties. Workstation networks and mainframes with system support staff have quite different management strategies. Portable computers used with such larger systems are, however, very likely to be used in a way that requires the user to exercise management skills. Our examples use mainly MS-DOS PCs since these are the most common.

The reader will notice some repetition of ideas we feel important; we also have tried to keep sections of the book self-contained.

The distribution mechanism for this book is an experiment in a new form of publishing using the Internet. We did not intend this to be the case. Unfortunately the publisher who commissioned the book as a venture into a new subject area decided to retreat in the face of recessionary pressures after we had submitted a typeset manuscript. Interest from other publishers did not transform itself into a contract. Our response has been to pay to have the work professionally reviewed — as a good publisher should — and to then edit and produce the work in a form that users can print out for their own use.

The current work has been formatted to reduce the number of pages from about 300 to about 200 by choosing margins that use more of the page area on traditional letter-size paper. We believe that A4 paper users will find that pages fit this size also.

Your comments are welcome.

John & Mary Nash, Ottawa, September 1994

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The book (and related materials) may be obtained by anonymous FTP from:

MacNash.admin.uottawa.ca

The full work is approximately 200 pages long and the PostScript files occupy about 4 megabytes of storage.

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Part I: Panorama

To get a good idea of the lie of the land, one finds a convenient tree, hill or building and exploits the larger field of view gained by height. As a preliminary to the detailed study of the application of personal computers (PCs) to scientific computation, we will take such a panoramic view. First, a chapter on the aims (and non-aims) of this book, which concern the way in which scientific problems are solved and the role of computations in such solutions.

Chapter 1

Introduction and Purpose: How Scientific Problems are Solved

1.1 Background
1.2 Goals
1.3 The scientific method and our audience
1.4 Computer configurations of interest
1.5 Computing styles

This book aims to help ***researchers*** who are not computer specialists to use PCs profitably and efficiently. It is especially concerned with the strategies and tactics that enable users to carry out their ***scientific*** work in all aspects — technical, administrative and educational — with the aid of PCs. We do not claim that PCs are the "best" answer for scientific computations but point out that they deserve consideration. Indeed our message is that there is no uniquely "best" approach to scientific problem solving, but that there are generally several options that will provide satisfactory results with modest expenditure of time and money. It is toward reasoned consideration of the PC option that we direct our energies here.

1.1 Background

The PCs of this book are primarily those of the IBM PC family, with the Apple Macintosh also kept in mind. We will use the abbreviation ***PC*** to refer to machines of ***both*** the IBM PC (that is, MS-DOS) family and the Apple Macintosh. Because we have less familiarity with Atari and Commodore machines, there are few references to them. Workstations based on the UNIX operating system, such as SUN, NeXT, IBM RS6000, certain Hewlett-Packard machines and many others, have not been used as examples, mainly because our use of such machines has been limited. The ideas presented in this book can nevertheless be applied to such machines, particularly if the reader is the system manager. The software and manner of use of workstations is, in our opinion, qualitatively different from that of PCs and Macintoshes in that the workstations are less independent machines than parts of larger networks. While many PCs are also connected in networks, the type of central support provided is more likely, we think, to be limited to

non-scientific applications. Thus there is a qualitative difference between the PC world and the (UNIX) workstation world in the technical support provided to the user for scientific computations.

We note that both IBM PC and Macintosh can be operated under variants of Unix, and that OS/2 is another choice of operating system for IBM PC users. As we write, Microsoft is introducing Windows NT. We will mention such environments as appropriate, but they are not critical to our examples.

The realities of present-day PCs are as interesting as the publicity that surrounds them. However, there is a lot less glamour to be found in the reality of PCs than in the advertising copy. This introduction presents the authors' goals in writing this book, suggests the type of reader who will find it most useful, and declares several topics that will not be covered.

We will caution that advertised products need to be evaluated carefully. New products may be able to serve us, but obstacles or restrictions mentioned in the fine print or omitted entirely may prevent easy resolution of our problems. While users are now less likely to resort to doing their own programming than a decade ago, there are still many computational problems that require such brute-force efforts. Furthermore, the existence of commercial software that solves only one problem is not necessarily helpful; it is difficult to justify spending hundreds of dollars to solve a problem that may be a small part of a larger task.

An annoying aspect of today's rapidly developing computer world, at least from the point of view of the ***computist*** — the person who must perform calculations — is the constant stream of statements, articles, lectures and papers that describe "new, improved" hardware or software. The realities of life in the world of technical computation, be it in engineering, natural sciences, economics, statistics or business, are that funds are not available to acquire each new piece of apparently useful electronics or program code. Furthermore, the cost of learning and evaluating a single new product is high. The pressure to bring out a new product ahead of competitors is such that errors are probably present in the first (or second or third or . . .) models delivered. This leads to contradictory evaluations of products in the literature, forcing prospective users to spend much valuable time and effort to discover the true utility of the product for their own situation.

There is, of course, pressure among the user's own community to use the "latest and best." Salespeople, industry writers and futurists have successfully created a collective faith in the ongoing rapid change in computing. New products are supposedly obsolete as soon as they are delivered. While we all like to be modern and up-to-date, much of the panic and hurrah is a myth. The truth is no less interesting, but does not have the glamour and air-brush artwork that should, in any event, be left for the cover of fashion magazines.

We have studied computation and performed calculations for more than twenty-five years. In that time, many new and interesting devices have been brought to market. There have been substantial decreases in the real costs of computing. In 1968, we paid $200 (Canadian) for a second-hand Monroe hand-cranked mechanical calculator. In 1980, we bought the Sharp PC 1211/Radio Shack Pocket Computer for $279 (Canadian). This machine was capable of quite sophisticated programs in BASIC and had a large repertoire of special functions. In 1992, a modest PC with 640K memory and floppy disk drives can be bought for under $500 (Canadian) and a PC/AT with fixed disk for under $1000. Clearly, these are great advances, and the Monroe is now a fondly regarded antique that nevertheless still functions perfectly. In its time it fulfilled a need and was used to solve many problems similar to those still coming across our desk today. In turn, the other machines will serve their time before being replaced. In fact we disposed of our first generation personal computers late in 1991 after over 13 years of solid service.

The useful lifetime of computers continues to be several years. There are sound business and operational reasons for this. One cannot consider equipment with a useful lifetime of less than five years as a good investment, though we may expect the uses of equipment to change over that lifetime. Similarly, manufacturers wish to convince us that their products are the last word in technology, but must have long enough production runs to keep their costs to a minimum. Thus many "innovations" are cosmetic and

designed to respond to marketing pressures.

In the practice of computation the changes observed in the last twenty-five years have been quite gradual. Several commendable efforts have been made to produce quality mathematical software packages and libraries. Despite the success of some of these efforts and the appearance of several new journals dedicated to specialized computation, there is still a vast body of very low quality programs in use that have been purchased, borrowed or stolen. These have frequently been installed without regard to the effects that a different computing environment may introduce into a calculated result.

1.2 Goals

To the chagrin of developers of quality mathematical software, poorly designed programs will correctly solve more than 99% of the problems presented to them. The expense and effort of good program development is spent mostly to prevent disaster for a few cases in a million. This "insurance" aspect of quality software is difficult to sell to users. A user who is happy with, but ignorant of, results from a poor program is unlikely to change programs if it means, as it usually does, a considerable effort and cost. Knowledgeable staff are seldom available to help the scientific user in the implementation of programs to carry out calculations. Unlike programs to process data or control functions, the results of computational programs are rarely right or wrong absolutely. That is, success in obtaining reasonable results is not necessarily a sign that the calculation has been correctly performed. Worse, correct performance in a number of cases may only lead to a false sense of confidence in a program destined to give erroneous output in a future calculation. If this output is the basis of decisions — business investment, government policy, vehicle design or aircraft navigation — we have the seeds of catastrophe. With increasing reliance on computations and simulations in all fields of human endeavor, the possibility and likelihood of occurrence of disasters large, and small, because of software failure, are an unfortunate reality in all our lives. We address such topics in our related work on technological risks.

One objective, then, of this book is the realistic evaluation of what may be accomplished with the computers that are commonly available to those of us who must perform calculations.

The second concern is the choice of ***strategies*** and ***tactics*** to make the most of the capabilities while avoiding or overcoming the limitations, diversity or inconsistency. Much of this material is common to all computing and data processing, be it on large, general-purpose machines, PCs or even a calculator, pencil and paper. In this we wish to avoid gimmicks and tricks, instead emphasizing a scientific approach. That is, we test claims, measure performance, deepen our understanding of what works and what does not, gradually improving our computing tools and our abilities to use them as we develop a solution to a problem.

A third goal will be avoiding unnecessary expense. Those with money and time to throw away we thank for buying our book. They need read no further. Others with slimmer budgets will hopefully find some useful tips to keep costs down.

In summary, this book is intended to be a guide and handbook to the calculation practitioner who must produce correct answers to problems that can be stated mathematically. With this in mind, an index is provided to enable quick reference use of the material. It is our hope that the text is interesting, comprehensible, and informative to users.

Having stated the goals of this book, it may be assumed that objectives left unmentioned will not be pursued. However, the diverse and turbulent activity concerning PCs has created a climate where readers may expect a different book from that which we have written. Therefore, a short list of topics that are ***not*** addressed is presented here.

- There is no comparative shopping guide to computer hardware, peripherals or software. The examples that do appear are there to serve as illustrations of the text. One reason for not attempting such a catalog is that it is difficult to keep it accurate in detail as manufacturers make alterations and

introduce their "new" products. Another reason is that we prefer to write from experience, which clearly cannot be products just released today.

- There is no attempt to present mathematical software formally in this volume. In other works (Nash J C, 1990d; Nash J C and Walker-Smith, 1987; our magazine columns) we have discussed methods for solution of many mathematical problems. We do, where appropriate, mention some sources and examples of mathematical software. We point to sources and advice on their use, but do not include machine readable software.
- There is no attempt to provide an all-purpose handbook for every PC owner. While we sincerely feel there are useful ideas here for all who work with computers, the focus is on calculation and its practitioners as described below.

1.3 The Scientific Method and Our Audience

In all technical fields of endeavor, quantitative methods are assuming an increasing importance and use. Heightening our understanding of phenomena, natural or man-made, quantitative measures bring a level of detail compared to simple qualitative descriptions of observed objects or events. In business decision-making, numerical rather than descriptive information is vital. In engineering, accurate calculations of the strengths of structures and materials are important in saving millions of dollars in unnecessary effort and fabric, while at the same time such results are critical to the integrity and safety of the structures built.

Quantitative methods are an outgrowth of the scientific method, which may be summarized as follows:

- Careful observation of the system of interest;
- Formulation of a model explaining the system's behavior;
- Testing of the model by comparison of its behavior with that of the real system;
- Further observation, model refinement and testing.

From the natural sciences, the scientific method has in recent years spread to social sciences and business. Not all applications have been either well-founded or well-executed, especially when the scientific method is taken to imply the use of a computer model. Models are popular because they are much less costly than experiments or prototypes. Their limitations derive from our imperfect understanding or poor approximation of the system in question. In a social model of consumer buying habits, we may be content with very rough indicators of how a large group of people react to changes in prices or policies, since the alternative is a complete lack of information. For aircraft flight simulation, however, we wish to mimic the behavior of an airplane very precisely so that the pilot can practice maneuvers without risk to life or property, while saving fuel and avoiding airport charges.

Models and related quantitative methods (the spectrum of statistical and data analysis tools) require calculations to be performed. It is to those who must carry out these calculations that this book is directed. The special interest is PCs, because calculations are increasingly being carried out in such computing environments.

1.4 Computer Configurations of Interest

PCs may be purchased with an extremely wide range of options and it is necessary to define the type of machine that is the focus of this book.

For our purposes, we will be interested in machines that are can carry out serious computations, which implies they must be able to run reasonably sophisticated software. The key word here is "reasonably." In 1980, such software was operated in a machine with a processor, memory, video display and keyboard,

with 5.25 inch floppy disks for information storage. By the beginning of the 1990s, a fast fixed disk had become more or less essential, in addition to the floppy disks (now 5.25 inches and 3.5 inches) that are used as a medium for supply and exchange of data or programs. Furthermore, a large enough main memory size is likely to be important so that scientific problems involving matrices and vectors can be solved without heroic measures to manipulate memory and disk space.

To the basic machine, we would generally add a printer, which should support some form of graphical output so that the user can plot as well as print information. This implies some form of dot-matrix printer, or its higher-resolution cousins, the laser or ink-jet printer. We also believe communications with the outside world are important. If telephone lines are the means of communication, then a modem is needed (Section 2.2).

The above requirements can be met by many different examples of machines in the IBM PC and Macintosh families.

1.5 Computing Styles

Throughout this book we will discuss ideas that relate to ***computing style***. That is, we will be interested in ***how*** users get the job done, with the "job" referring to scientific computations and related data processing. Our experience has been that, even in the physical sciences, style counts as much as substance. Scientists, engineers, economists and statisticians can easily get as excited or angry about cosmetic details as about fundamental theories. In this we are as guilty as others. For example, we do not particularly like mouse-controlled interfaces, though we have colleagues who swear they are the only reasonable approach. We hope readers will find our treatment "permissive," allowing each user to select his/her own preferred mode of operation.

Style also refers to the choices of ***what*** parts of one's work are performed with a PC. Some users employ just one computing platform, their PC. However, most scientists use more than one computer for their work and we will try to point out the major advantages and pitfalls of multiple platform computing as we proceed. In particular, we will try to raise alarms about situations where data might be awkward to transfer between platforms. Such "glitches" invariably cause great consternation. After all, the data is "right here on this diskette," yet neither action, prayer nor curses will release it.

At the same time, we will try to encourage users to maintain their data and program resources in a state where they can be moved across machine boundaries and shared with others. The synergy that results when like-minded researchers can easily exchange ideas and information is of immense value. In our own experience it is highly rewarding, at times accompanied by moments of scintillating intellectual insight that would never arise without the interaction of other workers.

Chapter 2

Data processing capabilities of PCs

2.1 Non-mathematical data processing related to calculation
2.2 Communications — Access to remote data
2.3 Automated data collection
2.4 Input, output, edit, and selection
2.5 Scientific text processing
2.6 Macro-editors and data converters
2.7 Graphics
2.8 Report writers
2.9 Programming and program development
2.10 Administration of research

This chapter concerns the data processing tasks that do not generally involve arithmetic. Even so, these tasks may be a very important part of our ***overall*** scientific computing effort. We take the viewpoint that a problem is not truly "solved" until the results have been convincingly reported. Thus preparing reports, talks and papers, along with a variety of other work that supports and permits the solution of problems, is scientific computing.

2.1 Non-mathematical Data Processing Related to Calculation

While this book is about scientific computing, it is rare that PCs are engaged in formal calculation work for more than a small percentage of the time. The primary reason for this is that PCs serve their users as data and word-processing tools, as well as engines to perform computations. In contrast, a high-performance supercomputer will generally be fed tasks by other computers. We do not expect such number-crunching boxes to occupy their expensive cycles waiting for keyboard entry or mouse clicks.

Because PCs act as a doorway to calculations, we shall point out how they prepare for and control calculations and how they help manage and report results. PCs are also used to direct tasks on other computers, or gather data or bibliographic citations from remote sources. These tasks, while tangential to scientific computing, are nevertheless essential to the advancement of research. Especially in the social sciences and statistics, we may need a great deal of clerical effort before calculation starts.

Clearly such work is not mathematical in nature. The main goal is to move, transform and put in order various quantities of data so that calculations can be performed, results organized and analyzed, and reports written. In the remainder of this chapter we shall look at the capabilities of PCs to help in this work.

2.2 Communications — Access to Remote Data

Because workers must communicate with their colleagues, a large part of any researcher's time is spent in written and oral communications. Letters are giving way to facsimile transmissions (fax) and electronic mail (email) exchanges. Some workers are also using direct machine-to-machine linkages, either via informal or organized attempts at group working (see for instance, the entire issue of the Communications

of the ACM for December 1991).

In sharing ideas, we must choose between direct interaction — the real-time, online, face-to-face or telephone exchange — and indirect communication — letters, email, fax, bulletin board exchanges, voice mail, or similar offline (time-independent) information exchange. Our own preference is offline: we like to read and sort messages at our convenience. Call Waiting or mobile telephone service offer to keep us always in touch. Following our policy throughout this book, we stress that each user of technology should carefully analyze his or her own situation. PCs are a part of such communication choices.

From our perspective, the important feature is ***connectivity*** — the fact that a PC can be linked to whatever source of data or information the user requires. There are some difficulties:

- Physical obstacles exist in the form of incompatible hardware such as interface ports and connectors at either end of the connection we wish to make, lack of suitable linkages such as transmission wires, or modems operating under different physical protocols (Derfler and Byrd, 1991).
- Logical obstacles occur when we do not have suitable accounts on the email networks of interest, or there is no gateway between our network and that of the person with whom we wish to exchange information, or the information is stored or transmitted in incompatible formats.
- Lack of training or understanding of the software and protocols may prevent us from establishing the connection. For example, we may not know how to log into a bulletin board, or if we do know, we may not know the correct modem settings for the speed, parity and word size.

Increasingly, users of PCs are connected to Local Area Networks (LANs). These should serve to simplify and speed up the connections we are likely to make. However, they may inhibit the worker who needs to do something out of the ordinary. LANs are usually managed for the benefit of a perceived "majority" of users. As LANs get larger, or are linked together, Wide Area Networks (WANs) are beginning to appear.

Increasingly, academic and other research environments are being linked together by special high-speed networks. These allow for rapid electronic mail, file transfer, and remote computer operation. There have been some unfortunate abuses of these systems in the form of unauthorized access and destructive programs (viruses, worms, etc.), but the benefits appear to outweigh the costs by a wide margin. The networks now link most parts of the world and connections and email are increasingly reliable. This has fostered the development of electronic newsletters and journals, special database servers to supply particular software or data, and a variety of electronic "conferences" (Krol, 1992; Stoll, 1990).

For PC users, it is important to note that while the networks transmit binary data, there may be nodes between us and a source of information that insist on working with text information. To allow the binary data to cross such a node, it is common to encode the binary data as printable text characters. The receiving computer reverses the coding. Two common formats for such exchange are UUENCODE and BINHEX, for which programs may be found in a variety of public repositories. There are also ways to transmit binary data across modems directly (Nash J C, 1993a).

2.3 Automated Data Collection

Researchers are in the business of gathering data. Measurements used to be taken with simple instruments and recorded on paper, traditionally in bound, hard-cover laboratory notebooks. Analysis was with pencil and paper. With electronic technology has come a capacity for instruments to provide output directly in digital form, suitable for direct input to computers. There is an increasing use of computer technology for control and calibration of these same instruments. PCs have frequently been used as both control and data-gathering devices (e.g., Okamura and Aghai-Tabriz, 1985). Instruments with auto-answer modems connected to the telephone network allow remote measuring stations to transfer data to a central site. We suggest readers investigate the possibilities of automated instruments with care, since data collection is generally done in real-time and must necessarily interfere with conventional machine operations.

Optical scanning equipment, though designed for optical character recognition and for the input of graphic material, can provide data to be processed in a variety of ways. There are cameras for input of still or video images. Researchers studying sound or electro-magnetic signals have a variety of instruments for inputting raw data. MIDI interfaces allow two-way transmission of musical information between instruments, synthesizers and computers. We have used scanners with moderate success to process photos and other images for use in reports and also to convert a typescript of a century-old diary into machine-readable form.

A variety of other interface mechanisms are used between computers and measurement devices.

2.4 Input, Output, Edit, and Selection

PCs are well suited to the task of entering, correcting and transforming data. It is relatively easy to write particular programs that provide a very friendly user interface yet carry out extensive error checking for well-structured problems. That is, if the problems are always of a specific type, a data entry program can be prepared straightforwardly to allow non-specialists to enter the data.

Preparation of a general data entry program is much more difficult. *A priori* we do not know the structure, type or precision of the data to be expected. Is it numeric or alphabetic? Whole numbers, fractions or mixed? Four digits or ten? How is each data element to be identified? Typically we, along with many users, employ a text editor and enter our data as simple lines of text information, though this allows no immediate control on the elements we are keying in. Statisticians use the word "edit" for the process of checking data elements to see if they are "reasonable"; the word "imputation" is used for the substitution of reasonable values for missing entries.

Similarly, a general data transformation program is difficult to produce, but special ones are easily implemented on PCs. Spreadsheet packages come close to being general data transformation programs. They have the great advantage that they are generally well known by non-programmers. They are easy to use for data entry. Editing individual entries to correct small errors is not difficult, but more global editing, such as a repeated find and replace, may be more awkward. They also generally lack a way to prepare general "scripts" that can be applied to many worksheets (Nash J C, 1993b). Simple graphs can be prepared easily. Most spreadsheet programs also incorporate some database management functions, but their strengths are the straightforward manipulation of tabular data.

Most PC database management programs also offer some attractive features for data entry, edit and selection. In particular, we may quite easily "program in" checks for absurd data. For example, a traditional concern with census data in the United States is the number of women who report multiple children and also report their age as under 14 (Sande I, 1982). Database management programs generally require more effort to use, in our opinion, than spreadsheet programs, but they offer greater flexibility.

2.5 Scientific Text Processing

Since the preparation of technical papers and reports is a primary data-processing task of PCs, it is important to consider the possible approaches we may take. There are several special-purpose text-processors designed to handle scientific material. In particular, the input and editing of mathematical and, to a lesser extent, chemical formulas are useful requirements. Such formulas are only slightly more difficult to write down on paper than the prose that usually surrounds them. However, as far as we are aware, all computer text processing systems make formula entry much more difficult than text entry. This is because text is mostly ***linear*** in the way in which it is presented, that is, one word follows another, left to right across the page in European languages. Formulas require us to recognize a variety of horizontal and vertical spacing rules, all of which can have very important meanings for the writer and reader.

It is our opinion that the learning cost is the greatest barrier to the use of special-purpose scientific text processors. There are a bewildering number of features and choices to make, as well as several interface mechanisms to consider. Of these, we note in particular T_EX (Knuth, 1986), which is perhaps the most important of the ***mark-up languages***. In a mark-up language, all the material is entered as text in a standard alphabet with special commands embedded to indicate fonts, positioning, type styles, special symbols, underlining, etc. The commands use characters from the standard alphabet. T_EX prepares material for type-setting, but the source material is not particularly readable to the uninitiated. The alternative is a WYSIWYG (What You See Is What You Get) approach where the user selects and positions symbols, possibly with the aid of some built-in formatting rules. An extensive surveys of scientific text processing has been carried out under the direction of Dr. Richard Goldstein (Goldstein et al., 1987a, 1987b, 1987c).

As special-purpose scientific text processors have evolved, the general word-processing vendors have also sought to add scientific features to their products. This book has been prepared using WordPerfect 5.1 (abbreviated WP5.1 from now on) using an MS-DOS computer with a VGA screen. We chose to use WP5.1 mainly for reasons of ***safety*** rather than features or convenience. In particular, with the very large installed base of users, there was likely to be advice and assistance available to overcome difficulties and user-UNfriendly quirks, of which we encountered many.

2.6 Macro-editors and Data Converters

Scientific computation inevitably requires data to be edited or its format transformed so that programs can make use of it. Lack of appropriate tools for these tasks is perhaps the most common source of frustration for researchers attempting to use PCs in their work. Sometimes editing and reformatting can be accomplished with a suitable macro-editor as discussed below.

Most PC users have some form of text editor. Frequently it is the same editor that is used for preparing letters or reports. Unfortunately, there are some significant dangers for the unwary. Students who have learned a word-processor such as WP5.1 frequently do not realize that the "document" files saved by word-processors include a large amount of information on how the document is to appear on the page. This information is stored as bytes in the file additional to the text in which we are interested. When an application program such as a programming language compiler reads the file, anticipating only the text, errors occur.

Even as a tool for looking at results, word processors have deficiencies. For example, it is quite simple to build a spreadsheet of fifteen columns of numbers. Allowing 10 spaces per column, this is 150 spaces wide. If we import the "printout" from such a spreadsheet into a word processor, we may find that the pleasant tabular structure of columns and rows has become an almost unreadable jumble of numbers and column headings. The difficulties are:

- Word processors often allow users to set and change margins and font sizes. Text is then ***wrapped*** to fit the margins. That is, the line lengths are adjusted to fit the margins, not vice-versa. We need to set our margins wide enough to accommodate the 150 character-wide lines of our spreadsheet if we wish to be able to see the structure.
- Word processors usually allow proportionally-spaced fonts. In these, the number 1 may take less space than a number 9 or a 7. The column alignment is once again lost unless we specify that a monospaced font is to be used.

This does ***not*** imply that one cannot use a familiar word-processing editor, but care needs to be taken.

It is quite easy to find public domain or freeware editors that allow for the manipulation of the text alone. (NED — the Nash EDitor — is our own freeware contribution. At under 6K bytes, it is very small and fast, yet includes a help screen and mouse support. See Nash, 1990a.) Users may also find that there are convenient editing tools included with programming languages or even with the operating system. Microsoft, after many years of imposing the truly medieval EDLIN on MS-DOS users, incorporated the

Quick BASIC editor EDIT, in MS-DOS 5.0. Such tools serve very well to correct or adjust a few characters in a file but are less useful when many changes have to be made.

For manipulations that have to be repeated, we recommend a ***macro-editor***, in which the user can set up several sequences of commands that can be executed via a single keystroke. This vastly simplifies operations of removing unwanted commas in data files, stripping out or adding in spaces, and similar tedious but necessary operations.

When we have a large (>50K) file to manipulate we use the commercial version of NED. It can edit any file for which we have enough disk space. One common use of such editors is to search through large text files for information.

We find that we use variations on the above theme nearly every day. Clearly we could use a special text search utility like the UNIX facility GREP. We occasionally use file viewers that allow searching, but prefer a small set of very familiar working tools. Moreover, the editor allows us to buffer and extract pieces of the text in which we are interested.

Clearly a text editor cannot easily adjust a file that is encoded in some way. For example, spreadsheet data files contain a variety of different forms of data: numbers, strings, data ranges, printing and output control information, and graphs. The typical worksheet is saved in binary form and is not amenable to viewing without special programs. Similar comments may apply to the files saved by database management programs, though some packages advertise the important fact that information is stored in text files.

We usually find it easiest to extract information from spreadsheets or database programs by "printing" information to a text file and editing it with our text editor. We use the spreadsheet or database program to select ***which*** data we save to the file, as well as the ***order*** in which it is presented, while the text editor is used to adjust the detailed layout or format. Here we are following a strategy of choosing to use familiar tools and a tactic of using each to perform tasks for which it is best suited.

Alternate approaches exist. In circumstances dependent on the application and frequency of use, we may prefer to use the ***data translation*** facilities of programs we use. Spreadsheet, database, word-processing, and statistical programs frequently provide selected translation facilities, especially ***into***, but less commonly ***out of***, their native formats. We note, for example, the Translate facility of Lotus 1-2-3. When buying software, it is important to note which data formats can be used.

More generally, there exist programs that attempt to convert a range of different data formats, even across operating systems or computing platforms. Usage will depend on application. For example, MACLINK converts file and disk formats for a variety of word processing programs between the Apple Macintosh and MS-DOS families of computers. DBMSCOPY allows data exchange between a large collection of different database management and statistical programs. Graphics Workshop allows a variety of picture files to be transformed one into the other, mostly successfully, but always with the danger of some loss of definition or "out of memory" error. CorelDRAW and CorelPHOTO-PAINT have proved more flexible.

Unfortunately, data file formats are constantly evolving, so that the provision of "long-lasting relief" to the data format transformation problem is not likely to be found. Our strategy has been to try to save data as much as possible in text form, since users then have a reasonable chance to find some way to work with files we provide. In this regard, we note that both T_EX and PostScript, which essentially describe graphical information, are coded as text. PostScript files are rather difficult for humans to interpret, but there are many different machines — usually laser printers — that can do so. T_EX, however, we find easy to convert to simple text or to camera-ready material, even though we do not have the software to perform the manipulations. The main codes are simple enough to follow so that we can provide the equivalent word-processing commands.

2.7 Graphics

Some computer peripheral devices literally "draw" lines on either paper or a screen by moving a pen or an electron beam from one point to another, then another, and so on. For this reason, they are referred to as ***vector*** graphic devices. The TV screen and most computer monitors draw dots on a screen in a row of lines. To draw a picture, one must put the appropriate colored dots in the correct position in a large matrix of dots. They are called ***raster*** graphic devices. Working on the same principle, drawings can be output to dot-matrix printers, of which the laser printers are a high-resolution, small-dot version.

It is not trivial to use raster devices directly, since we think of drawing, e.g., with a pencil, in vector form. The "programming" of drawing is easiest with vector graphic tools, for example, the Hewlett-Packard Graphics Language (HPGL) that can drive not only plotters but also Laser printers and even numerically controlled machine tools. PostScript may also be considered a vector graphics language.

For research users, there are likely to be many reasons why graphical computing tools will be important:

- Research data is frequently best presented as a simple graph, for example, growth of plants or animals over time, chemical reaction kinetics, or spacecraft trajectories. Statistical distributions and data relationships can be visualized by a variety of data plots.
- Drawings of instruments, either in preparation for their construction, to illustrate what we propose to do, or to report what has been done, are now more easily prepared with Computer Aided Design (CAD) software than by recourse to a draftsman.
- In a technical report, we commonly need to include a photo. While "production quality" will require the actual photo, a reasonable image can be included in the draft or on the layout sheet by importing it into a word-processing document from an optical scanner.
- Image painting or drawing programs allow us to include logos or other designs to improve reports and slide-show presentations. Image painting programs give us control over the individual pixels in a bit-mapped image. For this book, we used CorelDRAW. It is also possible to consider hypertext forms (Taylor, 1991).
- Page layout programs may be considered as graphical tools if we have pictorial elements or fancy layouts in our reports.
- To convert paper documents to machine readable form, optical scanning with character recognition software can be used to provide a more or less correct machine-readable version. This is then manually edited to fix any errors in the recognition process.

Unfortunately, users of graphics must still ensure that all pieces of software and hardware can be organized to work together. Using color information in reports is still expensive, so color is usually re-coded as different shading or hatching, sometimes in ways that are not recognizable. As color output devices gain acceptance, this difficulty may become less important.

One area where graphics have become extremely important is in the interface to computer operating systems. Many scientific computists prefer the Macintosh desktop or the Microsoft Windows operating environment to a command driven system. For some applications, a pointer-driven graphical interface is essential; for others it may slow our work. In many cases the choice is a matter of personal preference, with software available to use in both types of environment.

2.8 Report Writers

Many scientific computations, for example linear programming computations, produce a very large quantity of output. While it is sometimes important to save the detailed information for future analysis, the usual output may not be in a form suitable for review by management or colleagues. To overcome the difficulty the volume of data presents, we may use a ***report writer*** to summarize the results and

highlight any important features.

Such report writers were a growth industry in the early 1970s, but since then have apparently become less popular. In part, this may be attributed to better reporting of numerical results by the scientific programs themselves. There is also a greater emphasis on graphical reporting of results that renders them more immediately accessible to users and their colleagues.

Nevertheless, users of PCs may wish to consider the creation and use of simple programs to sift and summarize results. For example, to compare run-time performance of several programs, we could use a simple filter program to extract the execution time information from files of console (screen) output. The program could be organized to tabulate our results roughly. The alternative would be to use a text editor to remove the unwanted detail of the results. In practice, we have often chosen the middle ground of using a macro-editor, which allows us to find and extract the required information by invoking sequences of commands with single keystrokes.

2.9 Programming and Program Development

Most scientific computations involve, at some stage, the use of custom-developed programs. Macro-editors are a help here in writing the source code. The compilation and linkage editing of the code to make a working program is clearly data-processing. PCs can take advantage of a very wide range of programming language processors. In our own case we find that we have access to the following programming tools (compilers, interpreters, assemblers) for MS-DOS computers:

- BASIC (several GWBASIC and QBASIC interpreters; IBM, Microsoft, Turbo, Quick and *True BASIC* compilers);
- FORTRAN (Microsoft 3.2 and 4.1, Lahey F77L 2.2 and 3.1, Watcom F77 Version 9.0);
- C (DeSmet 2.4 and 2.5; Eco C; Turbo C++ 1.0, 2.0 and Windows; Microsoft Quick C version 2.5);
- PASCAL (Turbo Pascal 3.01a, 5.0, 5.5, and Windows; Pascal-SC);
- 80x86 Assembly code (Microsoft Macro Assembler, De Smet ASM88).

With the above there are several different linkage editors. Some of the listed programming tools are out of date. Others, though dated at the time of writing, are still useful tools.

By far the most popular high level language in the early 1980s was BASIC, which is really a family of similar but hardly compatible dialects. Efforts have been under way for over a decade to standardize BASIC (Kurtz, 1982), but apart from Minimal BASIC (ISO 6373/1984) this effort has not had a great impact. A reason for the popularity of BASIC was that a version is supplied with most MS-DOS PCs. BASIC is, however, rare on Macintosh computers.

The use of BASIC is diminishing as users treat the computer as an appliance for information handling tasks; they are not programmers. Moreover, BASIC lends itself well to quick-and-dirty tasks, (Nash J C and Nash M M, 1984), but is not well-suited to large scale projects. For example, most BASIC interpreters allow only a single 64K memory segment to be used for program or data on MS-DOS machines. By contrast, Microsoft Visual BASIC offers a tool for Windows programming.

Scientific computing has traditionally been carried out in FORTRAN. FORTRAN compilers available for PCs are generally based on the 1977 standard (ISO ANSI X3.9 - 1978, American National Standard Programming Language FORTRAN). For computational efficiency, FORTRAN appears to be a good choice. The compilers generally support memory access to large arrays and there is a wide selection of source code available in the public domain. Unfortunately, FORTRAN compilers are not as convenient for novice users as, for example, the Pascal development environments from Borland Inc. Nor do they always supply the same level of functionality for controlling user interfaces such as Pascal or C compilers,

screens, keyboards, file handling or pointer device functions.

The use of various compilers and interpreters can be very tedious. The Microsoft FORTRAN compiler version 4.10 offers a choice of four different memory models and five different approaches to floating-point arithmetic. This presents the user with the tedious chore of specifying the correct disk\directory path for each compiler and linkage library (the pre-compiled code that provides the appropriate memory and floating-point choices).

When we have to compile and/or consolidate several pieces of code, it is better to automate the process. We may decide to use a BATch command file (Microsoft, 1991), which is essentially a pre-recorded version of our keystrokes. To consolidate source code segments, we have had considerable success using simple, though quite long, BATch command files (see Nash J C and Walker-Smith, 1987). MAKE, developed to ease the burden of building C codes in UNIX systems, appears in several forms accompanying C, FORTRAN and Pascal systems on PCs. This program takes a simple script (called the MAKEFILE) and builds our program from the appropriate pieces. A particularly pleasant feature of MAKE is that it is able to use the time-stamps of files to avoid recompiling source codes that have not changed since the last compilation. Thus it saves time and effort if it can. We have used MAKE in a C-language programming project aimed at the study of tumor growth.

The BATch command files can also be replaced with programs. Examples are given in Nash J C and Walker-Smith (1989b) in the BASIC program NLPDEX. In Nash J C (1990b), we suggest consolidation and execution of program code using a hypertext environment that allows the user to learn about available programs and data and then actually use them; this was demonstrated in Nash J C (1993b).

2.10 Administration of Research

We have already noted that researchers use PCs for preparing reports and performing a myriad of mundane tasks. Among these are the administration of their scholarly work. This involves, in our mind, planning tasks, preparing grant applications, tracking activity, preparing progress reports and administering research funds.

With research increasingly involving collaborations over distance, these tasks may require extensive use of email and file transfers. We may anticipate the eventual use of groupware — software allowing real-time exchange of computer messages for collaborative work via a network.

Clearly the PC is well suited to the development of work plans, using simple lists generated with a text or outline editor. Grant applications, while generally restricted in format, can usually be prepared using a word-processor. If there are several aspects to the same overall project, there will be considerable duplication of information.

To track activity, we like to use a diary system and extract information from it as needed. One of us (MN) prefers the traditional book form "planner" into which activities are recorded first as plans, later as activities. The other (JN) prefers to keep a "to do" list using a text editor and to transfer the "to dos" to activities with additional comments once completed. The choice is, once again, personal, and the computer a possibility rather than a requirement.

Chapter 3

Computational capabilities of PCs

3.1 Good news
3.2 Application problems
3.3 Component computational problems
3.4 Component symbolic problems
3.5 Getting things to work

The PCs introduced in the previous chapters have not conventionally been regarded as tools suited for serious computation. Early PCs had limited memory and slow execution rates that are not, by choice, the characteristics of a number-crunching engine, especially as the processors usually lacked floating-point (REAL number) arithmetic instructions. Moreover, the programming tools were usually interpreters of limited capability with quirks or errors in exception handling and special functions. This chapter points out where PCs and their software are likely to be able to carry out scientific computations.

3.1 Good News

A number of technological and commercial developments have vastly improved the capabilities of PCs for scientific computation:

- The development of high-performance floating-point co-processors with well-defined properties thanks to the efforts of a number of workers, particularly W. Kahan of Berkeley, toward the IEEE Floating-Point arithmetic standards and concurrent development of the Intel 80x87 and related devices;
- Larger memory capacities and address spaces;
- Faster, more efficient interfaces such as video-display adapters, memory managers and disk controllers;
- Fast, large and inexpensive fixed disks;
- More capable operating software allowing better use of available hardware, such as disk or memory caches (Section 8.3), printer buffers (Section 11.8), and utility software (Chapter 10);
- Full-feature programming language compilers;
- Reliable application packages, such as modern statistical software.

Interest in manipulating graphical images for video games has provided an impetus for large memories and fast processing. Computers with these features are commodities like any other consumer electronic product. In consequence, it is now possible to buy a PC with roughly the raw processing power of a typical university central computer of a decade ago and to pay less than $5000 for it.

Recognizing this computing power, developers have produced some powerful scientific software. For the user — and the reader of this book — the issue is finding and choosing the right software at the right price for particular problems. Since many scientific problems have different names or descriptions in different subject areas, this can be more difficult than we would like. In this chapter, and indeed in the rest of the book, we will try to explain some of the jargon that is associated with various problems. Also we will try to point to the component sub-problems that commonly arise in many classes of scientific computing, since users can "put the pieces together" if they know what pieces they need.

Our goal is to recognize when our machine can perform desired tasks, and if it can, whether it can do it sufficiently quickly for our needs, with acceptably low human effort involved. We take the position that the central obstacle to successful scientific problem solving usually lies in one or more mathematical sub-tasks. There are, of course, many ancillary tasks to be performed, often requiring most of our programming and management effort. These are not ignored, but they are generally not the ***critical*** obstacle to the use of a given computer in carrying out scientific work. That is, one or more of the mathematical sub-problems may prove insurmountable and prevent the use of the PC in the overall solution of the scientific problem.

3.2 Application problems

Scientific and technical computing clearly has more variations than we can discuss in a book of this size. However, the main types of problems can be listed. These are:

- Analytic problems, that is, those involving solution of equations or finding of roots or extrema — the manipulation of existing data to extract information;
- Simulation problems, where we synthesize plausible data a number of times to explore possible outcomes to particular situations;
- Transformation or presentation problems, where we are trying to recast existing data into a new form.

It is useful to recognize these three types because analytic problems are "finished" when we have a solution. However, we decide how many sets of conditions to specify for simulations. That is, they can be open-ended. Transformations and presentation problems may involve several cycles of experimentation to achieve a desired "view" of our data.

In the next two sections we mention the names of some mathematical problems to which application problems are often reduced. Much of the work of problem solving is learning how to do this efficiently in both human and computer effort. Of course, we have afterwards to interpret the results so that they may be understood.

3.3 Component computational problems

This long section lists and briefly describes some classic problems of computational mathematics. It also provides a notation we can use in later chapters.

Numerical Linear Algebra — Matrix Calculations

A matrix is a rectangular array of numbers. Within a matrix A that has dimensions m by n, that is, having m rows and n columns, the i,j element of A occupies the row i, column j position. This simple structure of numbers forms a building block of linear algebra. It has been applied in almost all subject fields, both directly or as a part of other numerical methods. The most common general problem types addressed by numerical linear algebra are:

- *Linear equations,* that is, finding the solution values x_j , for $j = 1, 2, \ldots, n$ to the n equations

(3.3.1) $$\sum_{j=1}^{n} A_{ij}\, x_j = b_i$$

We shall generally use the matrix form of these equations

(3.3.2) $$A\,\boldsymbol{x} = \boldsymbol{b}$$

- *Least squares approximations.* Here we wish to find a set of values x_j , $j = 1, 2, \ldots, n$ such that the sum of squares

(3.3.3) $$S = \sum_{i=1}^{m} (b_i - \sum_{j=1}^{n} A_{ij} x_j)^2 = \sum_{i=1}^{m} r_i^2$$

is minimized, where

(3.3.4) $$r_i = b_i - \sum_{i=1}^{n} A_{ij} x_j$$

Again, this may be written in matrix form as

(3.3.5) $$S = \mathbf{r}^T \mathbf{r}$$

where ^{T} denotes matrix transposition, and

(3.3.6) $$\mathbf{r} = \mathbf{b} - A \mathbf{x}$$

Note that A is now rectangular (m by n), whereas, for linear equations it was a square matrix.

- *Matrix decompositions,* including the eigenvalue decomposition. These problems aim to find products of other matrices that are equal to the given matrix A. The matrices that make up the decomposition have special properties. Some particular decompositions are:

  · the singular value decomposition

(3.3.7) $$A = U S V^T$$

where U is an m by n matrix of orthogonal columns such that $U^T U = 1_n$, the identity of order n, V is an n by n orthogonal matrix so that $V^T V = V V^T = 1_n$, the identity of order n, and S is a diagonal matrix having non-negative elements.

  · the eigenvalue problem (square matrices)

(3.3.8) $$A X = X E$$

where X has some normalization and E is diagonal. For symmetric matrices where

(3.3.9) $$A^T = A$$

the eigenvalue problem is straightforward, but it becomes increasingly difficult when the matrix is non-symmetric or complex.

  · the QR decomposition (or orthogonalization)

(3.3.10) $$A = Q R$$

where R is upper-triangular or right-triangular, that is

(3.3.11) $$R_{ij} = 0 \quad \text{if } i > j$$

and Q is m by n orthogonal

(3.3.12) $Q^T Q = 1_n$

· the LU decomposition (A square)

(3.3.13) $A = L U$

where L is lower-triangular and U is upper-triangular

(3.3.14) $L_{ij} = 0$ if $j>i$

(3.3.15) $U_{ij} = 0$ if $i>j$

(Thus U and R have the same structure; the different mnemonics are purely historical.)

There are many variations on the above problem types depending on the matrix properties. For instance, a matrix may be categorized by:

- Size, that is, how large are the number of rows, m, and the number of columns, n;
- Presence of complex elements, otherwise the matrix is real;
- "Shape", that is, "tall" if $m >> n$, "fat" if $m << n$, square if $m = n$;
- The pattern of non-zero elements, for example, upper- or lower-triangular as presented above, diagonal if $A_{ij} = 0$ if $i \neq j$, banded if $A_{ij} = 0$ if $|j-i| > k$, where k is a small integer.
- The existence of mathematical properties such as positive definiteness or norm of the matrix, or properties about the values, e.g., a Toeplitz matrix, which has all elements on any diagonal of equal value.
- The proportion of non-zero elements to the total, where a small proportion of non-zero elements gives a ***sparse*** matrix, whereas a high proportion gives a ***dense*** one.

Band matrix

```
x x x 0 0 0 0 0 0 0
x x x x 0 0 0 0 0 0
x x x x x 0 0 0 0 0
0 x x x x x 0 0 0 0
0 0 x x x x x 0 0 0
0 0 0 x x x x x 0 0
0 0 0 0 x x x x x 0
0 0 0 0 0 x x x x x
0 0 0 0 0 0 x x x x
0 0 0 0 0 0 0 x x x
```

Lower triangular matrix

```
x 0 0 0 0 0 0 0 0 0
x x 0 0 0 0 0 0 0 0
x x x 0 0 0 0 0 0 0
x x x x 0 0 0 0 0 0
x x x x x 0 0 0 0 0
x x x x x x 0 0 0 0
x x x x x x x 0 0 0
x x x x x x x x 0 0
x x x x x x x x x 0
x x x x x x x x x x
```

Hessenberg matrix

```
x x x x x x x x x x
x x x x x x x x x x
0 x x x x x x x x x
0 0 x x x x x x x x
0 0 0 x x x x x x x
0 0 0 0 x x x x x x
0 0 0 0 0 x x x x x
0 0 0 0 0 0 x x x x
0 0 0 0 0 0 0 x x x
0 0 0 0 0 0 0 0 x x
```

Tridiagonal matrix

```
x x 0 0 0 0 0 0 0 0
x x x 0 0 0 0 0 0 0
0 x x x 0 0 0 0 0 0
0 0 x x x 0 0 0 0 0
0 0 0 x x x 0 0 0 0
0 0 0 0 x x x 0 0 0
0 0 0 0 0 x x x 0 0
0 0 0 0 0 0 x x x 0
0 0 0 0 0 0 0 x x x
0 0 0 0 0 0 0 0 x x
```

Upper triangular matrix

```
x x x x x x x x x x
0 x x x x x x x x x
0 0 x x x x x x x x
0 0 0 x x x x x x x
0 0 0 0 x x x x x x
0 0 0 0 0 x x x x x
0 0 0 0 0 0 x x x x
0 0 0 0 0 0 0 x x x
0 0 0 0 0 0 0 0 x x
0 0 0 0 0 0 0 0 0 x
```

Bordered matrix

```
x 0 0 0 0 0 0 0 0 x
0 x 0 0 0 0 0 0 0 x
0 0 x 0 0 0 0 0 0 x
0 0 0 x 0 0 0 0 0 x
0 0 0 0 x 0 0 0 0 x
0 0 0 0 0 x 0 0 0 x
0 0 0 0 0 0 x 0 0 x
0 0 0 0 0 0 0 x 0 x
0 0 0 0 0 0 0 0 x x
x x x x x x x x x x
```

Due to the great variety of types of matrices, there are many hundreds of problems and methods to solve them, but few users will want to explore such specialization unless a particular class of linear algebra problem is solved frequently. Few users have the resources and energy to acquire and maintain a large collection of software, so will generally prefer a few more general tools of wide applicability.

Matrix Calculations Without (Explicit) Matrices

In our experience only a few real problems have necessarily involved matrices much larger than 20 columns or rows. We say "necessarily larger" because many large problems are the result of injudicious problem formulation (Chapter 13). However, there are some linear algebra problems that come about when other problems are approximated, for example, differential equations problems. In such cases, the linear algebraic problems need not be solved using arrays of numbers.
Iterative methods build up a solutions by applying corrections to some initial guess to it. These methods are particularly suitable for sparse matrix problems. For the linear equation problem, the solution vector $\boldsymbol{x}$ satisfies Equation 3.3.2. An iterative method begins with some vector

(3.3.16) $\boldsymbol{x}^{(0)}$

Each iteration computes a correction $\boldsymbol{d}^{(i)}$, so the new approximation to the solution is

(3.3.17) $\boldsymbol{x}^{(i+1)} = \boldsymbol{x}^{(i)} + \boldsymbol{d}^{(i)}$

We repeat the process until the vector $\boldsymbol{x}^{(i)}$ satisfies some convergence or termination criterion (Nash J C, 1987d).

Most methods that use matrices implicitly need to use the information that would be recorded in a matrix either piecemeal, for example a row at a time, or as the product of the matrix multiplied by some vector. In either case the whole array does not have to be stored in the computer memory. Instead it can be read into memory in pieces from backing store (disk). Alternatively, only the non-zero elements of the matrix need to be stored if these are relatively few in number (see Section 7.8). Finally, we may be able to generate the matrix elements from a formula.

Clearly, methods that use matrices implicitly are very useful in situations where an array cannot be stored in memory. These methods were first developed for early computers that had minuscule memories by today's standards. However, the problem sizes have generally increased over the years, so that problems of the order (n) of several thousand solution elements are now common. Simply put, there are always problems too big to fit in memory.

Modern PCs can employ these methods easily. The principal obstacle to their easy implementation is, once again, the diversity of problem types. Methods abound for various specific matrix structures and properties, and these implicit methods add yet another dimension of choice, e.g., the generation of matrix elements by formula, or row or column-wise access to stored values. Thus it is likely that a user must tailor existing programs to his or her exact problem. Getting a particular program running may be hindered by small but awkward differences in the way a compiler handles integer and real numbers or how it accesses memory to manipulate sparse matrices.

Special Functions and Random Number Generation

Mathematical methods for many types of scientific problems result in solutions expressed as special functions. Most scientists and engineers take for granted the availability of trigonometric, logarithmic and exponential functions. However, statistical distribution functions such as the error function, Student's t-distribution, chi-squared or Fisher's F statistic are not usually part of a traditional programming language, though they are commonly included in statistical packages (see Myrvold, 1991). Similarly, the functions derived from classical differential equations may need to be specially coded, e.g., Bessel

functions, hypergeometric functions, elliptic integrals. Some of these special functions may be present in packages such as MATLAB or GAUSS, or in symbolic manipulation systems like ***DERIVE*** or **Maple**.

In this area of computation, the major limitations are:

- Finding a method that computes the answer to the needed precision;
- Fitting that method into the framework for the rest of our problem, e.g., in an appropriate programming language or package.

The first of the above difficulties may be overcome by a diligent search of the literature (see Sections 13.3 and 13.5) but the second obstacle can require considerably more expense or ingenuity. We may choose to replace the programming language compiler or interpreter, or to buy or program machine code routines that carry out the calculations to a sufficient number of digits, or to develop some modification of the numerical methods that works satisfactorily in the available precision.

A particular class of special functions is pseudo-random number generators. Many programming language compilers or interpreters include a function that allows a more or less random sequence of numbers to be produced. Unfortunately, many generators are unique to the particular programming language compiler or interpreter, so that results are awkward to repeat across different computing environments. Worse, the properties of such generators are rarely documented by the producers of compilers or interpreters.

Pseudo-random number generators use totally deterministic processes that produce sequences of numbers that seem "random" according to some property such as the correlation of each number with its near neighbors in the sequence. However, truly random sequences will show no discernible correlation between numbers that are 1,2,3 or 100 places apart in the sequence. Most of the common generators used for producing pseudo-random sequences have weaknesses, particularly in this last property. This may be very important in some applications where pairs, triples or quadruples of random numbers are needed, such as some methods for approximation of multiple integrals (Lyness, 1986).

Another difficulty of some pseudo-random number generators embedded in compilers, interpreters, or packaged software is that the user may be unable to select the point in the pseudo-random sequence where he or she wishes to begin. This is very important for simulation and related techniques where repeatability of calculations is needed. For games, the user will usually want the sequence to begin at some chance location.

There is no particular reason the user cannot program his PC to provide the wanted generator. With a little effort, this can usually be quickly accomplished. Again, the capability of the PC is not in question, but ease of use is a serious issue. Realistically, this is also a difficulty on any machine, though most computing centers will have several random number subroutines in their program libraries.

Thus, the capabilities of PCs for calculating special functions, including random numbers, are quite adequate to such tasks. With floating-point co-processors (such as the Intel 80x87) now widely available, PCs are better suited than conventional mainframes for such applications as lengthy simulations, where overnight or over-weekend "runs" are possible. The ease of implementation will continue to depend on user access to suitable software.

Interpolation and Numerical Differentiation

Interpolation and numerical differentiation are classical problems in numerical analysis. Primarily they are a part of more elaborate numerical methods. The methods use various formulas involving differences between tabulated values of a quantity of interest. A serious problem may arise if the precision of floating-point arithmetic is too short to allow the differences to retain enough information. For example, if a function is tabulated to six figures but changes only in the last two digits, the difference will have only two digits of information. This may or may not be adequate, depending on the application. Worse, limited precision may also affect the reliability of the calculation of the original function values. These difficulties

are common to all computing systems.

Because interpolation and numerical differentiation algorithms are small, they can be easily implemented on PCs. An experienced practitioner can program and run an interpolation or differentiation more quickly than he can access a library routine. Indeed the sub-program "CALL" may involve almost as much program code as the actual calculations.

Summation and Quadrature — Numerical Integration

In summation, PCs are only handicapped when data files are too large to be handled. Programs for summation, e.g., in computing the mean and variance of data, are modest in length, even if one is cautious to preserve accuracy (Nash J C, 1981f; Chan et al., 1979; Nash J C, 1991a).

Programs for the summation of mathematical series are also generally quite small, for example in the approximation of special functions, the evaluation of integrals or the calculation of areas of surfaces. Since programs tailored specifically to special functions on a particular machine architecture must usually be custom programmed, mainframe and PC users have until recently faced the same tasks. Some contributions to mathematical software collections (see Section 13.5) have attempted to be independent of computing platform.

Because so few functions are integrable, that is, because no analytic function exists for the integral of most functions, a classical problems of numerical analysis is ***quadrature*** or numerical integration. Students of elementary calculus are probably familiar with the simplest of numerical integration methods called the trapezoid rule. This uses the value of the function at a number of points,

(3.3.18) $f(x_i)$ for $i = 0, 1, 2, \ldots, n$

with $x_0 = a$ and $x_n = b$, then sums the areas

(3.3.19) $A_i = 0.5\ (x_i - x_{i-1})\ [f(x_i) + f(x_{i-1})]$

for $i = 1, 2, \ldots, n$, to give the approximation

(3.3.20) $$\int_a^b f(x)\, dx \approx \sum_{i=1}^{n} A_i$$

Clearly this can be coded as a simple, straightforward program. However, quadrature methods have been developed that are much more sophisticated either in the integration formula used or in providing an error estimate for the difference between the true integral and the approximation made to it. Obviously the true integral requires an infinite number of infinitesimally small areas. Thus, there is an error made in choosing the step size

(3.3.21) $(x_i - x_{i-1})$

as well as accumulated rounding errors in summing the quantities A_i. Furthermore, the trapezoid rule assumes the function $f(x)$ is linear over the interval x_i to x_{i-1}. More complicated rules exist that allow differently shaped interpolating formulas to be used but more evaluation may be required.

As the integration formula gets more complex and if an error estimate can be calculated, the program to do all the work becomes more complicated and executes more slowly, even when the function is simple to integrate. For example, in many regions a function may be smooth and almost linear, while in others it may change very rapidly, making numerical integration difficult. To handle such problems efficiently, methods have been devised for adaptive quadrature (Lyness, 1970; Kahaner, 1981). The programs involved

are quite complicated, though Kahaner and Blue (Kahaner, 1981) showed how to do adaptive quadrature in Microsoft BASIC.

For multiple integration, summations are in several dimensions. Here each problem may require a special program for its solution, particularly if high precision is needed (Lyness, 1986). However, for low precision integration it is possible to use a Monte-Carlo method. (See Dahlquist and Björck 1974, p. 460.) This method simply treats the integral as a volume in some multi-dimensional space. Using a random number generator, points are generated in this space. The integral is then the proportion of points "within" the volume of interest multiplied by the volume of the space considered. There are many mechanisms using symmetry and extrapolation to improve the precision and to reduce the work in such methods. A principal weakness is that reliance on the "randomness" of the points severely undermines the efficacy of the method.

Numerical Solution of Ordinary Differential Equations

The numerical methods that have been evolved for solving ordinary differential equations (ODEs) were transferred successfully to early PCs (Field, 1980). As with quadrature methods, there are packages of methods such as that of Gear (1971) that adapt to the problem at hand. Implementing a large system of software for ODEs may pose a difficulty that not all the system will fit simultaneously in the memory of a PC, especially if there are addressing constraints.

If we have problems of a single type, then we may be able to use much simpler software. It is straightforward to program a method such as the Runge-Kutta-Fehlberg (RKF) which will integrate one, or a system of, well-behaved ordinary differential equations over a modest range in the integrand (Kahaner, Moler and Nash S G, 1989). Should an ill-conditioned problem be attempted, however, one may have to settle for imprecise results and / or have to use a very small step-size. A small step-size will make the integration painfully slow.

A common class of "awkward" differential equation describes two or more processes for which the time scale is vastly different. Such stiff equations are the subject of special methods. These may be poorly suited to general problems.

For special cases, such as eigenvalue or boundary value problems, it may be possible to reformulate the problem so that one solves a set of linear equations or a matrix eigenvalue problem, thereby using well-tried linear algebra routines. Alternatively, various methods transform the integration of an ordinary differential equation into a function minimization or root-finding problem.

Numerical Solution of Partial Differential Equations

Partial differential equations (PDEs) are generally difficult to solve. We note that the subject of PDEs constitutes a large proportion of classical mathematical methods for the physical sciences (Morse and Feschbach, 1953; Margenau and Murphy, 1956; Stephenson, 1961). Traditional methods for their numerical solution involve large computer programs and extensive arrays of working storage. After all, we must typically try to find a function of several variables (for example x, y, z and t for the three spatial dimensions and time) over a region bounded by some oddly-shaped function. Furthermore, we usually need approximations not only to the function but also its partial derivatives with respect to one or more of these variables.

Special methods have been devised for many individual problems in order that particular features may be used to assist in developing a solution. Indeed, one colleague who works in this area believes the difficulties are such that one must exploit the special features of each problem. Software is developed for each problem.

Clearly, memory limitations will handicap this computational task. Multigrid methods appear to offer a possibility of compact solution methods (McCormick, 1982). At the time of writing, there are few general sources of software for solving PDE problems, though this situation is rapidly changing. Interested readers

will need to keep in touch with developments via the literature or electronic newsletters (e.g., NA Digest for numerical analysis; send an electronic mail message to na.help@na-net.ornl.gov for information).

Integral equations and integro-differential equations are a class of problems with which few workers have much experience, including ourselves. The software seems to be specialized to particular problem types and as yet confined to research environments.

Function Minimization and Optimization

Besides application problems that are naturally formulated as optimizations, many mathematical problems reduce to such forms. When the number of constraints is very few, the problem is usually called function minimization. A maximization problem is trivially converted to a minimization by multiplying the objective by -1. When the number of constraints is large enough that satisfying them is the main focus of our attention, the problem is then referred to as Mathematical Programming (MP). This nomenclature is confusing. It is particularized to problems that have linear, quadratic or nonlinear objective functions (LP, QP or NLP), have integer arguments (Integer Programming) or are associated with sequential decision processes (Dynamic Programming).

Various methods have been developed that are compact and easy to implement and use (Nash J C, 1979a, 1982b, 1982c, 1982e, 1990d; Nash J C and Walker-Smith 1987). For special cases, such as the nonlinear least squares problem, similar developments have been observed (Nash J C, 1977b, 1990d; Nash J C 1982b). Even when memory space is extremely limited, the Hooke and Jeeves algorithm (Nash J C, 1990d) may be used that has been implemented on "computers" as small as programmable calculators.

Mathematical programming methods have generally been much less amenable to use on personal machines. (An exception may be made to Dynamic Programming.) The main reason is that it is traditional to write the linear constraints in a large matrix, called the tableau. For many linear programming problems of interest, this tableau is large and sparse. As mentioned above, methods for handling sparse matrices are often not easily transported between computers. However, we know of implementations of MINOS (Murtagh and Saunders, 1987) on Macintosh computers and are ourselves installing LANCELOT (Conn, Gould and Toint, 1991) on an MS-DOS machine. Generally, however, math programming software for large-scale problems remains expensive.

A related issue concerns how we enter math programming problems of interest into whatever software we wish to use. The volume of data to specify the initial tableau may be a source of difficulty. The required data format may be uninformative to the reader. We may prefer to use a modelling language such as GAMS. Once the problem has been specified, it can be important to know if special conditions apply. There are extremely efficient algorithms for some types of math programming problems (Evans and Minieka, 1992).

Root-finding

Closely related to optimization, and often sharing similar algorithmic approaches, is the problem of solving one or more nonlinear equations, or root-finding. Such problems are very common analytic problems in all areas of study. They are frequently very difficult conceptually and numerically because of the possibility of multiple solutions and severe scale variations from one region of the variable space to another.

3.4 Component Symbolic Problems

Not all computations need be numeric. Computer manipulation of symbols is clearly possible — this is the basis for all text processing and database management — to the extent of performing mathematical manipulations. Until quite recently, this type of computation was largely reserved for mainframes, since the particular operations of algebraic manipulation may require large amounts of memory. The 640K

memory addressing limit of MS-DOS (see Section 7.1) still poses some difficulties, and some available software for symbolic mathematical manipulation will only run on MS-DOS machines with advanced architecture and extra memory (see, for example, a review of *Mathematica* in PC Magazine, March 31, 1992, vol. 11, no. 6). By contrast, David Stoutemeyer of the University of Hawaii, Honolulu, has for many years been showing the world how to do such computations on very small machines. His MuMATH and ***DERIVE*** contain a respectable spectrum of capabilities in algebra, integration, limits, differentiation and special functions, though we still needed to use the extended memory version for some test problems in a recent review (Nash J C, 1995).

A typical symbolic problem is the development of analytic expressions for gradients and hessians for differential equation and minimization problems. For such applications, we note that there are also automatic differentiation programs (Griewank, 1992; Fournier, 1991) which "differentiate program code" rather than produce analytic derivatives. A different task occurs in some statistical calculations (Baglivo, Olivier and Pagano, 1992) where symbolic "computation" of expressions may permit exact rather than approximate statistical tests to be performed. One can even prove theorems in some situations.

Combined symbolic and computational tools for problem solving are becoming more widely available and easy to use. Their application to user problems remains a challenge.

3.5 Getting things to work

The message of this chapter is threefold:

- PCs may have physical or logical limitations to the solutions of a particular sub-task that prevent us from solving our problem;
- Such obstacles should be identified before we do all the programming and related work;
- Finding appropriate software we can use without many hours of programming and testing is the main obstacle to use of a PC.

This message is primarily not just for PCs — it applies to any situation where we want to change from one computing environment to another.

Whereas two decades ago, almost all scientific computing involved some form of programming, many users now accomplish their work without ever working with FORTRAN or Pascal or C. "Programming" is still going on, sometimes almost explicitly in high level languages such as GAMS or MATLAB, but more often in such tools as spreadsheets, statistical packages or optimization systems.

As an early example of such uses, we note the investment analysis of Kahl and Rentz (1982) who discuss a complicated depreciation analysis problem (called Capital Cost Allowance in Canadian tax law) under conditions prevailing before and after the November 1980 Federal Government of Canada budget. The problem was quickly and easily solved without requiring any knowledge of programming.

PART II: Computing environments

The next eight chapters are concerned with the computer facing the user. This is as much a function of the software as the hardware, but the current marketplace offers so many plug-in options that the familiar boxes which house well-known PC systems may hold entire replacement computers. With this caution, we now turn to the study of the computing environment that presents itself to a user. Users who are familiar with computer hardware and software may wish to skim this material, which provides a base of information about PCs so that implications for scientific problem solving can be addressed in later chapters.

Chapter 4

Will a PC suffice?

4.1 Hardware
4.2 Software
4.3 Interfacing, communications and data sharing
4.4 Peripherals
4.5 Operational considerations
4.6 Issues to be addressed
4.7 Programming effectively
4.8 The software development environment
4.8 Input/output problems — bugs and glitches
4.9 Debugging and troubleshooting
4.10 Precision problems
4.11 Size problems
4.12 Utilities and support
4.13 Summary

Every computing device has its own strengths and weaknesses. For purposes of calculation in particular, some machines are clearly more attractive as tools in that they provide greater speed, better precision, more memory capacity, more data storage or better software support. This chapter attempts to provide a comparison between PCs and other computers based on the above criteria.

4.1 Hardware

The actual electronic components of PCs are quite similar to and sometimes the same as those used in larger machines. There are simply fewer pieces — less memory, fewer processor parts, fewer power supplies, fewer input/output channels. Higher performance of mainframes and workstations comes from parallelism in the processes — winning the race by being able to do many things at once. PCs are rapidly closing this gap. Most microprocessors, until recently, handled 8 or 16 bits at a time, but 32-bit processors are now common.

There are many factors that contribute to the time required to execute a given program. The word size and cycle time, while important basic measures for theoretical speed, have little to do with the ***measured*** time for a particular job. Computer purchasers should remember that price and performance are the main considerations for any piece of equipment. How a given performance level is achieved should be immaterial, be it PC, workstation or mainframe.

A more serious matter related to the word size has been the address space of the machine. Most computers work with Random Access Memories (RAMs), meaning that any single element of data can be retrieved or stored equally quickly. To do this, memory is arranged as an array of pigeonholes or cells, each of which has a location number or address. Of course, each cell can only store a certain amount of data. Since addresses are data when used within programs, there is a relationship between the word size (memory cell capacity) and the maximum address allowed. Many 8- and 16-bit processors use a 16-bit address. That is, the 8-bit machines must use two memory cells for each address. The 16-bit address space means memory cells can be numbered from zero (0) to 2^{16}-1 This is the 64K limit common to many early PC systems. At any one time, such computers can access only 65536 = 2^{16}-1 memory cells. This means that program, data and operating system functions must all be fitted into this maximum space. Whenever a new function is added to the system software, the amount of memory available to the user's program and data is correspondingly reduced.

For example, in a machine that stores a floating-point number in only 32 bits or 4 bytes, a matrix 100 by 100 requires 40K bytes of memory, leaving very little room for the program to work with it. Clearly users who must have such arrays in memory in order to solve their problems are going to be hard pressed to make them fit. On typical PCs of the late 1970s, the Intel 8080, Zilog Z80, Motorola 6800 and Mostek 6502 processors all imposed limits of this type. Some imaginative solutions were invented to overcome the problem. For example, clever use of special input/output or other instructions allowed the processor to look at different ***banks*** of memory, one at a time. This is like the movable stacks in some libraries. A patron can move the wheeled shelves to select one set of books at a time. The Intel 8086 and 8088 microprocessors used a similar mechanism to expand a 16-bit processor bus to a 20-bit memory address, to access 2^{20} = 1,048,576 bytes (or 1 Megabyte) of memory. The "640K limit" of 8088 based PCs was due to design choices related to display and other devices mentioned below.

Processors allowing for larger address spaces are better suited to the matrix problems of the previous paragraph. The Motorola 68000 family of processors and the more recent members of the Intel 80x86 family can address large amounts of memory directly without special tricks. For Intel-based machines, however, backward compatibility with existing software, especially operating systems, may mean that users cannot use this capability easily.

Another address space limitation of many PC systems is the use of memory mapped input/output or similar functions. As a historical example, the Intel 8080 and Zilog Z80 computers have OUT instructions that allow data currently in the accumulator of the CPU to be directed to a given I/O channel. Other systems, notably the Mostek 6502 of early Apple, Commodore and Atari computers, simply "write" the data to a specified memory address that contains an output channel instead of a memory device. Memory mapped I/O is common, especially for displays. Of course, each address used for I/O is unavailable for programs or data. Worse, we generally lose address locations in blocks simplify the design of the addressing circuitry. Other hardware functions that may use memory addresses for either control or buffering functions are disk controllers, network adapters, some floating-point processors, and ROMs (read-only-memories) that hold the startup software of the computer or provide special control functions,

such as our own ***SnoopGuard*** security access device for MS-DOS computers. The startup software is commonly called the BIOS (Basic Input Output System).

Certain essential software also takes memory away from problem-solving. The operating system, of course, must occupy some space to control all processes and manage the machine resources. Any program that we want resident or always ready to work must have interrupt handlers to activate the working parts of the program. Sometimes the whole program remains in memory. On MS-DOS PCs, such "terminate and stay resident" or TSR programs are very common for handling screen savers, keyboard buffers, and other useful functions. Device drivers use memory to operate RAM-disks (see 8.5), provide special keyboard emulations or display characters, or allow access to such peripherals as optical scanners, nonstandard tapes, disks or CD-ROMs. In the case of RAM-disks, disk caches or print buffers, memory space is needed to store data if this is taken from the main system memory.

Integrated program development environments and debuggers may use up a lot of memory, since much of the code stays resident. Trends to different operating system principles, as in the Microsoft Windows approach, while having a high overhead cost in terms of system resources, offer a certain freedom from the memory squeeze.

A different limitation for PCs concerns the ways in which devices are connected. Even if there are sufficient physical connectors, we may find that there are not enough circuits to run all our devices at once. In particular, the IBM PC design is notoriously limited in terms of ***interrupt request*** (IRQ) lines. These carry signals to tell the processor that it should pay attention to something happening with respect to a device. An example concerns communication ports. On our own machines, we have had to limit the ways in which we use Microsoft Windows because there are not enough IRQ lines to fully support internal modems that are set up as the third serial communication port on two of our machines.

Because PC systems have fewer discrete components than mainframes, they ought to have an intrinsically higher reliability. Counterbalancing this is the fact that they tend to be used in less than ideal environments — unfiltered electrical power, dust, heat or cold, humidity and general rough handling all add to the potential sources of faults. However, the use of interchangeable circuit boards and/or socketed components makes servicing usually quite easy.

In summary, PC users must carefully assess the processing, disk and memory resources ***available*** for problem solving rather than the raw or total resources implied by the PC hardware.

4.2 Software

The software for PCs is, we believe, a much greater obstacle to their use in scientific problem solving than the hardware. We may arbitrarily divide software into the following four categories:

- The operating system, which enables us to execute all other software and to send data to or receive it from peripherals;
- Utilities, which allow the user to do certain housekeeping functions such as copying or listing files;
- Programming language translators, to compile or interpret programs written in other than machine code;
- Application programs, that is, all the rest.

We will look at these categories in reverse order. Programs for a given application need not be drastically different just because they are to be run on a PC. Primarily, we want to be sure our task is feasible in terms of the actual working memory or disk space available within the application program. More positively, PC application software may access low-level machine functions for speed. Also, since we are the manager of the PC, we can also choose to let inefficient programs run for hours or days at a time if this is the least-cost method of achieving our goals. On a practical level, however, we need to know that

the execution time to get a task done is not so long that it will inhibit use of the PC.

We have already seen in Section 2.9 that practically all main stream programming languages can be used with PCs.

It is usually in the area of housekeeping support that PC systems are at a disadvantage. At nearly all mainframe or workstation sites there are systems programmers to help handle housekeeping tasks. On PCs, utility programs that are not provided in or with the operating system must be acquired separately ***by the user***. There is no shortage of choice of tools, as almost any PC trade magazine will illustrate. In fact, the wide selection is a source of difficulty, since the user must choose between several attractive choices. However, with each selection costing money, buying each set of utilities will draw resources away from the scientific software budget. Freeware or public-domain utility programs exist, but the chore of evaluation requires much time. Since we are usually dealing with programs that move, modify or delete files, program errors can have serious consequences, so untested utilities are worse than none at all.

Operating system software controls all the activity in the PC. Since many PC systems are configured with a unique combination of processor, memory and peripherals, the user must usually make at least minor modifications to the operating system to allow the processor to use the resources available to it. Configuration management (Section 11.8) extends to most major applications packages such as word processors, desktop publishing software, CAD programs, compilers, file managers, or drawing programs. When we add a new resource (printer, plotter, scanner, mouse, video adapter, network adapter) to our system, we have to adjust all affected software. An advantage of the newer operating environments such as Microsoft Windows or IBM OS/2 for Intel-based PCs, or Finder for Apple Macintosh, is that the operating software is nominally the only place where such adjustments are made.

With increased memory sizes in PCs, operating system (OS) software has tended to become bloated. Sometimes users have had to reinstall "old" versions of their OS because critical applications programs would no longer operate under the "new" system. Our view is that operating software should be as small as possible. First, the operating system takes time to load; as each program terminates, the command processor is generally reloaded to memory, with load time proportional to its size. Extra OS features that we do not use still require some computing effort to bypass and the memory and disk they occupy can be better used for other purposes. Also, the larger the code, the easier it is for accidental errors or viruses to corrupt it. Finally, the more features there are, the larger the manual through which we have to sift to find a particular item of detailed information.

4.3 Interfacing, Communications and Data Sharing

PCs are well suited to being connected to other computers or data handling devices. PCs can be reconfigured to a specific task, whereas a mainframe must usually serve many users and cannot be radically altered to suit just one application. Moreover, some components of a PC system are programmable; that is, their properties may be changed by sending special control instructions. An obvious example is a dot-matrix or laser printer to which font descriptions can be down-loaded.

The disadvantages are that the user may have to do the work of interfacing or pay quite heavy fees to have someone else do it. On the hardware side, simple cables may cost over $200 for a custom-made item that has parts worth only a few dollars. The most commonly needed cables needed cost less than $20.

Miniaturization has presented some scientifically trivial but administratively unpleasant obstacles such as connectors that do not match. For example, the serial connector on the original IBM PC is a male DB 25 plug. This was and is a commonly available component. To reduce size, and noting that not all of the 25 pins were used, manufacturers sometimes switched to a DB 9 plug. An added level of confusion existed with early IBM PC-compatibles by using a DB 25 ***female*** connector for the serial port. Gender changers and adapters are fortunately available inexpensively from many suppliers, though we have on occasions been told by ignorant employees of some stores that "that kind isn’t made."

Another problem is that the transmit and receive lines may need to be swapped using a device called a ***null modem***. To simplify our own work, especially in travelling, we have found it useful to have a cable with both male and female DB 25 connectors at each end of a 6 to 8 foot length of ribbon cable. This, with a null modem and some gender changers and 9—pin to 25—pin adapters allows us to make needed connections. Once we have established the right connections, a simpler cable can be obtained. We have also found the cables supplied with the Laplink file transfer software to be very useful.

PCs handle data communications quite easily. The main mechanisms commercially available are either Local Area Network (LAN) products or modems designed for use with the standard telephone network. We will not deal here with special equipment for use with private telephone lines or satellite channels.

There are so many forms of LAN hardware that we will not attempt more than a cursory description of the possibilities. The important aspects are that simple cabling — either coaxial cable or telephone-like multiple wire cable — allows very high rates of data movement between computers. The applications of such high-speed transmission are that a user can work with data on another computer as if it were present on the local fixed disk. Software operating the LAN may have strong influences on PC configuration, performance and user practices.

Modems, though much slower, also allow for the transport of data between machines. Ironically, this is often via the intermediary of a mainframe computer. We use this technique to make class notes available to students via a shared disk area on a university mainframe. Such mainframes are commonly nodes of the international academic and commercial networks, and provide access to many electronic mail and file transfer facilities (see Krol, 1992).

4.4 Peripherals

Practically every type of input, output or storage device can be attached to PCs, though certain types are favored. The main mass storage mechanism for PCs has evolved from the flexible disk to the high-capacity fixed disk. ***Flexible (or floppy) disks*** can store data in a bewildering variety of sizes, densities, recording mechanisms and formats. We have found that it is helpful to describe these by the type of machine, capacity, and physical disk size rather than an adjective preceding the word "density". We tend to use IBM PC 360KB 5.25 inch disks for distribution of the relatively small files associated with our own work and IBM PC/Macintosh 1.44 MB 3.5 inch disks for archiving data, for the work of individual projects and when travelling. Apple chose a variable speed drive for its computers so that more data can be packed into the outer tracks of the diskette surface than the inner ones. This contrasts with fixed rotation speeds in the MS-DOS world, but many Macintosh machines now read and write the 1.44 MB fixed-speed format.

Capacities have been evolving in both Macintosh and PC families of 3.5 inch disks. This can be a nuisance for users, but manufacturers seem aware of the need for backward capability so "old" diskettes can still be read. Despite the difficulties of standardization, flexible disks are cheap, quite reliable, and offer a satisfactory method of storing and moving data and programs for PCs. With proper packaging and some luck in the postal system, they are a means by which data can be transferred from one machine to another.

In contrast, the ***fixed (or "hard") disks*** cannot normally be exchanged from drive to drive but are sealed in a dust-proof case. Such systems offer compact, high volume storage on platters that have been decreasing from 14 to 8 to 5 to 3.5 to 2 inches in diameter. The major problem with such disks is backup, because the high volume of data requires a good deal of time for transfer to another medium. Indeed, a significant part of the expense of any fixed disk system is a backup mechanism, such as tape cartridges.

On mainframes, the reel-to-reel 0.5 inch tape was the primary removable data storage medium for many years. Drives are expensive because the sophisticated mechanical tape handling system must start and stop the tape very rapidly without stretching it. Someone had the good sense to recognize that the data could be recorded steadily at a slower speed if the controller could buffer the data. Such streaming tape drives can be offered at quite modest prices when the same idea is applied to compact ***cartridge tapes***.

PCs use practically every imaginable ***printer***. The most common type is the dot matrix variety. So-called "letter quality", daisywheel impact printers were initially the common method of obtaining output with an acceptable "business" look. These have almost disappeared, thanks first to competition from multi-strike dot matrix printers and later to laser or ink-jet printers. The latter achieve an amazing diversity of type fonts and graphic designs by clever use of software, either running in the PC or within the printer itself. (The printers are themselves often controlled by quite powerful microprocessors and memory.) Multicolor versions of various types of printers are challenging the pen-plotter role.

In turn, pen ***plotters*** have achieved much of their development thanks to PCs. Initially aimed at the specialist technical market, they are now a tool for business. With the wider market base, prices have dropped considerably, but the popularity of pen-plotters is low compared to that of graphic printers. An important niche market for plotter technology is a cutter in which the pen of the plotter has is replaced by a knife. This allows stencils or other masks to be cut, so that signs and displays may be created more quickly. Large plotters attached to PCs are also used industrially for preparing cutting plans, circuit diagrams or engineering and architectural drawings.

Visual displays for PCs and workstations continue to evolve. From the user point of view, it is important to note that since the quality of the image displayed is dependent on the number of dots on the screen and the number of colors that can be displayed, a high-quality display demands much memory to store the image. (This refers to raster displays, and does not apply to vector-graphic devices, which are much less common.) If this memory is taken from the system's main memory, there is less available for our programs. If it is a separate memory, the speed with which data can be transferred to the ***video memory*** may affect the speed of our whole machine. Indeed, the video memory of the machine used to write this material is over 14 times "slower" than the rest of the memory. In serious computations, we must avoid writing to the screen if we want our results quickly.

There are many ***pointing devices*** for the interactive use of PCs. These include light pens, mice, trackballs, and even head motion pointers.
Devices such as scanners and digital cameras are becoming common for input of graphic data. Also available are interfaces to musical instruments or to sources of sound and video data, and laboratory interfaces for control of equipment or data acquisition.

4.5 Operational Considerations

The PC has become such a common piece of equipment that one may forget that it is still a computer. As such it imposes various demands on its users for hardware, software and data maintenance. The hardware of a PC is a lot easier to accommodate than that of a mainframe in that no raised floor or special power are required. However, as we shall note in Chapter 11, the absence of specific requirements does not mean that we should ignore common sense when choosing an operating environment.

We have already noted that the software for a PC will require ***configuration*** depending on the particular peripherals to be attached. New or upgraded software may also mean that the configuration (system generation) must be repeated. This is particularly so for operating system upgrades. Worse, we must also check all programs that directly use the operating system to ensure that they will still execute correctly. This can be sufficient reason for deciding to stick with an "old" version of the operating system, particularly if its deficiencies impose only minor inconvenience to our machine use. We think that configuration is an onerous chore with which software developers burden the user. Several times we have had to spend the better part of a day making configuration changes so new software would work. This is time lost to scientific work.

Finally, our own data must be maintained in good order and there is usually no one we can rely on to do this but ourselves. Thus, all backup and house-cleaning are the responsibility of the user, very different from the automatic file maintenance of most centrally supported machines.

Operationally, the pros and cons of PCs devolve from the power of decision granted to the user. We have

control of where and how the machine is to be used, and must assume sole responsibility for those decisions. In the rest of this chapter, we turn to strategies for coping with the difficulties that attend the use of PC for scientific calculation. Readers can choose among the ideas discussed — the PC is a private calculating and data processing engine. Why heed the advice of others if we can discover ways to meet our goals in a manner convenient to our own habits and tastes? We hope the sections which follow aid that discovery.

4.6 Issues to be Addressed

If we are fortunate enough to be able to choose between several computing platforms, then we first need to know which of them can carry out our tasks. This book deals directly with PCs, but the same approaches can be used for any computer. We will want to know if an available computer can carry out our (scientific) work by means of suitable organization of the machine, the tasks, or both.

The next seven chapters look at the practical, non-scientific details related to deciding if our PC can, or can be made to, perform required tasks. Chapter 5 considers the management of data, of files and of programs, probably the thorniest problem for users of PCs. While not all scientific computing requires that we program, Chapter 6 discusses ways to make our efforts effective when it is required. Since memory size is critical to our ability to fit our problems in the PC, Chapter 7 considers this matter. If size questions can be answered positively, we then need to decide if the speed of computation is sufficient, and timing is investigated in Chapter 8. The question of programming errors and their detection and repair, either in our own programs or in those we acquire, is the subject of Chapter 9. Chapter 10 suggests some utility software for the support of our work. The physical care of PCs and their accessories is the topic of Chapter 11, which also touches on configuration management.

Following the housekeeping matters — that inhibit effective computing to an extent that we devote about half this book to them — we turn to problems of a type likely to be encountered in scientific computation and some approaches we may make to their solution. The general steps in problem solving are the meat of Chapter 12. Chapter 13 looks at the important matter of formulating problems in a manner suitable for correct and efficient solution on our PC. The rest of the book, apart from a final chapter on choosing one's own strategy, consists of case studies in problem solving. Our goal there is to suggest ideas for the solution of the user's own problem — ***your*** problem. As a warning that there may be very great differences in the time required to carry out scientific computations across PC hardware and software, Chapter 18 presents a study of the execution times for three almost identical algorithms in a selection of their implementations. Chapter 19 shows some ways performance of different software may be compared using graphical data analysis tools. The same tools may be used in analyzing other sets of data.

Since our message is that it is critical to try out ideas if there is a question of PC capability or performance, much of the book mentions the kinds of tests and tools appropriate to answering such questions. We conclude in Chapter 20 by summarizing some of the ideas we have developed in a quarter-century of working with limited-capability computers.

Chapter 5

File management

5.1 File creation and naming
5.2 Types and distributions of files
5.3 Cataloguing and organizing files
5.4 Back-up
5.5 Archiving
5.6 Version control
5.7 Loss versus security

This chapter considers the thorny problem of file management - how to keep track of our program and data resources. We think this is the ***biggest*** problem for all computer users, no matter what the size of their machine. The task does not depend on the computer type or the application involved. The only areas in which PC practice is different from that of a mainframe are the mechanisms for file security and the utilities available to aid the user.

We note that we want:

- To have data protected from destruction and loss (backup and archiving);
- To be able to find data (i.e., files) easily (name recognition and avoiding duplicate names).

In the following sections we will consider various aspects of file management, be they physical, logical or human. Some suggestions for coping with the problems will be made, but the major burden unfortunately rests squarely on the shoulders of the user. Knowing what to do and how to do it counts for nothing in file management — we still have to do it!

5.1 File Creation and Naming

The main unit of "permanent" memory on computers is the ***file***. This is simply a sequence of words (bytes) of data that has a ***name*** and some ***access mechanism*** so that the computer can read the data. Presentation or use of the data is handled by programs. Data may represent counts, text characters, picture elements (pixels), program code in source, object or executable form, or variously coded forms of any of the above items.

A file created on one computer may not be usable on another, so it is important for the user to be aware of the ***compatibility*** of the file with his or her machinery. In our experience, simple text files, using printable characters of the ASCII 7-bit standard set, are the only files that can be transferred and used with any assurance between systems. Word processing files and binary data files are notoriously awkward to transfer (Nash J C, 1993a).

The access mechanism to files is determined by the computer we are using, its operating system and the software used to create the files. The user, however, generally has a choice in the naming of files. The goal should be to ensure that names chosen are meaningful within the context of the work or subdirectory at hand and within the name length and character restrictions imposed by operating or application software. Note that directories and subdirectories are themselves files and should also be appropriately named.

The MS-DOS file system has been criticized for having many shortcomings. One of these is that the filenames may not exceed 8 characters in the main part of the name and 3 characters in a filename

extension. Typically the two parts are separated by a period (.) though other ways of writing the two parts exist. The blank character is not allowed in names although it is sometimes possible by error to get a blank embedded in a name. This generally leads to some awkward work to correct the name, or even to delete the file.

The filename extension is often used to suggest the function of a file. Indeed, the MS-DOS operating system treats files with the extensions .EXE or .COM as executable. Files ending in .BAT are sequences of operating system commands and may also be "executed". Naming non-executable files with such extensions can lead to unexpected results. For example, it may be tempting to name a file of comments on a lecture as LECTURE.COM. Later, forgetting that the file is a text or a word processing file, we may try to execute it.

Operating systems may permit characters other than letters or digits in filenames. For example, MS-DOS allows us to use

$ % ' - @ { } ~ ` ! # ( ) & _

The last of these, the underscore (_) is quite useful if we would like a "space" in the name e.g. MY_FILE.TXT. However, take care as some application programs may not allow the use of all of the above characters. To avoid errors, it is therefore advisable to use only letters and numbers. Foreign or graphics characters in filenames or extensions may cause some software to react in unpredictable ways.

Filenames in MS-DOS are handled as if in upper case letters, but they can be entered with any mix or upper or lower case. That is, the filenames are case insensitive for MS-DOS. UNIX is case sensitive.

For MS-DOS there are several characters that should not to be used in file names or extensions, namely

? . , : ; = * \ / + " > <

Indeed, the ? and * characters are ***wildcards***: the ? takes the place of a single character, the * takes the place of any character string starting at the location of the asterisk in the filename or extension.

The Macintosh FINDER allows for longer filenames — 31 characters as the maximum. The names can be upper or lower case and the name displayed stays in the case in which it was entered. However, we cannot create two separate files AAA and aaa. That is, the case sensitivity extends only to the display of names, not to search or use. The long names may include spaces and special characters. Thus the Macintosh names can include quite a large amount of identifying information. Unfortunately, transfer of the files to other systems may force us to use a more restricted set of names.

The choice of names and extensions is, for the most part, a personal one. We can nevertheless suggest some we have found useful. Above, we have mentioned that MS-DOS (and other operating systems) may use the extension as an indication of the file usage. Besides .COM, .EXE and .BAT we have

.SYS	system files
.OVL	overlay (for an executable program)
.BAS	BASIC source code
.OBJ	object code (input for the LINKer)
.FOR	FORTRAN source code (though .FTN also used)
.PAS	PASCAL source code
.C	C source code
.H	C header file

Several applications create specially named files. Unfortunately some of the names are conflicting or overlapping and may include:

.DTP DeskTop Publishing file
.DOC document file (used by several word processing programs and also generically to indicate DOCumentation)
.TXT text file, also used by some database programs for databases stored in text form
.WK? worksheet for various spreadsheet programs
.TIF graphics file (Tagged Image Format) used (in different ways!) by various drawing, photographic and fax programs
.ARC an archive file, not always in the form used by programs such as ARC (Systems Enhancement Associates)
.LZH an archive file created by LHA (Haruyasu Yoshizaki, 1988)

In our own business work we have used extensions such as the following to keep track of common types of files:

.BID bid
.INV invoice
.LET letter
.LST list
.MTG meeting
.PRO proposal
.REC receipt
.RPT report

When working with files that have specific temporal importance, we can also think of using abbreviated names for months, e.g., .JAN, .FEB, .MAR, etc. or for days of the week, e.g., .MON, .TUE, .WED, etc.

There are as many proposals for good file extensions as there are people using computers. Since summary directories do not show file time/date stamps and some software automatically updates this information when used to view the file, it is often helpful to include some temporal information in the file name, e.g., NASHJC.92B for the second letter sent to J.C.Nash in 1992. On the negative side, we may forget how many letters we have written this year to active correspondents.

Returning to the filename rather than the extension, we note that there may be ***reserved names***. MS-DOS reserves AUX, COM1, COM2, COM3, and COM4 for serial communication ports, PRN, LPT1, LPT2, and LPT3 for printer ports, CON for console input (keyboard) and output (screen), and NUL as a dummy device to which output can be directed. These predefined "devices" are always available to programs. For example,

```
COPY A:*.* NUL
```

checks that all files on A: are readable. Unfortunately, documentation of these device names is scattered through various parts of the MS-DOS manuals and books about this operating system. Worse, in a recent attempt to move files from a UNIX system to a PC, a series of files related to "conversion" had filename CON with different extensions. As they were downloaded by modem, the communications program cheerfully copied them to the screen rather than the disk!

5.2 Types and Distributions of Files

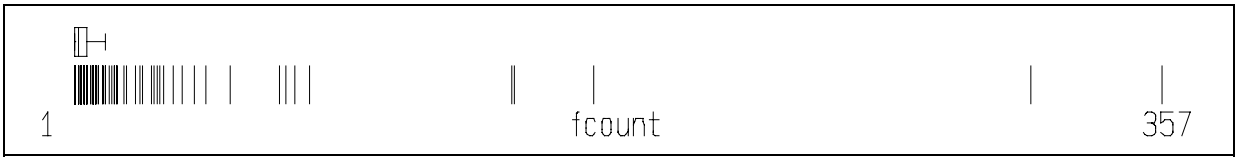
To give meaning to the discussion, we present here a brief analysis of the files found on just one of our IBM-class PCs. The purpose of this is to present a snapshot of a file collection, indicating the number, size distribution and general usage of files in a machine. We want to control the files — to make sure we do not lose information but are not overwhelmed by too many copies and versions of each file. Clearly the characteristics of a set of files will depend heavily on interests and inclinations of the user(s), but the ideas are general.

At the time the snapshot of all files was taken, there were 2474 files or directories in the fixed disk. Of

these 1119, or about 45%, we could identify as system or software files, while 1355 (about 55%) were files created by the user(s). This is a very high ratio of operating and support files to application files. The ratio can be expected to be lower in a system that is mostly dedicated to particular applications such as word processing. Our uses, involving testing and evaluating software, weigh the balance in favor of system and support files.

Some of the files on disk were duplicates; of these, few are intentional copies, such as safety or convenience copies of configuration files or style sheets that save us changing directories. We also noted some "temporary" files of various types as well as a few files of unknown origin. These should, of course, be deleted. The distribution of filename extensions is highly skewed, as shown below: some extensions are heavily used, but many appear once, suggesting our discipline in naming files is imperfect.

Figure 5.2.1 Distribution of filename extensions in sample set.



5.3 Cataloging and Organizing Files

Whenever files are stored, we would like to know and possibly have a list of the following information:

- File name;
- Location of primary and backup copies;
- Date and time of creation and/or modification;
- Length of file;
- Format or type of file, i.e., how it is structured;
- Description of contents

We know of no operating system for which such a complete list is automatically kept. Nevertheless, the six points above provide a set of desiderata to which we may aspire.

In what follows, we will be referring to our entire collection of files, both on-line and stored on external media. In practice, unless we are very assiduous, we will not even have a record of file names and locations. While most PC operating systems include file lengths, there may be no information about the file format and the time/date stamp of the file is only meaningful if the computer that created it had a correctly set clock/calendar. Moreover, users are often careless in file manipulations — there is a strong temptation when "looking at" a file with an editing program to automatically save it again, thereby updating the time stamp. Some software is perverse enough to do this for us!

We strongly recommend that the date and time be checked every time a machine is started. To this end, we use our own small program (Pdate.pas) that displays the date and time in a format we find convenient. That is, we like to see:

Current date & time: 1991/7/2 16:46:30.36

Note that the date and time follow the ISO forms yyyy/mm/dd and hh:mm:ss.xx where xx is in hundredths of seconds. The clock in many computers is not capable of 1/100 second precision, but conversion of the fractions of a second to this form is convenient.

We often use ***redirection*** to put a time stamp on diskettes. For example, we can use the command

```
pdate >A:timedate.dsk
```

to put the current date and time line above into a file called TIMEDATE.DSK on the diskette in drive A.

Few computers have operating systems with integrated file management, where the catalog is continuously on line and dynamically updated. (The only one we have used was the GEORGE 4 operating system of the ICL 1906A computer in the early 1970s.) This reflects not only a limit on the physical resources - the size of the catalog of files may be too large to be kept continuously available ("on-line") — but also the organizational difficulty of registering changes to volumes that are not attached to the system. Users may take disks to other machines and add, delete or modify files there. How can we control or monitor such activity?

Operating systems do, however, provide the user with the capability to list the contents of a single directory on individual storage volumes (disks). How, then, can a consolidated catalog of a number of disks be made? Clearly, each filename must first be associated with the volume (we will use disk and volume interchangeably) on which the file resides, so disks must each be given a unique name or number. We may also want to note the subdirectory in which a file is found.

Thus the contents of each disk must be read, directory names extracted, filenames extracted and linked to directory names to make a full filename, and the unique disk identifier attached to each full filename. This list of extended filenames must then be sorted and displayed, with the short filename being the most likely sort key.

This task may present the user with several obstacles. First, the individual disks or tapes may have no unique identifiers if users omit to label disks or else supply non-unique names. Second, there may be no easy-to-use mechanism that allows the directory of an individual disk to be read as data by a program such as a cataloguing utility. In our own work we have made use of the operating system ***DIR*** inside batch command files rather than develop hand assembled machine code calls within programs. Once the data has been collected, the filename sorting and display must be done carefully so that duplicate names are easily recognizable.

To complicate matters, a single computer may be operated under several operating systems, each of which uses different conventions for storing the catalog directory of a disk. For example, both IBM PC class and Apple Macintosh family machines can be operated under variants of the UNIX operating system as well as their own flavors of system software. If we are running two different operating systems, we are forced to fragment our catalog. Unless there are very strong reasons for running more than one operating system, we recommend that only compatible operating systems and compatible versions be used within a single group of machines.

Our mention of versions raises "within family" differences. On the Macintosh, the System 7 FINDER on the Macintosh is different from previous versions. On IBM PCs, there are both generic (MS-DOS) and proprietary (e.g., PC-DOS, Compaq DOS) variants, and these all have a variety of versions.

We have felt strongly enough about catalogs to have developed two cataloging utilities, one for North Star DOS (Anderson and Nash, 1982) and one for MS-DOS machines (Nash J C and Nash M M, 1989). Programs that purport to do similar tasks exist in collections of shareware, but we have not seen any major commercial catalog program.

We note that a major reason for listing all files (with attributes such as length and time stamp) is that we wish to eliminate duplicate files where possible. Special programs exist that are designed to help in this task, but the catalog is a good starting point, since duplication may occur in the name rather than the file contents. Only the user can decide what files are to be eliminated and what ones kept. In some case we may need to run file comparisons to decide where the differences lie. We note that saving a file to the wrong directory is a frequent cause of multiple versions of a single file.

Catalogs of files take time to build, especially if we include all the removable volumes that accompany

a computer or group of computers. In our own work we have found our use of catalogs decreasing with the linking of our machines into a network, since this simplifies our storage of files. One and only one machine is used to hold each group of files, for example, the material for this book lives on a machine identified as JOHN on a particular fixed disk drive and in a special directory. All faxes live on a machine called FAX.

5.4 Backup

We try to maintain two backup diskettes for each directory containing our own files. About four times a year we do a complete backup to tape to preserve the files and associated directory structure. This is a form of insurance against accidental loss of the information we are likely to want to use again. Some causes of loss of information are discussed in Section 5.7. Unfortunately, the fear of information loss leads many PC users to make too many copies of the same material. (We are culprits too!) During program development, one may save trial versions of programs, thus keeping several similar, but not identical, program files. Data files, too, may exist in multiple versions, for example, the manuscript of this book as it is being revised and edited. Later we consider version control methods. Here we concentrate purely on backup.

The first requirement for the security of copies of files is that they be somehow physically distinct. For floppy disks, this means two disks. For fixed disks, copies may be made to a sequence of removable disks or tapes. It should be noted that many PC systems have a single ***physical*** fixed disk that is partitioned into more than one ***logical*** disk for organizational convenience. We do this ourselves to let part of our data to be write-protected.

Once a file exists on two separate physical objects, we need to think where we are going to keep them. For safety against fire, flood and other perils, the two copies should be in different locations, possibly in special containers to protect them against shock, dirt, moisture, heat or stray electromagnetic radiation. Of course, when updates are to be made, we may have a long walk to fetch the disk or tape for revision. In our own work, we usually accept the risk of storing short term backup files in our office. Original copies of our operating and commercial software or data are kept in a relatively inaccessible "master set" of disks out of normal reach. Disks in the "master set" generally have the write-protection mechanism engaged. For files that would be difficult to replicate from other sources of information, we keep a copy in our "security set" in another office at a different location.

Some readers may be unfamiliar with the write-protection that exists for practically all magnetic recording media. This is a physical mechanism to prevent writing, though reading is still allowed. For example, on cassette tapes there are small square tabs that may be broken off to prevent recording. On half-inch tape a write-permit ring must be inserted in a groove in the reel. 5.25 inch floppy disks use a notch that is covered to write-protect the disk. 3.5 inch disks are protected by opening a slider on a small square window.

Carrying out the backup is the most dangerous step, because it may involve having both primary and backup media (disks, tapes, etc.) in the machine simultaneously. For example, a power failure while both volumes are being accessed could cause physical damage to both. There are ways of organizing the backup to minimize such risks, but at the cost of more complexity for the user.

Backup should, where appropriate, be built into programs. It is easy to add a small amount of code to most programs that presents the user with a series of instructions to make a backup copy of data files. An example dialog might be:

Machine: DO YOU WANT A BACKUP OF YOUR DATA (Y OR N)?
User: Y
Machine: TAKE YOUR DATA DISK OUT OF DRIVE 1, PUT IN BACKUP DISK. ARE YOU READY?
User: Y

Machine: COPY MADE

Some programs ***always*** make a backup copy of a file. This can be a nuisance and fill disk space unnecessarily. Nevertheless, it is a easy task to erase all files of type .BAK for example. We even have a utility program that removes several different types of temporary files from all directories on a disk at once.

Programs may make backup copies of files at periodic intervals. WordPerfect does this. We find it annoying to be asked to wait while the program saves information, but the idea is useful in the general office environment where file-saving discipline may be slack.

The backup described so far is for individual files and represents localized backup against loss of data for a specific purpose. If we wish to answer the threat of loss posed by catastrophic failure of a fixed disk, then we need a more extensive mechanism for saving both the files *and* their organization, that is, the directory structure. We now turn to consideration of "full" backup.

The goal of a full backup is to mirror the contents and organization of the file system on a machine by copying all the files and directories onto backup media (disks or tapes). We strongly urge users to evaluate the costs and benefits of backup strategies before undertaking any serious exercise in backing up a system. Back-up takes time and effort, as well as resources in the form of equipment and media. However, we quickly improved our own back-up discipline when a neighbor's house burned down in mid-afternoon on a public holiday, while the occupants were home, and with such speed that the family dog perished.

File backup is amenable to risk/benefit analysis (Nash J C and Nash M M, 1992). The costs of data loss will depend on the particular file collection under consideration. We can ascribe time-costs to the tasks of recovering lost files. Moreover, following an approach like that outlined in Section 5.2, files can be partitioned into several categories so that costs can be ascribed to losses of each type. For example, we may have:

- Files we care very little if we lose (temp, old drafts of papers, Junior's video games, etc.);
- Commercially available files (Lotus, dBase, DOS, WordPerfect, etc.) that can be replaced at well-known cost;
- Proprietary files. These are almost impossible to replace, but how much are they worth? Their value is in the time required to rebuild them multiplied by our labor cost.

Once categories of files have been established and approximate values assigned, we can work out the total value of each category by multiplying number of files times approximate value of each. If the value is less than direct and time costs of backup, why should we do a backup? The most striking outcome (Nash J C and Nash M M, 1992) of such an exercise — easily carried out with a spreadsheet program — is that, on balance, it may ***NOT*** be worth backing up the whole file system. Saving the "important" files usually will have a net benefit. The conclusions depend on the particular costs, times, and values used.

Such an analysis underlines the need to be selective in how we do backups. We stress that it is important that the back-up save the system organization, that is, directory structures and configuration files.

An important adjunct to using risk/benefit analysis is the estimation of values for files. Clearly, if a user is unable to put a cost to losing a file, it is not worth the bother of backing it up. We believe the exercise of estimating file values is in itself helpful to users in assessing the relative importance of different aspects of their work.

On a practical level, back-up software should be chosen carefully to match personal needs and convenience. We make the following observations:

- Back-up to diskettes is very tiresome for all but the smallest collections of files. Tapes are much more convenient, especially for saving system organization and configuration.

- There are significant performance differences between backup software. Some carry out the writing of data very quickly. Moreover, the efficiency of storage may vary widely, so that fewer backup volumes may be needed with some backup software than others.
- Some backup software saves data in a form accessible to regular programs. While may be less efficient in time or in storage space, it simplifies recovery of a single item.
- We know victims of the following horror story. Backup is done in a regular, almost religious, way. Then, when a fixed disk "crashes" the data cannot be restored. We recommend testing any backup system for both backup and restore before putting much faith in it. Note also that files saved by the MS-DOS BACKUP under one version of DOS cannot be restored by the RESTORE of another version.
- Performing a "restore" to a new system is a fast way to configure it for use. (Don't violate copyrights in doing this.)
- For networked systems, software that allows backup from one machine using a storage device on another can be very helpful, since it minimizes some physical and logical work of the backup operator (Us!). We use Norton Backup Version 2 for this reason. It is also possible to backup one system by mirroring its fixed disk (or critical portions of it) on another machine's fixed disk. Note, however, that this may not provide adequate security against fire or flood damage.

5.5 Archiving

Closely related to backup is the question of archiving. At some stage in every project there are materials to be put away for safekeeping. We do not wish to lose the information, but there is not likely to be a regular usage for some foreseeable time. Alternatively, we may wish to package several files together for shipment to a colleague or for distribution. If we can also compress files as we archive them, we reduce the storage burden on our machine, though we cannot use the files directly.

Over the years, many workers have developed ***ad hoc*** or formal programs to carry out the archiving task. On MS-DOS machines, there are many programs both commercial and shareware. We use the program LHA, which has the benefits of a small size, a single program for all functions, and quite good compression ratios. (Not all archiving programs carry out compression.) LHA is, however, slightly slower in our experience than some other programs available.

When packaging software for distribution, archiving programs may offer several useful features:

- The files that make up the package are collected into a unit there is less chance for parts of the package to be mislaid.
- Some archive programs allow the de-archiving routines to be placed in the archive file and the file to be prepared as a "program". Thus the archive becomes self-unloading. We simply run the program. This eliminates the need for the recipient of the archive to have the de-archiving program.
- Compression of files into the self-unloading program or into the archive file reduces the disk space requirements and the telecommunications costs for transmitting the package over electronic mail or telephone lines.
- In some archivers, the unloader program allows a list of the contents of the archive program to be displayed. It is also helpful to have information on how the files have been packed.
- It is helpful if the archiver can capture file system organization as well as just the files. LHA allows the user to archive and restore entire directories including subdirectories, which is extremely helpful for moving or distributing packages of files.
- Archivers may have convenience features such as the capability for automatically deleting files that have been archived. Such features are helpful when we want to save many files into a single archive.

The idea of compression and dynamic unloading has caught the imagination of several programmers. There are several commercial and shareware products that will compress executable program files and attach an unloader to the compressed files. The advantages of such tools are mainly storage savings (though loading may be slightly delayed). In particular, use of compression often permits a package to be run from a single diskette, which is very useful when resources are limited, as in teaching environments.

Products that claim to "double" disk capacity apply compression to entire disks. For users who archive files regularly, the gains anticipated by "doubling" the fixed disk are quite limited, though we do use the program STACKER on our notebook computer. We caution that this program conflicted with other software installed on another of our machines and had to be de-installed at the cost of considerable effort.

5.6 Version Control

Due to reluctance to erase an active file while a new variant is being tested or to delete a file until one is absolutely sure the content of an updated file is correct, the ensemble of files may accumulate several versions of essentially the same information. Whether the failure to delete "old" files is deliberate or absent-minded, the extra files are a nuisance and a source of errors. We must be constantly watchful that the proper file is used.

The version control problem arises on all computers, large and small. The remedy requires discipline, and it is not a trivial task.

The problems multiply when several users, each with his/her own machine, are working on one shared project. Clearly everyone wants the latest version of each file. A complicating factor arises if these people are working at different locations. If machines can be physically connected, then we recommend that there be just one master copy of each file. We have adopted this strategy ourselves in preparing this book. By networking our machines, both of us can work on the same collection of files. The network software prevents both of us from having write-access to a single file simultaneously. Naturally there are overheads and occasional annoyances in such a strategy, but our experience is that the benefits clearly outweigh the costs.

When networking is not possible, we recommend adopting a system by which each file is assigned a token. This may be a physical object, for example a button with the name of the file. Only the user in possession of the token has the right to modify that file. This system works well when all users follow the rules. If they do not follow the rules, then it takes little imagination to predict the consequences.

Some measures that can be taken to help in maintaining the file ensemble in good condition follow.

- File storage can be systematized so that files of a similar nature or use are stored together. This permits the file ensemble to be segmented according to application and (hopefully) localizes all versions of one file. When we network machines, we let this process to be taken to its logical conclusion. When we work on exchangeable media such as diskettes, we can create pairs of diskettes for security but keep them organized in the same way.
- Listings of all data and programs in a given application area can be kept in a binder. Such listings should be dated. Changes can be noted on the listing, with the appropriate date. When the listing is heavily marked, it can be replaced. Old fashioned though paper may be, its human readability is self-evident, and the listing serves as both a documentation aid and a security backup. Listing programs should print the time and date stamp to help the above process.
- Unidentifiable files should be deleted.
- Users should choose a naming convention to identify temporary files that, if found in the system, can be erased without concern for their contents. Examples are files with the extension. TMV, or any files that start with the letters TEMP.

- Programs that create temporary work files should automatically delete them at the end of successful execution. We wish all commercial vendors would note this recommendation.
- For programs under development, users should consider using working disks or directories that are kept separate from the main file ensemble, or else using RAM-disks.
- The use of archiving programs to save the entire set of files at a given point in time can be helpful if we need to keep versions. This reduces the problem from one of maintaining version records for all the files to that of keeping track of the (dated) archives.

5.7 Loss versus Security

Loss of information contained in the file ensemble is the ultimate fault that we would like to avoid. Most, though not all, causes of degradation of the file ensemble are human in origin. Rarely do machine errors cause loss of information already successfully recorded.

Failure of the disk controller is unlikely to be only in the write circuitry. Moreover, read-after-write options are available on most systems and should be used to detect either drive or disk media faults (e.g., scratches).

Some of the ways in which human error can lose information follow.

- We record data on the wrong disk or forget to record it.
- Disks are handled roughly or we allow dirt and dust to accumulate.
- We make programming errors that write incorrect data.
- We are forgetful and fail to backup files immediately or fail to destroy unwanted files thereby creating a source of confusion.
- We reformat a disk containing wanted information.
- We commit a typing error that deletes data or copies from "old" to "new" during backup, thereby nullifying an update.

There is no magic cure for file degradation. Every user makes some mistakes in learning how to use his or her system effectively. Anyone who has accidentally erased a file built over much time and with much effort knows how much that experience teaches of the value of caution thereafter.

To our list above we add the possibility of intentional damage to our data. This can arise by virtue of:

- Vandalism or theft, that is, physical damage or loss of equipment;
- Intentional alteration of data for whatever motive;
- Damage by computer viruses, that is, programs designed to cause nuisance or destruction.

We do not consider intentional destruction to be a major threat to scientific users of PCs, except for computer viruses. Viruses have become a large issue because of the general practice of moving diskettes from machine to machine in an uncontrolled manner. Control requires appropriate discipline.

- It is useful to scan all diskettes that have been in "foreign" machines with a program that looks for commonly known computer viruses.
- Fixed disks of software can sometimes be write-protected, for example using our ***SnoopGuard*** device. Unfortunately, some operating software makes this difficult to do by requiring write access to several configuration files.
- Programs can be used that continuously monitor the system for suspicious activity.

- Programs can be run periodically that check for changes characteristic of the behavior of viruses.

All the above relate to detection of viruses. The only sure fix after detection is restoration of files from backup. Hence good backups are essential.

Security against unauthorized access can be accomplished in several ways. First, we recommend good conventional physical security. Doors have locks, as do filing cabinets, and they should be used if there is a risk of unauthorized entry. If machine use is a problem, there are a variety of hardware devices available that require keys, access cards or passwords to be used before part or all of a PC's resources can be used. Our own product (SnoopGuard) is an example of a password access control device. It also allows for screen blanking with password restore, a feature we believe is useful in environments where users may need to prevent information (e.g., medical or personnel files) from being seen by unauthorized persons.

Logical methods may also be used to prevent access to data. Files may be encrypted or otherwise locked in some way by the software that permits access to them. The DR DOS alternative to MS-DOS incorporates such a feature, but it is easily defeated. Several database packages let files or records be "locked". Encryption of a file is more secure, but our opinion is that it causes rather than prevents loss of data when users forget the "keys" or passwords to undo the encryption. This is even more dangerous when access control is implemented by encrypting the directory tables of a fixed disk. We have heard of several cases where physical errors, forgetfulness or disaffected employees have caused loss of the encryption keys leading to the loss of all data and programs on a fixed disk.

For data that must be kept secure, we recommend removable media. This may be as simple as using diskettes. Alternatively, several vendors offer high capacity removable disk drives that behave in essentially the same way as regular fixed disks. The removable media can be secured by regular lock and key methods.

A security measure that is often overlooked is the ***procedures manual***. This is no more nor less than a simple booklet of rules or standards to follow. By providing simple steps to follow for file system backup and a regular schedule for so doing, a procedures manual forces a small amount of order on an otherwise undisciplined situation. We recommend the practice. Alternatively, the instructions for several common difficulties can be pinned on the wall or a cork board so they are readily available. Of course, if not used, these measures are a waste of time.

Chapter 6

Programming

6.1 Programming tools and environments
6.2 Cross-reference listing and data dictionary
6.3 Flowchart or other algorithmic description
6.4 Structure and modularity
6.5 Sub-programs — data flow
6.6 Programmer practices

We now consider general ways to make programming easier. These mainly concern programming style, especially where memory space is limited or special resources of the machine must be used for reasons of speed or other necessity. While scientific computations are increasingly performed without traditional programming, users must still bring data and algorithms together in an appropriate way. This is still a form of programming and the ideas of this chapter generally apply.

6.1 Programming Tools and Environments

Scientific computing, because it often involves new ideas, can require new procedures or arrangements of procedures. In the past this has implied that scientists have had to learn "computer programming" in the traditional sense of procedural programming languages. Much scientific computing still involves the writing of code in FORTRAN, C, Pascal or BASIC, but increasingly scientists are working with computational environments more suited to their particular needs. These allow large blocks of computation to be performed at a single command, and integrate many graphical, statistical, numeric and data management tasks in convenient packages.

There are now many packages in use for statistical analysis, engineering analysis, forecasting, solution of differential equations, signal processing, image enhancement, and a host of other computationally intensive subjects. While these overcome the need for the user to program the ***detail*** of the computations, any package that allows the user to issue a sequence of commands is being "programmed". Packages requiring the user to issue commands one at a time from a console, without the possibility of execution from a stored script, are of limited utility. Such packages cannot be programmed; the user must remember and enter the commands, thereby working for the computer rather than vice-versa.

Many computational packages even present themselves like programming languages, for example, most of the major statistical packages, the matrix language MATLAB, or the modelling software GAMS. MINITAB even allows the commands of an interactive session to be automatically saved (by the JOURNAL command) for later re-execution. Here the important aspect of these packages is their capability of execution under the control of a command script, even if there is an interactive capability to let us test ideas in a quick "walk-through".

The idea of scripted calculations can be carried further using various mechanisms for stringing together existing programs. In the MS-DOS environment, we have the BATch command language to automate commands. Various mechanisms exist to enhance the MS-DOS batch commands, including "compilers" that allow faster execution and the invocation of one string of commands from another. We have been interested in hypertext scripts (Nash, 1990b). Hypertext processors of various types exist on all common computing platforms. Unfortunately, there does not appear to be a scripting language to tie together existing programs that is platform independent (Nash, 1993a). Sometimes we can use traditional

programming languages to launch executable programs.

Another way to glue together preprogrammed computational building blocks is to use a subroutine library and write the "glue" in a regular programming language that can call the subroutines easily. This is a time-honored approach in scientific computing. It is well supported by commercial and publicly available collections of routines, particularly in FORTRAN.

Whatever route we decide is appropriate, it is important to have available tools to support the writing and running of the programs we create. Convenient and reliable tools save us much time and effort. It is worthwhile choosing carefully and discarding unsuitable editors, compilers, debuggers or programming "environments". One great nuisance of our own work, involving the testing and evaluation of many such products, is that each differs in the commands, control mechanisms, presentation, and other interface details. Continual change between different interfaces is inevitably inefficient and error-prone.

6.2 Cross-Reference Listing and Data Dictionary

When developing a program, it is inevitable that one chooses names for variables in a way that suits our own convenience and taste. After some time, or in merging two programs, we may have conflicting or inappropriate uses of a single variable name. An aid in sorting out such problems is a cross-reference listing.

A cross-reference listing should itemize variables, functions and labels (line numbers) according to where they occur and their usage in a program. In Figure 6.2.1 we give a typical example for a program written in FORTRAN and compiled with the Lahey F77L compiler. Here we have set a compiler switch to generate a cross-reference listing. Such a feature is quite common in compilers, but hardly universal.

Alternatively, we probably can find utility programs to create cross-reference listings. In the past, we have used the now-dated PFORT Verifier (Ryder and Hall, 1979) that also checks conformance of the program with the FORTRAN 66 standard. FORTRAN programming tools are also available from commercial vendors such as the Numerical Algorithms Group (NAG). In our own work we have not felt justified in spending money on such tools, since we have had the benefit of compilers that will generate a form of the listing required.

The same cannot be said of BASIC or PASCAL. We extensively modified a program for preparing cross-reference listings for BASIC programs to polish the code published in Nash and Walker-Smith (1987). Similarly, in checking the PASCAL code in Nash J C (1990d), a program called TXREF, attributed to Michael Roberts, was obtained via colleagues from the Turbo (Pascal) Users' Group.

The main assistance of such programs may come from incidental features. In PASCAL, for example, we noted our most common error was that comment braces would not be closed, so that part of the program that we wanted to execute would then be inside a comment block. TXREF displays the comment level so such errors are easy to detect.

Similarly, C programmers frequently are concerned that the begin.end braces for blocks are unbalanced. Some programming editors, such as BRIEF, will format the display to show the balancing of such blocks. A similar problem exists with the ***begin*** and ***end*** constructs in PASCAL, and we have found that the TXREF program also helped in this regard.

Cross-reference listings help us to check that the data we are using is correctly named. Where possible, we should also check that it has the correct type. Furthermore, we can track the variables and/or the information they carry from routine to routine within the whole program. Such tracking is useful in

Figure 6.2.1 Listing with cross-reference table for a FORTRAN program to compute cube roots by Newton's method. The listing was edited to fit the page.

```
  F77L - Lahey FORTRAN 77, Version 3.01    10/28/92  14:45:07          PROGRAM _MAIN     Compiling
Options:/N0/N2/N7/NA/NB/NC/ND/NE/NF/H/NI/NL/P/R/S/NT/NU/
Source file Listing

  1  C      CUBEROOT.FOR  -- A FORTRAN PROGRAM TO COMPUTE CUBE ROOTS
  2  C                       USING A SAFEGUARDED NEWTON'S METHOD
  3  C
  4  C                       SOLVE Y = X**3 BY SOLVING
  5  C                         F(X) ==  X**3 - Y = 0
  6  C
  7  C
  8         REAL X,Y,XOLD,FVAL,DVAL
  9  C      X, XOLD HOLD OUR ITERATES, Y = NUMBER TO FIND ROOT FOR
 10  C          FVAL IS FUNCTION VALUE, DVAL ITS DERIVATIVE
 11         INTEGER ITER
 12  C      TO COUNT THE ITERATIONS
 13  C
 14  C      GET THE NUMBER Y
 15         WRITE(*,950)
 16   950   FORMAT('0 ENTER THE NUMBER FOR WHICH ROOT IS DESIRED ')
 17         READ(*,900) Y
 18   900   FORMAT(F10.0)
 19         WRITE(*,951) Y
 20   951   FORMAT('0 Y = ',1PE20.12)
 21  C
 22  C      PROVIDE AN INITIAL APPROXIMATION FOR THE ROOT
 23  C
 24         X=Y/3.0
 25         IF (ABS(Y).LT.1.0) X=3.0*Y
 26  C
 27         WRITE(*,952)X
 28   952   FORMAT('0 INITIAL APPROXIMATION TO CUBE ROOT = ',1PE20.12)   29  C
 30  C      SAVE 'OLD' VALUE
 31  C
 32         ITER = 0
 33    10   XOLD = X
 34         FVAL = (X*X*X - Y)
 35         DVAL = (3.0*X*X)
 36         WRITE(*,953)ITER,FVAL,DVAL
 37    953  FORMAT(' ITN.',I3,' (X**3-Y) = ',1PE16.8,' DERIV =',E16.8)
 38  C      SAFETY CHECK
 39         IF(FVAL.EQ.0.0) GOTO 20
 40  C      CHECK ON DERIVATIVE AND SAFETY SETTING
 41         IF (DVAL.EQ.0.0) DVAL=Y
 42  C      DVAL = 0.0 IFF X HAS BECOME ZERO. CUBE ROOT HAS SAME
 43  C         SIGN AS NUMBER Y.
 44         ITER=ITER+1
 45         X = X - FVAL/DVAL
 46         WRITE(*,954) X
 47  954    FORMAT('   NEW X = ',1PE16.8)
 48         IF (X.NE.XOLD) GOTO 10
 49  20     WRITE(*,955)X,ITER
 50  955    FORMAT('0 CONVERGED TO ',1PE16.8,'  AFTER ',I3,' ITNS')
 51         STOP
 52         END

Symbol Cross-Reference Listing -
Reference types:  =-Assigned; /-DATA; d-DO Index; f-FORMAT
Usage:  i-Input; o-Output; r-Argument; s-Specified; u-Used
------------------------------------------------------------------
 Name     Type       Class      Line <reference type - see above>

Abs                 GENERIC     25u
Dval     REAL       VARIABLE     8s   35=   36o   41u   41=   45u
Fval     REAL       VARIABLE     8s   34=   36o   39u   45u
Iter     INTEGER    VARIABLE    11s   32=   36o   44=   44u   49o
X        REAL       VARIABLE     8s   24=   25=   27o   33u   34u
                                 34u   34u  35u   35u   45=   45u
                                 46o   48u  49o
Xold     REAL       VARIABLE     8s   33=   48u
Y        REAL       VARIABLE     8s   17i   19o   24u   25u   25u
                                34u   41u
```

Figure 6.2.1 (continued)

```
Label Cross-Reference Listing -
Reference types:  a-ASSIGN; d-DO Label; @-FORMAT Statement; f-FORMAT
Usage: g-GOTO; i-IF; s-Specified; r-Argument
------------------------------------------------------------------
Label        Line <reference type - see above>

00010         33s   48g
00020         39g   49s
00900         17f   18@
00950         15f   16@
00951         19f   20@
00952         27f   28@
00953         36f   37@
00954         46f   47@
00955         49f   50@
```

Figure 6.2.2 Data dictionary for the cube root finder of Figure 6.2.1

Symbol	Meaning and comments
DVAL	Temporary variable to hold the value of the derivative of the function f(x) = (x**3 - y); this is f'(x) = 3 x**2
FVAL	Temporary variable to hold value of f(x) = (x**3 - y)
ITER	Iteration counter
X	Approximation to the cube root of Y which is refined by the Newton iteration.
XOLD	The last approximant for the cube root of Y. Used for the convergence test.
Y	Number for which cube root is wanted.

verifying that the correct data is used throughout the calculations and is an aid in documenting the code for users or those who must maintain or upgrade the code later.

When the cross-reference feature is not available in a compiler nor in a separate program, we must do the job "manually". This is most likely when we are trying to document scripts for special purpose packages, e.g., **Stata** or MATLAB. While we would not recommend doing the full cross-reference task by hand, for most programming or command script languages it is straightforward to list variables by routines (functions or procedures). Such a listing is sufficient for following the data flow within programs. To build the list we could use a text editor to add the function or procedure name to the variable declarations, then sort on the variable name after some stylistic cleanup.

Extending the idea of a cross-reference listing is a data dictionary. This literally gives the meaning of each data element, though it is also useful in recording the structure and format of such elements. A typical data dictionary lists the name, purpose and structure of each variable or array. Clearly, the cross-reference listing can serve as the basis and even the recording sheet for such documentation.

6.3 Flowchart or Other Algorithmic Description

The previous section concerned data structures, where they occur in programs (cross-reference) and why (data dictionary). We firmly believe this is the correct precedence, that is, we should understand the ***data*** before considering the ***procedures*** that such data must undergo. Understanding the algorithmic processes implies that we have a way of writing them down. In sum, the listing of the working program represents such a record. Unfortunately, even modern structured high level programming languages generally are imperfect as tools for description of algorithms to humans rather than computers.

What is desirable is a description of what we want the PC to do in words we can understand. To this end, many programmers use some simple method for describing the algorithmic processes. Two approaches

are the flowchart and the step-and-description pseudocode.

Flowcharts are diagrams with arrows showing the control transfers within the program. Variously shaped geometric figures are used to denote different types of processes within the algorithm. The use of flowcharts seems less common now than previously, especially in describing scientific computations.

The pseudocode, or step-and-description approach uses simple numbered or labelled steps and statements in plain language to explain what is going on. Comments should be liberally used, particularly if the reason for a given statement is not obvious. A number of authors have used various pseudocodes having a formal syntax, for example, the introductory text for beginners by Dyck, Lawson and Smith (1979). In mathematical computations, different forms have been employed by Lawson and Hanson (1974) and Nash J C (1979a). Nash J C (1978b) gives some reasons why such a informal presentation of an algorithm may be preferred to a program listing. In passing, it is worth noting that two pseudocodes have become full-fledged programming languages, APL (Iverson, 1962) and PASCAL (Wirth, 1971). In our own work, we generally use descriptions close to PASCAL. MATLAB is becoming common as a way to describe numerical algorithms.

6.4 Structure and Modularity

In recent years, structure in programs has become a much publicized virtue. Good programmers have always kept their programs tidy and well-arranged so that they can be easily documented, debugged, altered or maintained. They write their computer programs so that it is obvious what they are doing. Formalizing such arrangement or tidiness of programs has become a fashionable and at times lucrative occupation.

Since there are many programs written by those who do not know what they are doing, the use of tools and programming practices that force some order on the chaos is to be welcomed. However, the movement can have the same fervor as a temperance meeting. Our personal practice is to strive for well-ordered programs that are easy to comprehend, without slavishly following the dictates of structure. For small experimental programs, we have sometimes produced some shockingly unstructured code, most of which is soon discarded.

Fundamentally, we wish to subdivide any program into parts, each of which has only one pathway "in" and one pathway "out". Clearly, any program can be organized artificially to have just one beginning and one end. To be useful however, the structuring must divide the range of processes into sensible pieces so that each can be considered by itself. Our recommendation:

Divide the program into the largest pieces that can be conveniently considered by themselves.

We wish to avoid any procedure that alters the state of several variables. Such a procedure may have too many options or features, much like a fancy kitchen appliance or workshop tool. This is the wrong type of structuring.

At the other end of the spectrum, a frequent mistake of novice programmers who have just been taught macros or subroutines is to put each small loop or calculation in its own sub-program. The resulting main program becomes a difficult-to-read collection of CALLs. The difficulty experienced when one tries to read undocumented APL programs is closely related to this type of over-structuring; each operator performs several actions and looks like a CALL to a short subroutine. If the functions performed do not need to be considered at the detailed level, it may be better to ignore the individual operators and lump together several small routines into one.

The issue of GOTO commands in any programming language has been hotly debated in the computer science literature. Knuth (1974) presents a moderate viewpoint with wisdom and humor. Clearly, it is a good idea to avoid jumping around all over a program, since this makes it difficult to break up into pieces

that can be conveniently considered one at a time. Nevertheless, there are occasions where a simple jump over several lines of code is the most straightforward and understandable means to accomplish a task. It can sometimes be useful to be able to execute the same segment of program code in more than one situation, yet not set up a separate procedure or function. A balance must then be struck between an easily understood program and one that avoids unreasonable code duplication. In our opinion the C language constructs ***break*** and ***continue***, or their equivalents in other programming languages, can be as troublesome to understand as the GOTOs they implicitly replace.

As a convenient set of programming rules, we try to keep in mind the following ideas:

- Sections of code should not extend over more than one page in length. This allows us to see all of one section of code at once.
- Each section of code should, if possible, have one entry point and one exit point. For multiple branching (***case*** statement in PASCAL, ON...GOTO... in BASIC, ***switch*** in C, computed GOTO in FORTRAN, or similar construct), the individual branches can be replaced by subroutine calls to make the code more readable, but the calls should be documented to tell the reader what is done by each of them.
- Every section should have sufficient comments or remarks to explain its fundamental purpose.

6.5 Sub-programs - Data Flow

In most computer languages, including many of the command scripts for computational packages, there is the provision for building sub-programs to carry out frequently-used and (hopefully) well-defined tasks. FORTRAN, in particular, probably owes much of its popularity to the relative ease with which users may call subroutines to compute, for example, the normal (Gaussian) distribution probabilities, or to invert a matrix.

The importance of the sub-program in any programming language is that it isolates the task to be done and allows us to focus on doing the best job we can on that task alone, without concern for the larger goal. In particular, we should ***not*** have to be concerned with the names or functions of particular variables apart from those involved in the present calculations. The sub-program has its own ***local*** data structures (variables, arrays, etc.) so we do not have to worry about inadvertently changing some value in a way that has perverse consequences for the whole of our program. Unfortunately, things are never that simple, and the transfer of information between calling and called routines is a frequent source of errors. Setting up the calls can involve much work.

The simplest subroutine is the GOSUB . . . RETURN structure in BASIC. However, users of "old-fashioned" BASIC must be very careful to recognize that the code invoked by GOSUB is really a part of the main program, with which it shares all the variables and arrays yet defined. While executing, the subroutine may generate more variables, which are in turn grist for the mill of other parts of the program.

This becomes particularly nasty when a subroutine is called from a loop. The subroutine code may alter the looping parameter, with disastrous consequences. In some dialects, variables may be used for input/output channel numbers. Changing such a variable to a nonexistent device number will usually cause the system to "hang".

Other languages may pose fewer dangers in this regard, but they are hardly immune to them. We have made the same mistake in FORTRAN at an early IBM OS/MVT site. The interesting outcome of attempting to "read" a record from a line printer was that a 12 inch diameter bell of the fire-alarm variety just inside the front cabinet of the IBM /360 model 50 machine started ringing. It was an indication that the operating software — down to the hardwired ***monitor*** (like the BIOS on today's PCs) — had detected an unrecoverable error. Among the regular programmers at this site it became a matter of pride to "ring the bell".

Clearly, the operators of the system could have saved much aggravation if simple checks for valid calling arguments were built into the internal functions and subroutines of the FORTRAN compiler used. When writing sub-programs, we ***strongly*** urge readers to include such checks. While they require additional lines of code and may slow the overall execution of the program, the checks serve to document what we expect as input to the sub-program. If execution time becomes an issue, the lines of code constituting checks can be commented out or bypassed with some sort of compile-time or run-time switch. We regard the presence of such code as a form of documentation for all users. Once we can be assured that the calling routing will never present unacceptable inputs, the checks can be set aside.

The actual passing of data to and from sub-programs is another matter. There are several mechanisms, each of which presents its own concerns.

Argument lists for functions and procedures provide the most obvious mechanism for passing data. Suppose we want to compute the natural logarithm of a variable named X. Then we could write

```
Y = ALOG(X)
```

in FORTRAN. Similar statements can be used in other languages. Unfortunately, none provide a way to keep control if X has a non-positive value, or even a value that is so small that the logarithm cannot be computed within the available arithmetic. A better alternative would be

```
Y = OURLOG(X, FAILED)
```

where FAILED is a Boolean (LOGICAL) variable that is TRUE whenever the logarithm cannot be computed. In such cases we may want to provide Y with some default value, which in IEEE arithmetic (IEEE, 1985) might be the NAN (Not-A-Number) value. An alternative is to use the NAN to signal that the log function has failed, but we need to be sure that this ***convention*** is followed universally within our programs if it is to have any value in protecting against errors.

Notice that FAILED is now an argument passed from the called to the calling routine. Thus we introduce the issue of direction of flow of information. This is frequently a source of confusion and errors. In PASCAL, variables whose values are passed back to the calling routine (they may also be passed into the routine) must have the prefix ***var*** in the definition of the function or procedure. We have experienced more "bugs" than we would like to admit from omission of the ***var***. Worse, the internal arrangements of compilers for argument transfer are such that some variables are called by value — their values copied and, if passed back, copied back. Others are called by location, that is, their address is passed to the sub-program, so we cannot avoid changing the values in such arguments if they are operated on within the sub-program.

Several difficulties arise. Because arguments are usually defined by their positions, simple confusion in the order of arguments in a call can have unexpected effects. Some arguments may define values for which we would like to use a constant. If the call is by location, we can actually change the values of a "constant". We once changed the value of "3" to "10" by such an error. In C, the arguments of a function are usually ***push***ed onto a stack. This includes arrays, so that it is easy to overflow the available stack space. We have experienced this type of difficulty in C, trying to translate FORTRAN code for the timing study of Chapter 18.

We have already mentioned that BASIC assumes ***global variables and arrays***. This is also the case for the "languages" defined by several statistical and numerical packages. In other programming languages we may wish to define global variables to simplify argument lists in calling sub-programs. In particular, it can be extremely tedious to transfer all the data relating to a large problem via explicit reference in an argument list. We may also want to avoid the transfer of information about the computing environment such as the machine precision, range limits and other "default" information.

We think the main concern with the use of global variables is that both programmers and users may forget that they are in play. We believe that they should be used in simplifying programs, but that they ***must*** be documented in the sub-program and preferably mentioned in the calling program. Otherwise we

can quickly find ourselves using global variables we believed were local.

The FORTRAN construct of COMMON allows for global variables, but is best used in the ***labelled*** COMMON form, so we can segment the global variables according to usage. This offers a convenient partitioning of the data that is global to several routines. For example, one block of common can be reserved for exogenous data, another for machine environment, another for working storage, etc.

The transfer of data to a sub-program can also be accomplished by storing the data first in a structure (array, record, file, etc.) from which the sub-program can then extract it. C explicitly defines structures and passes ***pointers*** to the structures rather than the structures themselves.
This approach is straightforward to use, is very efficient of computer time, but may lead to errors if we are not careful to ensure both main and sub-program use exactly the same pointers and definitions.

Files are another possible data transfer mechanism. In particular for users with fast disks (or large pseudo-disks or RAM-disks), a reasonable choice for passing a large amount of information to a subroutine is to have the main program write a file and the subroutine read it again. Moreover, it offers the potential for segmenting the execution of a program should we wish to check results, carry out another task, or simply have some safeguards in case of error in later computations.

Another type of subroutine call is that to a machine language routine. This is not a topic commonly offered in courses, yet it is important to many users of PCs who wish to interface calculations with data received from some unusual external or internal device. One example is the job of controlling temperatures in experimental equipment by turning on heaters or fans.

Most PC language dialects offer methods for invoking machine code or linking to assembly language routines. However, the mechanisms can be complicated and are not for the faint of heart. Personally, we have only carried out such operations via well-defined operations in BASIC (on 1970s vintage PCs) or by execution of operating system calls from Turbo PASCAL on MS-DOS PCs.

Typically, the major difficulty is that the program constructs for transfer of information require us to fill registers or memory locations with data before we make the transfer of control. Similarly, after return from the routine, we may have to unload data. We resort to machine language calls only when there is no other way to accomplish the task, or where the advantages are too great to overlook. In such cases, we recommend keeping the calling mechanism as simple as possible.

A special case is a call to execute another program. In PCs, it can be extremely useful to be able to launch one program from within another program. For example, in the middle of a data analysis, we may want to invoke a text editor to allow us to alter the values of some numbers. To set the properties of a printer it may be useful to call up the operating system command shell to reset some parameters. The facilities for making such transfers of control are provided in most programming languages. They are straightforward to use, but we caution users to take note of all the details that must be accounted for.

The different approaches to passing information to sub-programs are not equivalent in their demands on computing resources. To underline this, see Figure 8.1.2, where different methods for calling sub-programs were used.

6.6 Programmer Practices

Every programmer wants to program effectively. Where the target computer is a mainframe, the programmer may need to anticipate a range of inputs that could cause program failure. The PC user may be prepared to suffer the occasional "crash." Indeed, practices designed to save our own time rather than that of the PC, or to "get the job done" may be higher priorities than an elegant source code. Therefore, our perception of efficient programming on a PC concerns the ease of use or ease of modification to a far greater extent than the speed of execution. This does not excuse, however, a lack of ***programmer***

documentation to show the state of development of a program code.

We are ready to allow programs that are incomplete in the sense that they will not trap all invalid input data. A warning comment should be provided. We are less comfortable with the use of nonstandard special features of a programming language or computer. Tricks that use "undocumented features" are equally unwelcome. This is simply because such enhancements cost many hours of work if we decide to run the program on another system, or even to modify it for another problem on the same PC. Programming is fun and a great learning experience — one of us (JN) enjoys it immensely — but it earns the scientific programmer and user no money, no credit for research done and no love from his or her boss. One must keep a proper perspective on the time and place for monkeying with the system. An informal cost-benefit analysis performed mentally has, at times, served us well and prevented monumental waste of time and effort.

The main strategy that we recommend for effective programming is simplicity. If you must use the fancy advanced programming tools in a programming language, then at least describe what these do, so that the user who must implement the program on a PC without the particular feature can arrange to get the task completed in more pedestrian fashion. Even better, replacement code can be provided in the commentary or in documentation. In any event, the documentation should make note of any unusual or possibly confusing structure.

Chapter 7

Size Difficulties

7.1 Determining data storage limits
7.2 Choice or adjustment of data structures
7.3 Usage map
7.4 Restructuring
7.5 Reprogramming
7.6 Chaining
7.7 Change of method
7.8 Data storage mechanisms for special matrices

This chapter deals with the situation where memory available to the user is not large enough to hold the program and data to solve a given problem. The proposed solutions change the program, though it may be cheaper to physically increase the memory capacity. For some PCs and operating systems, however, there have been ***address space*** limitations on the amount of memory that may be accessed at any given moment. Note that it may be possible to enlarge the memory available for programs by making temporary or permanent configuration changes in the PC setup.

7.1 Determining Data Storage Limits

If we have run out of space for our programs or data, we first need to know or find out what are the true limits. The first limitation is on the ***physical memory*** — the total main memory installed in our PC. The amount of main memory capacity is detected automatically by the start-up software of our system. Usually there is a test run to ensure memory integrity before loading the operating system, which has to keep track of the memory since this is a key system resource it has to manage.

The ***user memory*** is generally significantly smaller than the physical memory. First, we must allow for the program code and working storage needed by the operating system for its own functions. Increasingly — and we believe this is due in many cases to sloppy programming — the operating system is demanding such a large part of the memory that user programs will hardly fit. Besides allocating memory for user programs, the operating system also controls its allocation RAM-disks, printer buffers, file I/O buffers, network facilities, or disk caches.

The architecture of the processor, the electronic design of the PC, and the operating system will all define limits on the amount of memory we can access and may exclude certain addresses. The original IBM PC design has led to some annoying limitations on the amount of data that can be addressed in it and its successors. Historically, the Intel 8080 processor used a 16-bit address space allowing for 65,536 or 64K addresses, each storing one byte of information. To partially overcome this address space limitation, a switching scheme is used that allows several banks of 64K of memory to be used, but only one at a time. By appropriate programming we can then work with much larger amounts of memory, but at the cost of developing quite complicated software. A similar ***bank switching*** idea is used in the Intel 8088 processor (the processor of the original IBM PC and XT) that manages to combine a 16-bit address with a 16-bit ***segment register***. The segment register is multiplied by 16 and added to the 16-bit regular or ***offset address*** (Scanlon, 1984), allowing for a total of 2^{20} or 1,049,576 or 1 megabyte of memory. Where necessary, we will specify the 20 bits as 5 hexadecimal digits rather than use the complicated segment:offset notation that is ***not*** unique and confusing.

When IBM designed the original PC it was decided to further reduce the available memory for programs, including the operating system, to just 640K. The remaining addresses were reserved for ROMs, disk controllers, video adapters, and other devices.

Programming languages may complicate the issue of memory. Many early compilers and interpreters for MS-DOS PCs used only a short form of addressing involving the offset address. This means that programs had to fit both code and data in a single block of 64K of code. A minor improvement made in those compilers allowing 64K for code and 64K for data. More modern compilers have fewer restrictions if the correct compiler and/or linker switches are set. Read the manual carefully!

More recent Intel processors, along with the Motorola 680x0 processors used in the Macintosh, can address very large amounts of memory directly. Unfortunately, there is much "old" but still useful MS-DOS software around. Some mechanisms for running the "old" programs within a more flexible environment are beginning to appear. There are also schemes that allow large address space software to be run alongside MS-DOS, e.g., Microsoft Windows and IBM OS/2. Other approaches involve the use of special memory management software such as the Phar Lap or other DOS extenders that allow programs to use the large address space yet be launched normally from within DOS.

Various utility programs, e.g., the MEM instruction in more recent versions of MS-DOS, will allow the user to determine the maximum amount of regular memory available to programs and data. For PCs based on Intel 80386 or later processors, configuration adjustments supported by various memory management software allow some functions to be moved to regions of the address space beyond the 640K limit. Typically, the space available for user programs may be increased by 60 to 70K, which may be enough to allow us to avoid other measures.

On the practical level, we can only truly find out the maximum size of programs and data structures by experiment. Our recommendation is to perform such trials ***before*** making a commitment to a given programming environment. By varying parameters that define the size of large arrays or other constructs in small test programs, we can quickly, if inelegantly, learn the outside limits on such structures. We illustrate the approach in Figure 7.1.1. Comments in the codes reveal our findings.

7.2 Choice or Adjustment of Data Structures

If we cannot carry out a computational task by either reconfiguring our PC to gain more usable memory or by adding physical memory, then we must reorganize the calculations. This essentially means choosing different ways to store data or using a different method for solving the computational problem. Here we look at the data structures.

An obvious method for reducing the memory requirement of a task is to reuse a variable or array so that it holds more than one piece or block of data at different stages of the calculation. This reuse of data structures is a very common feature of many algorithms, especially those developed in the early years of automatic computation. It is easier said than done. First we must find out what data is needed at each stage of a program and then arrange for it to be stored appropriately for use in calculations.

Some programming languages allow certain data structures to be defined only for the duration of a given block of code. Indeed, variables and arrays used in FORTRAN subroutines, which are not in the argument list (calling sequence) nor in COMMON, are supposed to be local and not defined when the subroutine is reentered (ANSI 1978). In practice, however, compiler writers may not bother arranging that memory be released when not needed. It is simpler to assign space for each subroutine separately, even if the total exceeds what is available. It is the user who must work to squeeze his or her program into the memory available. C programming does allow for explicit allocation and release of memory, though it is still common for programmers to forget to release storage.

Early PCs had with user memory limited to about 30,000 bytes, so we reused even simple variables to

keep programs as lean as possible. However, bigger gains come from reuse or restructuring of arrays. Array space can be saved in the following ways:

- Rectangular matrices should be dimensioned to conform to the problem. An array declared 20 by 10 will have over 100 unused elements for a 12 by 8 problem. Some programming languages (e.g., C) allow dynamic redefinition. This needs to be done carefully.
- An array may be reentered from disk rather than saved. For example, to solve linear equations

(7.2.1) $A\ x = b$

we may decompose the matrix A. Such decompositions often overwrite the original matrix, so that no extra storage is needed. Once a solution x has been found, we no longer need the decomposition, and can reread the matrix into the same storage to compute the residuals

(7.2.2) $r = b - A\ x$

- Matrix decompositions that have a special structure can employ different storage mechanisms (See Section 7.8).

Arrays can also hold non-numeric data. As with the examples just given, sensible choice of data structures can save memory requirements.

Figure 7.1.1 Use of simple programs to determine array size limits.

a) BASIC

```
0 LET M = 16385
20 DIM B(M)
30 FOR I = 1 TO M
40 LET B(I) = I
50 NEXT I
60 PRINT "DONE m="; M
70 STOP
80 REM for GWBASIC 3.23  m=15047
90 REM for Turbo BASIC 1.1 m=16382
100 REM for QBASIC 1.0, MS BASIC 6.0,
 QuickBASIC 4.00a m = 16383
110 REM for TRUBASIC after conversion from
 this code m =37500
120 REM was accepted, then it gave an out of
 memory error.
```

b) PASCAL

```
program sizetest;
const
  maxsize = 8084; {biggest is 10808 in TP5.5}
  { 8084 in TPW, but then runtime error 105 }
  {10809 in TP5.0                            }
  {10820 in TP3.01a TURBO.COM                }
  { 6487 in TP3.01a TURBOBCD.COM             }
  { 8114 in TP3.01a TURBO-87.COM             }
{vary the above number until program
     will not work}

var
  big: array[1..maxsize] of real;
  i  : integer;

begin
  for i:=1 to maxsize do big[i]:=i;
  writeln(
  'DONE SIZETEST for maxsize = ',maxsize);
end.
```

7.3 Usage Map

Ideally, we would like data structures to be named for the data they hold. When data is no longer needed, its corresponding data structure should be cleared so memory is freed. This is not always possible and so we reuse data structures, but then must keep track of what data elements are in each data structure — a source of possible confusion.

To effectively reuse data structures, we must know when particular data elements are required and when their use has ended. A usage map is any record of the active data structures at some given program milestones. We know of no programs that prepare such a map, but important aids are the cross-reference table and the data dictionary (Section 6.1). The usage map can become complicated when many data identifiers or program milestones are involved. It helps to group data elements in sets.

The main task is to record the program milestone after which a given date element is not needed. Jumps in the program (GOTOs) make this difficult to work out. We have found even well-structured programs have quite messy usage maps, and only recommend their preparation:

- Where we need to adapt a program to a slightly larger problem;
- Where there are clear opportunities to reuse large data structures.

Such retrospective attempts to reduce the space requirement of a program mean that the original design could be improved.

7.4 Restructuring

When the program and data will not fit, and reasonable chances for reuse of variables or arrays have been exhausted, yet we still need a little more memory, restructuring the code to make it shorter may help.

In particular, several sections of similar code may be replaced by subroutine calls to a single sub-program. Certain parts of a program that are nonessential to the calculation may be deleted or split into programs that are to be chained with the main calculation (Section 7.6). Output may be vastly simplified, even to the detriment of readability, thereby saving the space of all the descriptive text in print commands. Two or more loops over similar indices may be combined. Rather than use many assignment statements to put data into variables or arrays, we can use special programming features or read values from a file. In BASIC, the DATA statements require space that can be released by such a restructuring.

We recommend small experiments to decide which approach is most economical of space. The resulting code may be less simple or readable, but necessity takes priority over elegance, though some changes to branching may save code yet render the structure more transparent. Figure 7.4.1 shows a small example. The truncate function INT replaces a loop structure, but we must add a PRINT to ensure subsequent PRINTs start on a new line when N is not a whole multiple of 5.

Figure 7.4.1 Simple example of restructuring. Both program segments will print a vector V of N elements with 5 elements printed on each line.

A.
```
1000 REM PRINT VECTOR 5 ELEMENTS PER
          LINE
1010 FOR I=1 TO N STEP 5
1020 FOR J=I TO I+4
1030 PRINT V(J),
1040 NEXT J
1050 PRINT
1060 NEXT I
```

Size: 99 bytes

B.
```
1000 REM PRINT VECTOR 5 ELEMENTS PER
       LINE
1010 FOR I=1 TO N
1020 PRINT V(I),
1030 IF 5*INT(I/5)=I THEN PRINT
1040 NEXT I
1050 PRINT
```

Size 92 bytes

7.5 Reprogramming

An extreme case of restructuring is the complete reprogramming of the computation. This is not nearly the admission of defeat it may be taken to be. First, programs always grow and change with the tasks to which they are put. There are nearly always parts that can and should be simplified, especially after "patches" are made. Second, reprogramming allows variable and array names to be rationalized. Third, the experience gained with the program can be incorporated into improvements in the rewritten version. Patches and fixes can be cleanly made a part of the whole. Finally, documentation can be brought up to date.

Obviously, reprogramming is not a task to be undertaken without due consideration. Nevertheless it may be better than hours of frustrating work trying to restructure a much altered code, possibly without up-to-date documentation.

7.6 Chaining

Chaining is an "old" technique for handling size problems. We break up the task into pieces that can be run sequentially in a "chain". Some language processors allow for automatic chaining. That is, an executing program may command the PC to load and begin executing another program. While this technique still exists in some compilers and interpreters, it has largely disappeared as a formal tool. Users can, however, arrange for similar functionality in a variety of ways, in particular BATch command files in MS-DOS or programs that execute other programs, such as hypertext systems. We use "chaining" to refer to any form of this idea.

The primary requirements for successful chaining are:

- Suitable breakpoints in the task and
- A mechanism for passing data from one program to another.

The first of these requirements is dictated by the task at hand. Note that almost all problems have at least three common parts: initialization and input, processing, and reporting of results. Rarely can we not split a task into pieces.

The second requirement, that of data transfer, is sometimes provided for in the language processor. Compilers and linkers that permit ***overlays*** are performing such a job. We avoid such techniques in favor of simplicity. It is quite easy to write needed data to a file in one program, then read it again with the next program in the chain. The chaining tasks can then be accomplished by BATch commands or similar method.

Such "start-from-file" facilities in a program can be very helpful if we must carry out very long program runs. Our programs can be set up to periodically output a file with a standard name, e.g., PROGSTRT.DTA, that is always read when the program starts and which contains the status of the program. If it is necessary to interrupt the program to perform other tasks, or if power failure or other breakdown upset the progress of execution, we can simply restart without losing the whole of our work. This is especially useful for programs that use iterative algorithms.

7.7 Change of Method

The last way to overcome size difficulties is to change the method by which a solution is sought. This is really formulation and choice of method, which will be discussed again in Chapters 12 and 13. Normally we will not change the method unless there are strong motivations. In our experience, running out of space is such a motivation.

When changing methods for this reason, the main criterion is to reduce the overall memory space. We make our point by using the example of function minimization methods, for which Table 7.7.1 shows some typical working storage requirements for some well-known methods (Nash J C and Nash S G, 1988). Other factors, such as efficiency in finding a minimum and need for gradient information will influence our choice, but we can see that the Conjugate Gradient (cg) and quasi-Newton (qn) method both use function and gradient information, yet cg only requires a few vectors of storage, while qn needs a matrix. If the methods are not too dissimilar in performance, then cg can save us space as n increases. Generally Table 7.7.1 illustrates some signposts to reduced storage requirements we should watch for:

- The use of vectors instead of matrices;
- Iteration rather than direct solution;
- Short code length, even if there are many loops;
- Use of data implicitly rather than explicitly, e.g., a way to compute a matrix-vector product where we do not use the matrix itself;

- Segmentation of data, so we use it piecemeal from storage.

The divisions between restructuring, reprogramming and change of method are not always clear. An example of space-saving that merges the ideas is Algorithm 15 from Nash J C (1990d). This code is designed to solve the generalized matrix eigenproblem

(7.5.1) $A\ x = e\ B\ x$

for symmetric A and B, with B positive definite. That is, we want to obtain all the possible sets of eigenvalues e and eigenvectors x that satisfy Equation 7.5.1. Several techniques are available but most of those that solve for all the eigensolutions first decompose the matrix B, then develop a standard symmetric matrix eigenvalue problem. In the algorithm in question, we decided to use a Jacobi matrix eigenvalue routine to accomplish ***both*** the decomposition and the resulting standard eigenproblem. Thus the code length was considerably reduced.

Table 7.7.1 Working storage requirements for some function minimization methods. Only the leading term in n, the order of the problem, is given for storage requirements.

Method	Storage requirements	Function requirements	Work per step
Hooke and Jeeves	$2n$	f	O(n)
Orthogonal search	n^2	f	O(n)
Nelder Mead	n^2	f	O(n)
Newton	$n^2/2$	f, g, H	O(n^2)
Truncated Newton	$9n$ to $13n$	f, g	O(n^2)
Quasi-Newton	$n^2/2$	f, g	O(n^2)
Conjugate Gradient	$3n$	f, g	O(n)
Steepest Descent	$2n$	f, g	O(n)

f = function, g = gradient, H = Hessian

7.8 Data Storage Mechanisms for Matrices

Matrices often have a special structure that can be exploited to save memory space when solving particular problems. Matrices are so important in scientific computing that we include here a few tactics and structures that are useful. We will use v[ ] and a[,] to represent one and two dimensional storage arrays in computer programming languages.

An ***LU decomposition*** of a square matrix A, (used in elimination methods for solving linear equations) can often overwrite the original array. This is accomplished easily if one of L or U must always have unit diagonal elements. Suppose

(7.8.1) $L_{ii} = 1$ for $i = 1,2,. . .,n$

This can be "remembered" by the program and requires no storage. The other elements of the decomposition are stored as follows:

(7.8.2) U_{ij} is stored in a[i,j] for j >= i, since

(7.8.3) $U_{ij} = 0$ for $j < i$ (upper triangle)

(7.8.4) L_{ij} is stored in a[i,j] for $j < i$ (strict lower triangle) since

(7.8.5) $L_{ij} = 0$ for $j >= i$

Any ***triangular matrix*** can be stored in a linear array (vector). There are several ways of doing this, but one simple one (Nash, 1990d, page 82) is to use a row-wise ordering, which for a lower triangular form has the following equivalence:

Figure 7.8.1 Array storage ordering

[2 D] Array				[1 D] Array (vector)			
(1,1)				1			
(2,1)	(2,2)			2	3		
(3,1)	(3,2)	(3,3)		4	5	6	
(4,1)	(4,2)	(4,3)	(4,4)	7	8	9	10

The relationship can be written

(7.8.6) v[$i*(i-1)/2+j$] = A_{ij}

Note that we could also use a column-wise enumeration

(7.8.7)

1			
2	5		
3	6	8	
4	7	9	10

In which case the correspondence is

(7.8.8) v[$j*(j-1)/2+i$] = A_{ij}

For upper triangular matrices we must transpose these rules. Programmers making use of such techniques should be ***very*** careful to make sure that the correspondences are always correct. It is also worth noting that for matrices less than, say, 15 by 15, the extra program code will offset the storage saving of $n(n-1)/2$ matrix elements, where n is the order of the matrix. The break-even value of n can be found by testing.

These triangular schemes are appropriate for symmetric matrices, where

(7.8.9) $A_{ij} = A_{ji}$

Banded matrices, which have

(7.8.10) $A_{ij} = 0$ for $|i-j| > k-1$

where k is the band width, can be stored as a sequence of diagonals. Consider the case where we have a symmetric band matrix with band width $k = 5$. Thus we have

(7.8.11) $A_{ij} = 0$ for $|i-j| > 4$

Since the matrix is symmetric, the subdiagonal elements A_{ij} for $j < i$ are equal to the superdiagonals A_{ji} . We can store the data in a rectangular array a, with the following correspondences

(7.8.12) a[i,1] = A_{ii} for $i = 1,2,. . .,n$

(7.8.13) a[i,2] = $A_{i,i+1} = A_{i+1,i}$ for $i = 1,2,. . .,(n-1)$
[note: a[n,2] = 0]

(7.8.14) a[i,3] = $A_{i,i+2} = A_{i+2,i}$ for $i = 1,2,. . .,(n-2)$
[note: a[n,3] = a[$n-1$,3] = 0]

In this case, we store only $3n$ elements instead of $n^2 = n*n$ elements. Clever programmers probably can even use the three unused elements of a, i.e., a[n,2], a[n,3] and a[n-1,3].

Hermitian matrices are complex matrices defined so that

(7.8.15) $H = H^*$

where * represents the conjugate transpose. That is, if Re(x) is the real part of the complex variable x and Im(x) is its imaginary part,

(7.8.16) H_{ij} = Re(H_{ji}) - Im(H_{ji})

But the equality imposed means that the real part of H is symmetric, while the imaginary part is anti-symmetric (Nash J C 1974). Thus,

(7.8.17) Re(H_{ij}) = Re(H_{ji})
(7.8.18) Im(H_{ij}) = - Im(H_{ji})

Note that Im(H_{ii}) = - Im(H_{ii}), so that

(7.8.19) Im(H_{ii}) = 0

We therefore can store the real part of the Hermitian matrix in one triangular matrix, and the imaginary part in a triangular matrix with no diagonal. These can be put back together in a square array as follows.

(7.8.20) Re(H_{ij}) = a[i,j] for $j <= i$
= a[j,i] for $j > i$

(7.8.21) Im(H_{ij}) = a[j,i] for $j < i$
= a[i,j] for $j > i$
= 0 for $j = i$

There are so many mechanisms for storing ***sparse matrices*** that it is futile to try to survey them. We find two simple mechanisms useful.

- The array is stored as three linear arrays (vectors) that only mention non-zero elements: r[j] gives the row index of an element, c[j] gives the column index of that element and v[j] gives its value, for j = 1,2,. . .,E, where E is the total number of elements. Note that the triples of numbers (r[j], c[j], v[j]) can be written in any order, but that some orderings may be helpful for particular calculations such as matrix multiplication. We may even want two copies of the vectors at hand with different orderings of the elements.

Example: 5 by 4 matrix

1	0	0	2	r:	1	1	2	3	4	5	5
0	0	1	0	c:	1	4	3	1	3	2	4
3	0	0	0	v:	1	2	1	3	4	1	1
0	0	4	0								
0	1	0	1								

- The array is stored as a row-wise set of paired values giving the column-index and element value of each non-zero element. We can use two vectors C and V. A new row is indicated by a negative column index. In this scheme, we can no longer present the matrix elements in any order. Clearly, column variants of this scheme are also possible. For the example above, we have (row form)

c	v	comments
-1	1	"new" row, the first, column 1
4	1	same row, column 4
-3	1	new row, row 2, column 3
-1	3	new row, row 3, column 1
-3	4	new row, row 4, column 3
-2	1	new row, row 5, column 2
4	1	same row, row 5, column 4

Chapter 8

Timing Considerations

8.1 Profile of a program
8.2 Substitutions
8.3 Special hardware
8.4 Disk access times
8.5 Time/accuracy and other tradeoff decisions
8.6 Timing tools

Some applications of computation require answers within a specific time period. Any tracking problem, such as air or surface traffic control, satellite orbit management, or numerical machine tool positioning, must have answers quickly. How quickly may determine the hardware and/or software required for these "real-time" jobs. The machine must respond in a given elapsed time after receiving the data on which calculations are to be performed.

Many other situations arise where timing is important. Operators may lose interest and attention if response is too slow. A timesharing scheduler may demote a "long" job to a low priority in the job queue, or may charge more than we wish to pay. While less than two decades ago, statements like:

> *It is worthwhile thinking about a problem for an hour in order to save a minute of CPU time* (Quittner, 1977, p. 14)

reflected genuine concerns, we can now buy high-performance processors for so low enough prices that the issue is now to speedup computations for our convenience rather than for computer efficiency.

This chapter presents some techniques available to measure and reduce the execution time for a program. Because each problem has individual requirements, users must choose their own detailed path to attain acceptable speed.

8.1 Profile of a Program

To reduce the time requirement for a program we must know ***where*** time is spent. We can measure the time taken to execute a given segment of program code, count the number of times a given statement or group of statements is executed. We want to find the parts of the program that contribute most to execution time.

Such measurement of effort can be found from a ***profile*** of the entire program. This will record the number of times a statement was executed. It may give a subsidiary count to show how often an IF statement condition was TRUE or how many times a DO loop was entered or exited. Certain compilers may allow this to be carried out by invoking special features. Sometimes programs exist that will carry out the profiling. They may even estimate the time taken by statements. We generally prefer to build clocks or counters into programs ourselves to avoid high learning costs associated with other approaches, though we use the same ideas. We try to locate the time-critical portions of a program, not time every line of source code. Focusing on known time-consuming tasks, we attempt to discover bottlenecks so we can seek to overcome them. Some obvious features of our code to examine and time are loops, calls to sub-programs, and input/output functions.

We can often speed up loops, especially nested loops (loops within loops) by streamlining their coding.

Common actions can be moved outside a loop. Note, however, the counter example in Monaghan (1992). Figure 8.1.1 gives examples of loop simplification.

Some calls to subroutines or functions may be replaced by in-line code. A subroutine call may involve much work in transferring required information. Figure 8.1.2 gives an illustration in FORTRAN.

Figure 8.1.1 Illustration of loop simplification in cumulative binomial probability calculations. The codes compute the probability we get k or fewer successes in n independent trials with probability of success in a single trial of p.

a) Explicit calculation.

Note: $C(n,i) = n! / ((n-i)!\ i!)$

```
        FA = 0.0
        DO 10 J=1,(K+1)
C         LOOP FROM 0 TO K INCLUSIVE
          I=J-1
          FA=FA + C(N,I)* P**I * (1.0-P)**(N-I)
 10     CONTINUE
```

b) Partially simplified calculation using stored binomial coefficients

```
        DO 25 J=1,K
C     STORING BINOMIAL COEFFICIENTS
          BCOEFF(J)=C(N,J)
  25    CONTINUE
C       NOW COMPUTE THE CUMULATIVE PROBABILITY
        Q = 1.0 - P
        QT = Q**N
        FB = QT
        IF (K.EQ.0) GOTO 40
        PT = P/Q
        DO 30 I=1,K
C         LOOP FROM 1 (NOT 0) TO K INCLUSIVE
          QT=QT*PT
          FB = FB + BCOEFF(I) * QT
 30     CONTINUE
```

c) Calculation using a recurrence relation; no binomial coefficient calculation is carried out in this code.

```
        Q = 1.0 - P
        QT = Q**N
        FC = QT
        IF (K.EQ.0) GOTO 60
        PT=P/Q
        DO 50 I=1,K
C         LOOP FROM 1 (NOT 0) TO K INCLUSIVE
          QT = QT*(N-I+1)*PT/I
          FC = FC + QT
 50     CONTINUE
```

Timings in seconds and cumulative probabilities for 5000 repetitions of the above calculations (Lahey F77L, 33MHz 80386/80387 MS-DOS PC).

n	k	p	T(a)	FA	T(b)	FB	T(c)	FC
8	5	0.3	2.470	0.9887078	1.760	0.9887078	0.440	0.9887078
20	10	0.9	5.930	0.0000072	4.450	0.0000072	0.770	0.0000072
20	10	0.1	5.930	0.9999993	4.450	0.9999992	0.770	0.9999994

Figure 8.1.2 Effects of algorithm, option selection and use of in-line code versus subroutine call for several FORTRAN programs for the singular value decomposition applied to random sparse m by n matrices (many zeros)

Method (see list below)

m	n	I	II	III	IV
5	5	5866 (4039)	5505	10194 (6924)	8751
5	5	5866	5505	10194	8751
10	5	10867 (6539)	13103	12261 (7838)	10867
20	5	22503 (14473)	29403	38707 (18512)	32216
20	20	398950 (249360)	1211600	1320400 (954213)	1247400
40	5	44862 (24138)	70610	91839 (22214)	88329

Timings are in microseconds for execution on an IBM 370/168 under the MVS operating system and the FORTRAN G1 compiler. The singular value decomposition of matrix A into the matrices U, S, and V may be accomplished without the U matrix being computed explicitly. Figures in brackets show the times for this option.

I — the Golub/Reinsch method (see Wilkinson and Reinsch,1971)
II — a FORTRAN version of Nash (1979a), Algorithm 1
III — a FORTRAN version of Nash (1979a), Algorithm 4
IV — method III using in-line code rather than a subroutine call to accomplish plane rotations of a matrix

If a sub-program executes too slowly, we may be able to substitute a quicker but less general version. For example, it is not necessary to use a general-purpose sub-program to compute results if the input arguments have values in a specific range. Depending on requirements, we can replace the function call with a table look-up or a simple approximation. This is a time / accuracy tradeoff (Section 8.5).

The action of printing data or reading or writing to disk or tape is generally very slow compared to memory access, even with clever buffering schemes. It may be helpful to read data once into memory if we have space, so that there is no waiting for disk access when we need to calculate. Printing can often be postponed until a calculation is completed to avoid delaying progress within loops, or a print buffer used.

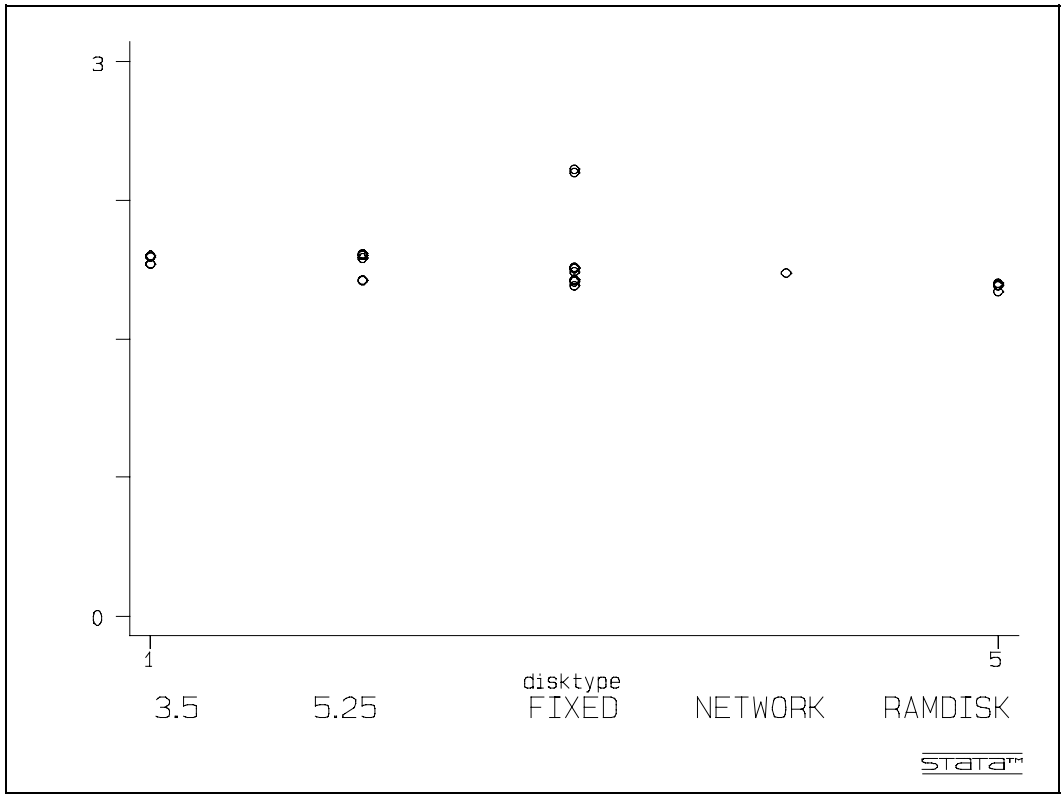
The approach just presented is only one form of a ***trace*** of the program execution. Facilities for tracing exist within many programming environments and "debuggers". One needs to be a frequent user of such tools to profit from their application. Since each tool takes time and effort to learn, we prefer to add our own trace when needed, but those who work with just one programming environment should know how to get the maximum information from its debugging, tracing or profiling tools.

In Figure 8.1.3, we show the effect of reading data into an array in computing the mean and variance of 10,000 numbers. Using standard formulas, a first pass over the data calculates the mean of the numbers and a second pass the variance and standard deviation. Alternatively we could a RAM-disk (Section 8.4) and avoid having to change our program.

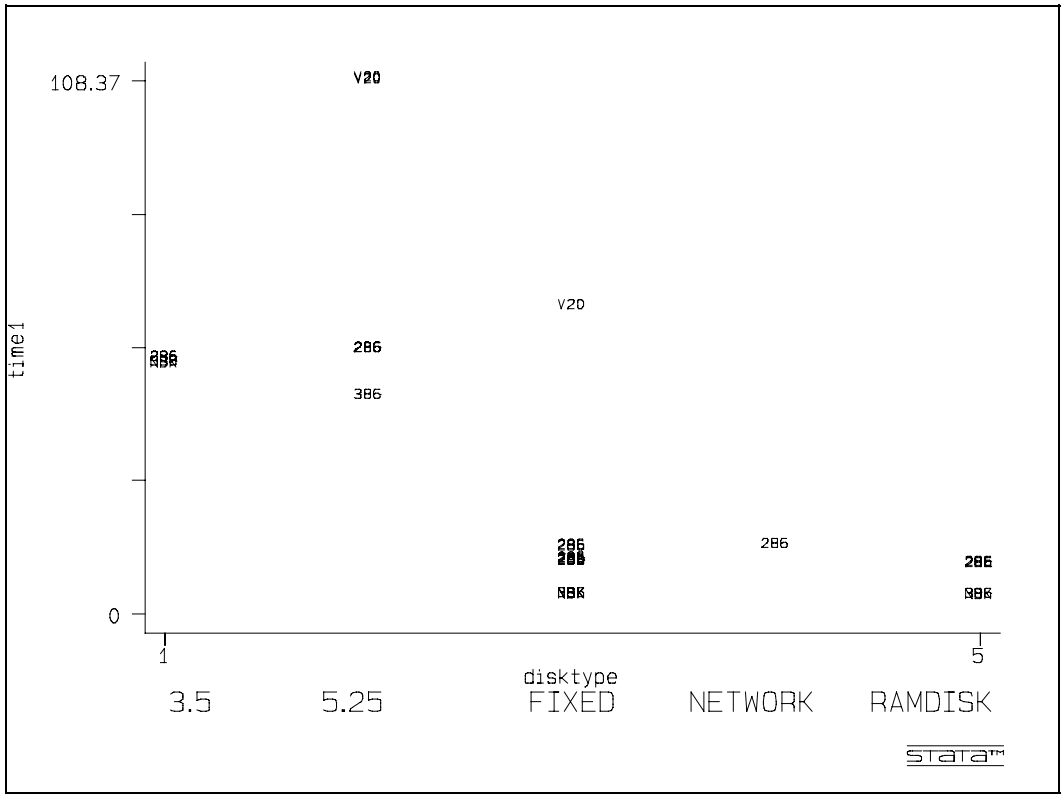
In carrying out profiling, the user may simply want to count the number of times a given operation occurs. Simple count and write statements accomplish this. Some examples, such as the number of function or gradient evaluations in function minimization tasks, are so common as to be a regular part of packaged programs. Others can easily be added by the user. We note, in particular, the availability of

Figure 8.1.3 Variance calculation using standard two-pass formula on different MS-DOS computers from different disk types.

a) Ratio time(data from disk) : time(data pre-read into array)



b) Actual times (seconds) for using pre-read to array.



a count of floating-point operations within the MATLAB mathematical computation system (Moler, 1981, Math Works, 1992).

One technique we have frequently used for following the progress of a program is to print different letters or symbols whenever a particular segment of code is executed (Nash J C and Walker-Smith, 1987, p. 151 and p. 167). This provides for a very succinct output that barely slows the program execution, yet it informs the knowledgeable user what the program is doing. In most programming languages, display of single characters need not force a linefeed, so very little screen or paper space is used to record quite a lot of information, though such displays may confuse the uninitiated. We need a key to the significance of the displayed characters or they are meaningless. Nevertheless, the technique is quick, easy to use and gives a rapid view of the relative usage of different parts of a program. The technique cannot be used if the display does not appear until a line is full, that is, until a buffer must be emptied.

8.2 Substitutions

The profile should tell us which parts of our calculation are "slow" so that we may consider what action to take to achieve a speedup. We consider the following possibilities:

- Speeding up the overall operation of the program by use of a better translator for the programming language;
- Optimization or use of machine code for key segments of the program;
- Use of additional processors in concert with the main processor.

If we consider replacing our programming language compiler or interpreter, we need to be reasonably sure that the new version will be faster yet provide correct code.

Table 8.2.1 Comparison of execution time on a 33 MHz 80386/80387 MS-DOS system for compilers and interpreters using the simple program:

```
40 FOR I=1 TO 10000
50 LET X=EXP(SIN(COS(1!*I)))
60 NEXT I
```

Compiler or interpreter	Time (seconds)
Microsoft GWBASIC 3.23 interpreter (does not invoke 80387)	26
Microsoft QBASIC 1.0 interpreter	9
suppressing 80387	51
Microsoft BASIC Compiler 6.0	5
suppressing 80387	50
Microsoft Quick BASIC 4.00a	5
Borland Turbo BASIC 1.1	3
suppressing 80387	19

Interpreters are like simultaneous translation at a meeting, converting source statements to machine instructions on the fly, while compilers do the translation once and for all. The situation is complicated by the existence of interpreters that attempt to simplify the source code before execution. Keywords in the source code can be reduced to 1-byte ***tokens***. Some compilers partially process programs to an intermediate (possibly machine-independent) pseudo-machine code or p-code that may be interpreted or compiled. The UCSD Pascal system was a popular example of such a translator. The line between compiler and interpreter blurs with such practices. Typically, however, compilers provide significantly faster overall execution speed than interpreters, though interpreted code has other advantages that may be important in certain circumstances. The speedup will vary greatly depending on the type of operations. Testing and measurement (see Chapter 18) are the only way to know for sure.

Assembly languages are tools for programming using the processor's actual instruction set. Generally, the large number of details that need attention when programming at so low a level make this unattractive for scientific computations, but the speedup may be worth the trouble. We have found assembly code routines to be useful in only a few cases. For example, on a first-generation PC (Anderson and Nash, 1983) we were able to sort numbers approximately fifty times faster using 8080 assembly coded than with BASIC, the only other programming language available. A lot of human work was required to get this improvement, needed because the time delay in BASIC was unacceptable for the application, which involved ranking sports tournament scores.

We may sometimes be able to obtain fast assembly or machine-code routines from commercial or academic sources. An example is found in the BLAS (Basic Linear Algebra Subprograms, Dongarra et al. 1979) that have been optimized for many machines. Many common matrix algorithms have been specifically coded as calls to the BLAS to ensure reasonable efficiency over a wide class of computer systems. The BLAS has been used as the basis for LINPACK (Dongarra et al 1979) and LAPACK (Anderson et al., 1992).

8.3 Special Hardware

If cost effective, consider adding extra hardware to increase throughput of data. This may improve performance with little human effort or intellectual energy. Special co-processors or ancillary circuit boards allow functions such as Direct Memory Access input/output (DMA), disk operations, floating-point arithmetic, or control functions to be performed very efficiently. Some examples are:

- Special graphical display boards that have their own onboard processor to speed up display functions;
- Disk doublers or data compression boards to provide fast but reliable enhanced data capacity;
- Special numeric co-processors for vector or matrix functions;
- Printer or communications buffers;
- Caching disk controllers.

The major concerns for the user in employing such add-ons are possible difficulties in installation and use. Co-processors designed to work with our existing system are usually easy to install. While very early software for PCs was unable to take advantage of the Intel 8087, this void was soon filled. First dual-version products appeared like the Borland Turbo Pascal 3.01a compiler with TURBO.COM and TURBO-87.COM. Most current software automatically detects the co-processor. If it is not present it is emulated by software, so results are (supposedly!) the same whether or not the co-processor is present, though computation time will generally be much longer without it. Some software requires a co-processor.

The 80x87 family of numeric co-processors is popular because of the large base of existing PCs using related 80x86 main processors, the high performance gain they give for low cost, and the conformance of these processors to a sensible standard for floating-point arithmetic (IEEE 754 April 1984). Consequently, there has been a demand for easy-to-use software to exploit these devices. The Motorola 6888x co-processors fulfil a similar role for the 680x0 main processors of Macintosh PCs and other machines using the 68000.

Manufacturers other than Intel and Motorola offer products that are replacements for the regular co-processor but claim better performance. They may offer better value for money, but timing tests are needed to check claims. Since factors such as memory transfer speed may affect performance greatly, the tests need to be carried out on a variety of machines. We have seen one serious case of overheating in a co-processor, but floating-point is often a heavy power user and circuits run "hot".

The speed of a co-processor should be matched to our system. In 8088 / 8086 class machines, and 80386 and later systems, the cycle speed for the co-processor is the same as for the main processor. This is not generally the case in 80286 machines. Our own 80286 machine uses a 12 MHz main processor but an 8 MHz 80287. In reviewing some statistical software, we discovered an error that only occurred on such a machine. It did not occur when the 80287 was disabled. We believe that the C compiler used to create the program tried to optimize performance by running the 80286 and 80287 in parallel. Since the 80286 runs faster, it wins the race and causes an error (Nash J C, 1992).

The devices just discussed are called co-processors. They execute commands that form a part of an instruction-set for the computer architecture to which they belong. The floating-point instructions are "ignored" by the main processor; the co-processor executes them and returns results for use by later instructions. The main and co-processors act together as one CPU (central processing unit). Some microprocessors, e.g., variants of the INMOS Transputer and the standard Intel 486 processor (but ***not*** the 486SX), have floating-point instructions built in.

Not all floating-point add-in hardware works as transparently as the devices just discussed. To obtain higher performance on some special tasks such as inner-product accumulation

$$\text{(8.3.1)} \qquad Inprod(x, y) = \sum_{i=1}^{n} x_i \; y_i$$

we may choose to acquire a special-purpose "vector processor". To use such a device, however, we must transfer data in and results out of it. These transfers must be very fast, or we will lose the advantages of the device's speed of calculation. We will need special software, usually provided by the device manufacturer or related companies, but may have to write some machine or assembly code to maximize performance.

8.4 Disk Access Times

Any data processing job involves getting data in and out of memory. In typing data at a keyboard this is obvious, as is the delay loading data from any serial access media such as a tape. Disk operations, even those on high-performance fixed drives, take precious milliseconds. Attention to disk data transfers may offer ways to reduce such delays.

Delays for transferring data from disk are made up of three parts:

- Seek time — the time required to move the read / write head to the track to which data is to be transferred;
- Latency time — the time for the disk to revolve until the data is under the head;
- Start-up time — if the rotation motor is deactivated when the disk is inactive. This is common for flexible disk drives, and is also used to save battery power for fixed disks on some portable PCs.

The delays can sometimes be reduced by program modification. Start-up time may be avoided by calling functions to spin the disk in anticipation of data transfer. We have used the trick of executing a READ or WRITE instruction that does ***not*** actually transfer any data. Similar tactics can be used sometimes to pre-position the read / write head to save seek time.

A more general improvement can be obtained by using a ***disk cache***. The idea is to move the data we are going to use to memory as in Figure 8.1.3, but now we do this at the system rather than application level. Most disk caching is done with hardware or with system software loaded with the operating system. Table 8.4.1 shows the results of some timings with Microsoft's SMARTDRV.SYS, which is a software cache. Note the significant speedup on write operations.

Direct reduction of seek or latency time is more difficult, since it involves changes to low-level code within the operating system. However, data placement on the disk may help to reduce either seek or latency time, if the workings of the particular drive are understood, and may have some important side benefits.

Seek time may be reduced if the file to be read is stored as a contiguous block on the disk. A ***sector*** is the physical unit of storage on the disk. The words "cluster", "block" or "bucket" are also used, possibly with special meanings. We number sectors from 1 to N, where N is the total number of sectors available for use on the storage device. Assuming our file is stored from sectors S to F inclusive, and each sector holds C bytes of information, our file can be at most (F-S+1)*C bytes long.

Unfortunately, files are often ***not*** stored this way. One of our earliest machines, a North Star Horizon, had an operating system (North Star DOS) that forced files to be created as contiguous blocks. This allowed for very little data to be appended to the file. To overcome this deficiency, most operating systems allow for extensions to files. These extensions need not be physically adjacent to each other. Typically, a file is initially assigned a minimum number of sectors. When more space is needed, a standard sized block of sectors is added. This is sometimes called an ***extent***. The operating system handles the creation and adjustment of the file space. Moreover, it will reuse space freed by the deletion of files, and may even avoid reuse of recently deleted space so as to improve the chances that the user can undelete (i.e., restore) accidentally erased files.

The ongoing use of a disk eventually has the operating system hunting for space all over the disk; files become ***fragmented***. This may delay data access. First, there is the directory management overhead — a file now has several entries that record where its parts are located and in which order they are to be accessed. Second, the read/write head must now move, possibly across several tracks, to get between blocks of sectors — adding seek time for each extent.

The remedy for such fragmentation is to ***defragment*** (or "defrag") or ***compact*** the disk. A variety of commercial and free software exists for such purposes. Our experience suggests a considerable variation in features, reliability, ease of use, and performance. Defragmentation of a large disk may take quite a long time — sometimes hours — especially with some slower programs.

In our experience, the time costs of fragmentation are usually minor, but there is a security advantage to contiguously stored files. If the directory of the disk is damaged, our data remains untouched but inaccessible. Many utility programs can read individual (physical) sectors of data. Indeed, the better ones allow us to search sectors for specific patterns of data. Therefore we may be able to locate a sector belonging to our file. If it is stored contiguously, we can simply search forward or backward sequentially until we have found and resaved all our precious data.

To find out the importance of disk fragmentation to data transfer times we wrote a small program to create a fragmented file and time the operations to do this. Starting with 2 text files, call them AAA and BBB, with BBB null, we repeatedly appended AAA to BBB, but in between each append operation, we created a new copy of AAA on the disk by copying AAA to F01, F02, F03, and so on. The F?? files are then between the extents of AAA. We timed the "append", the "copy" of AAA to F??, and then a "read" of the whole of BBB after each append and copy cycle. We did this for a 3.5" flexible disk, a fixed disk and a RAM disk on our 33MHz 80386/80387 machine, using a program compiled with Turbo BASIC 1.1 and files of two different sizes. The timings were saved to a file and edited for analysis by the statistical package **Stata**. To eliminate file size effects, we computed the operation time (*optime*) for a read, append or copy of a single line by dividing timings by the file size in lines. Graphs show very minor slowdown with increasing fragmentation except for flexible disk operations. To check that there was no

Table 8.4.1 Impact of disk caching and disk compressions. The disk cache is Microsoft SMARTDRV.EXE (from Windows 3.1) dated 10/03/92. The disk compression is STACKER version 2.01 dated 26/02/92. The test file consisted of 3147586 bytes in 100000 lines of text. The cache size was 1MB.

```
         write  read   copy          details
        12.46  11.54    25.1   Tower 486D66, nostack, cache
       176.64  10.82  266.01   Tower 486D66, nostack, nocache
cache  ======================
speedup 14.18   0.94   10.60

        29.22  28.51   56.25   Notebook 386DX33: cache, nostack
       236.79  24.38  479.44   Notebook 386DX33: nocache, nostack
cache  ======================
speedup  8.10   0.86    8.52

        25.05  24.93   48.94   Tower 386DX33, nostack, cache
        231.3  23.95  388.32   Tower 386DX33, nostack, nocache
cache  ======================
speedup  9.23   0.96    7.93
```

Stacked disk cache speedup. Note how minor the speedup actually is.

```
        22.46  18.01   96.34   Notebook 386DX33: c, cache, stack
        38.39  19.28  717.82   Notebook 386DX33: c, nocache, stack
cache  ======================
speedup  1.71   1.07    7.45

Stacked disk slowdown (NOTE: it turns out NOT to be slower!)
Nocache
       236.79  24.38  479.44   Notebook 386DX33: nocache, nostack
        38.39  19.28  717.82   Notebook 386DX33: nocache, stack
stack  ======================
slowdn   0.16   0.79    1.50

Cache
        29.22  28.51   56.25   Notebook 386DX33: cache, nostack
        22.46  18.01   96.34   Notebook 386DX33: cache, stack
stack  ======================
slowdn   0.77   0.63    1.71

       231.62 121.99  552.33   M286 12 nostack, nocache
        85.74  57.89  787.41   M286 12 stack,   nocache
stack  ======================  (There is insufficient memory to
slowdn   0.37   0.47    1.43     install a cache on this machine.)
```

hidden effect we modeled *optime* using a linear model

(8.4.1) $$optime = b_1\ fragments + b_0$$

Table 8.4.2 shows the results for modelling read times. We see that there is a pronounced effect for flexible disk files. For fixed disk files we see from R-squared that the model has very poor predictive power relative to using a constant read time, but fragmentation is still a statistically significant variable in the model. For RAM disk, fragmentation does not seem to matter, as we would suspect because there is no physical mechanism to explain a slowdown. Similar results were observed for append and copy times.

As a final note on defragmentation, one should ***not*** attempt to interrupt the process, especially during ***directory*** compaction. One of us (JN) started a defragmentation, realized there was a block of files that should be deleted first, and tried to halt the process by hitting the ESCape key. While we have had not difficulties in doing this when files are being moved around by the defragmenter (we use OPTune), here we managed to cross-link — that is, confuse the directory of — 100 Megabytes of storage. What a mess! Fortunately, we had backup of all but one file, which was short and available on paper. Still, several hours of cleanup were required.

Another possible time saving may come from the placement of sectors on each track to reduce latency time. Here we need to know how the sectors are ***interleaved***. That is, we need to know the ordering of the sectors along the track. For example, if there are ten sectors, they could be arranged in natural order

1 2 3 4 5 6 7 8 9 10

However, since it is sometimes impossible to read one sector right after another, sectors may be ordered

1 3 5 7 9 2 4 6 8 10

This gives the PC a chance (about half a disk revolution) to put sector 1 safely in memory before having to read sector 2. Few users will want to engage in the complicated exercise of adjusting their data to save time in this way. Still, the knowledge of how a particular disk works will be important in explaining specific types of performance of a program. Moreover, programs exist that allow for the changing of the "interleave factor" as well as to perform other disk maintenance tasks. An example is the program SpinRite.

The cure for slow execution caused by disk transfer times may rest, not in changing software or data placement, but in replacement of the disk drive with a faster acting one. Replacement drives with higher capacity or performance than original equipment may be available and require no software changes.

Another choice is to simulate the disk with a faster storage device. Using software, the relatively slow physical disk is simulated in fast memory. Data usually disappears when the power is turned off, though some suppliers may use a battery to preserve "disk" contents. This approach to creating a fast "disk" is variously called a semiconductor disk, pseudo-disk, RAM disk, or virtual disk. We ***always*** configure our machines to have at least a small RAM disk for scratch files and fast text editing. Most RAM disks use of system memory, but manufacturers have from occasionally offered special boards or boxes. The virtues of using RAM disk have already been shown in Figure 8.1.3 (b).

8.5 Time/Accuracy and Other Trade-off Decisions

For floating-point calculations, we may measure deviations from precisely known values for answers. We may, of course, not need ultra-precise results, and can possibly save time by sacrificing accuracy.

Iterative algorithms often produce successive approximations to the desired results, with termination controlled by measuring the difference between successive iterates or similar values. When the measure is smaller than some tolerance, the program stops. By making tolerances larger, the program will usually (but not always!) stop earlier, but the results may not be as "good". The difficulty is in finding or modifying software to get the right time and accuracy.

To obtain a "low accuracy" method, we need to understand how accurate the solution must be, then choose or adapt a method, possibly quite crude to achieve it. A simple example is the computation of the cumulative Normal (Gaussian) distribution by numerical integration. By increasing the number of integration points, we hope to increase the accuracy of the approximation to cumulative probability. Note that increasing the number of integration points does not necessarily increase the accuracy of the result, since there may be rounding errors in summing many small numbers. Table 8.5.1 shows a sample of results in both 8 and 14 digit arithmetic from a now-defunct North Star Horizon. The decision to use 8 or 14 digits is itself a time / accuracy tradeoff. Here, we also need more array space for more integration points, though the program can be arranged to need only a few storage locations independent of the number of integration points.

Table 8.4.2 Time penalty for file fragmentation as found by linear least squares regression of the time to read one line of a file versus the number of file fragments. We use R-squared as a measure of the success of linear model, with 1 indicating a perfect fit, 0 showing that fragments do not help to explain the read time. We give the t-statistic of the coefficient of "fragments". An absolute value < 1 for the t-statistic indicates that it may not be worth using fragments to model the read time.

	File of 720 lines		File of 120 lines	
	R-squared	t(fragments)	R-squared	t(fragments)
3.5" Flexible	0.8217	17.571	0.2365	5.510
Fixed disk	0.0833	4.243	0.1131	-5.024
RAM disk	0.0005	0.221	0.0241	-1.556

Table 8.5.1 Computing the probability that the standard Normal distribution has an argument less than 1.960 by integration. Times are given in seconds. Abramowitz and Stegun (1965) give a value of 0.97500210485178.

Number of integration points	8 digit FPBASIC value	time	14 digit FPBASIC value	time
2	0.94823555	0	0.9482355602402	0
4	0.97284807	0.1	0.9728480852968	0.1
8	0.97480306	0.2	0.97480304586296	0.2
16	0.97498101	0.4	0.97498100028943	0.4
64	0.97500182	1.6	0.97500181413367	1.9
128	0.97500208	3.2	0.97500206927061	3.9
256	0.97500187	6.4		
512	0.97500208	12.9	0.97500210430476	15.8
1024	0.97500223	25.8	0.97500210478352	31.5
2048			0.97500210484367	63.3

8.6 Timing tools

We strongly recommend ***measuring*** the performance of programs as they are actually used. Experts can only give opinions about performance. What count are test results. We urge users to watch for simple changes, such as using a RAM-disk for data input or disk cache for output, which can lead to dramatic speed improvements with minimal effort from the user. How then, should users conduct the timings?

When we started using PCs, we commonly used a stopwatch. This is reliable, but not very accurate for programs that run quickly. Fortunately, most computers now have usable clocks. The main worry is that the "tick" in many PCs is quite slow, typically about 1/20 of a second, even though times may be reported to several decimal places. We do not trust the timing of intervals of less than 1/4 second unless sure that the clock and the software to access it are capable of fine-resolution timings.

The software mechanisms to access clocks are a serious nuisance for programmers. The sub-programs provided are not standardized, so that timing of the same routine with several compilers may require us to alter the code for each compiler. Worse, the timing resolution may vary between compilers. Occasionally we may have to use the "time-of-day" clock functions, giving only 1 second timing resolution. Sometimes the time-of-day is provided as a string variable, which makes for more work.

A sub-program that returns elapsed time in seconds or hundredths of seconds since some starting point is wanted. We note, as did Cinderella, that strange things happen at midnight. A negative timing in Chapter 18 was corrected by adding 24*60*60 = 86,400 seconds.

A few programming environments provide no mechanism for accessing the clock. We can consider writing assembly or machine code routines to get the time. We did this some years ago for our North Star Horizon, although the manufacturer said such a program was not possible, and even spent a pleasant hour or so at the computing center of the Technical University of Vienna in 1980 showing others how to do it. There is a satisfaction in overcoming such programming obstacles, but only if the timing routines are used regularly can the effort be justified.

An alternative is to return to the idea of a stopwatch and build this into our computing environment. We find our MS-DOS program TIMER, for which partial PASCAL source code is given in Figure 8.6.1, to be very useful. This program "runs" the program we wish to time and gives us a report of the total elapsed time for the run. During the elapsed interval, we must load and exit from the program we are timing, so it is a good idea to work from a RAM-disk. Alternatively we can compile a "dummy" version of the

program in which the first executable statement is replaced by a STOP or similar command, so that we can time the program load. (Note that the rest of the code should be kept to give the load module the proper size.) Clearly, any statements that require input from the keyboard are also going to be timed. This problem can be overcome by arranging that all input comes from a file. Sometimes we can use input/output ***redirection*** to get data from a file. As an example, to time the program MYCOMPN.EXE using data in a file MYCOMPN.DTA, with output sent to a file MYCOMPN.OUT, we would issue the command

```
TIMER MYCOMPN.EXE <MYCOMPN.DTA  >MYCOMPN.OUT
```

Again, the default ("logged-in") disk drive containing the program and input files should be a RAM-disk to minimize the data read times.

When using computational or statistical packages, such as MATLAB or **Stata**, we cannot use this approach if we want to time how long it takes to run particular sets of commands within the package. Some packages provide timing commands, e.g., MATLAB offers a wall clock and a routine for using this to compute elapsed times in seconds. With other packages we may need to invoke operating system commands, e.g., in **Stata** we can preface an operating system command with an exclamation point and have it executed from within the package. With some ingenuity, one may be able to use such mechanisms to save a time stamp in a form readable by the package itself and thereby develop ways to time processes automatically. Lacking timing tools or a method for accessing external programs, we must get out the stopwatch.

All timings suffer from the possibility that events too fast for our "stopwatch" to register — everything happens between clock ticks. To overcome this, we put operations to be timed inside a loop. This is trivial to arrange, but we must then exclude administrative overheads of program startup or looping from our timings. As before, the answer is to develop "dummy" versions of programs that have the parts we wish to time commented out. The desired timing is then obtained as the difference between the timings for the "active" and "dummy" programs.

Sometimes we wish to compare performance of programs with or without numeric co-processors. Some authors claim the only sure way to "turn off" the co-processor is to unplug it. However, sometimes we can use operating system environment variables. Table 8.6.1 shows some settings for MS-DOS compilers. These control settings may not be listed in the index of a manual, or may be listed under headings we, the users, are unlikely to consider. In fact, we rely on trial and error and the timings to see if they work. This is how we decided that the co-processor could be suppressed for QBASIC 1.0 in Table 8.2.1.

Table 8.6.1 MS-DOS Commands to turn off 80x87 co-processor function for selected compilers. Some are case sensitive and require appropriate spellings. The relevant flags are set to null (that is, there are no characters after the equals sign in the SET statement) to restore functionality, e.g., SET 87=

compiler	*suppress 80x87*
Borland Turbo BASIC 1.0	SET 87=no
Turbo Pascal 5.0	SET 87=NO
various Microsoft products	SET NO87=Coprocessor Suppressed

Figure 8.6.1 Parts of TIMER2.PAS to time the execution of other programs in MS-DOS machines. Copyright J C Nash 1991

```
program Timer2; {Runs other programs and displays the time taken to do so.}
{$M 8192,0,0}          { Leave memory for child process }
uses Dos;              { To access the timing procedures in TP 5.5 }
var
  Command, parmstr: string;
  i, nparm: integer;
  hr1, hr2, min1, min2, sec1, sec2, hun1, hun2: word;
  dsec: real;
  lsec: longint;

begin
  writeln; writeln('TIMER2 (C) J.C.Nash 1991 -- execute & time DOS programs');
  writeln;  nparm:=paramcount;  parmstr:='';
  if nparm=0 then
  begin
    writeln('You MUST provide a program to run i.e. TIMER MYRUN.EXE');
    writeln('Give FULL path if needed,  i.e. D:\mydir\mysdir\myprog.exe');
  end;
  begin {at least 1 paramter (the program}
    command:=paramstr(1);
    for i:=2 to nparm do  parmstr:=parmstr+' '+paramstr(i);
  end;
. . .
  gettime(hr1, min1, sec1, hun1); dsec:=sec1+0.01*hun1; {start time}
    SwapVectors; Exec(Command,parmstr); SwapVectors;
    if (DosError<>0) then
    begin
      writeln('Termination with DosError =',DosError);
      if DosError=2 then writeln('?? wrong path to executable file');
    end;
    writeln('DosExitCode =',DosExitCode);
    writeln('TIMER2 start ',hr1:2,':',min1:2,':',dsec:5:2);
    gettime(hr2, min2, sec2, hun2);  dsec:=sec2+0.01*hun2; {end time}
    writeln('TIMER2 end   ',hr2:2,':',min2:2,':',dsec:5:2);
    dsec:=0.01*(hun2-hun1)+1.*(sec2-sec1)+60.*(min2-min1+60.*(hr2-hr1));
    writeln('Elapsed seconds = ',dsec:8:2);
end.
```

Chapter 9

Debugging

9.1 Using output wisely
9.2 Built-in debugging tools
9.3 Listings and listing tools
9.4 Sub-tests
9.5 Test and example data
9.6 Scripts and documentation
9.7 Resilience to I/O failure and disk problems
9.8 Tests of language translators

The word "debugging" entered the jargon of computers one August night in 1945 when a two-inch moth was discovered inside the Mark I at Harvard. According to Grace Hopper, "things were going badly wrong in one of the circuits of the long, glass-enclosed computer. Finally, someone located the trouble spot, and using ordinary tweezers, removed the problem, a two-inch moth. From then on, when anything went wrong with a computer, we said it had bugs in it." (SIAM News, 1992) "Debugging" has since become the accepted name for the process of correcting the faults in a program so that it runs as desired. In this chapter we shall consider how the user may best carry out this step, whether in a traditional program, in a command script for an application package or within the application program itself. Debugging skill cannot make up for poor program design and implementation, but errors are a part of all programs at various times in their life-cycle. It is important to have a strategy for finding and correcting them.

The chapter also considers software testing and validation, that is, the steps that go beyond merely satisfying ourselves there are no obvious errors. We want reliable performance in a variety of situations for an array of problems.

9.1 Using Output Wisely

The first step in removing errors is to find their cause(s). The cause may be quite distant from the resultant effect, both in execution time and lines of program code. To find the "bug", we must make the program tell us what is, and has been, going on by inserting commands to display or print information about the state of our computation. Eventually, when the program works perfectly, the intermediate output is a nuisance.

A useful tactic is a switch mechanism in the program so that intermediate output may be suppressed. Commonly a program variable provides the switch; if zero/***non-zero***, it permits/***inhibits*** the execution of output commands. Some compilers allow us to leave out statements at compile time by means of compiler switches. Then there is no runtime overhead, though we do have to recompile the program.

Another choice is to direct diagnostic output only to a screen so that it is not saved. We could also send it to a separate file, possibly on a RAM-disk. In either case writing to screens or files takes time. Note that the time to write to video memory is usually much slower than to regular memory. Table 9.1.1 shows regular and video memory write timings for three MS-DOS PCs.

If intermediate output is produced, it is obvious that it should contain sufficient information to enable the error to be found. The important pieces of information that must be transmitted are:

- The path taken through the program, so we can learn which program instructions were executed and in which order;
- The values of control variables such as arguments in logical expressions, looping variables, and flag variables;
- Values of selected result variables that indicate successful completion of various parts of the program.

We would add to this a requirement that all listings should have a time and date stamp. Most computational analyses require multiple "runs," so that a time/date for each is a minimal point of reference. Some software allows the user to provide titles or comments. However, we would value this less than the time stamp since users are notoriously lazy when it comes to providing meaningful commentary to individual computations.

Simply "turning on the debug switch" will seldom give enough information to allow an error to be corrected. One often has to insert additional output statements to find a specific error, especially if the difficulty involves an interaction between the program, data and computing system. Many systems limit line length for output, so a program may run satisfactorily for many months before particular input data causes it to split numbers across two lines, destroying the appearance of the results. Users may present least squares fitting programs with collinear data for which most are not designed. We have had trouble several times (e.g., in Nash J C, 1992). These limitations should, of course, be recognized during the design phase of program development and reported clearly to the user. Instead, tedious analysis of program flow and data are usually needed.

We now present an example of finding bugs by use of selected output. Suppose we wish to find the minimum of a function $f(x)$ of one variable, x, by using a quadratic approximation to the function. At three values $x=A,B,C$, we have $f(A)$, $f(B)$, and $f(C)$, and can fit a parabola (that is, a quadratic approximation) to the points $(A, f(A))$, $(B, f(B))$, and $(C, f(C))$. A partial program to do this is given in Figure 9.1.1.

To use this approximation inside a program that finds the minimal argument x_min and minimal value $f(x\_min)$ for $f(x)$, we would now have to find the minimum of the parabola, that is, by setting the derivative of the approximating function

(9.1.1) $$g(x) = A + B\,x + C\,x^2$$

to zero.

(9.1.2) $$g'(x) = B + 2\,C\,x = 0$$

so that our trial minimal argument is

(9.1.3) $$x_{trial} = -B / (2\,C)$$

For certain functions and/or sets of points, this estimate x_{trial} of the minimum may actually be near a maximum. The program, as written, does not check for this possibility. We can quite easily plot the points to see that they form a concave triple. If $A < B < C$ we would like $f(B)$ to be less than *(see overleaf)*

Table 9.1.1 Comparing regular and video memory write times (microseconds) using ATPERF (PC Tech Journal AT Hardware Performance Test,Version 2.00, Copyright (c) 1986, 1987, Ziff Communications Co.,Written by Ted Forgeron and Paul Pierce). Note that the 386 and NOTEBOOK machines are nominally equivalent in processor and speed.

	386	NOTEBOOK	286
Average RAM write time:	0.07	0.12	0.25
Average Video write time:	1.36	2.64	3.11

(9.1.4) $f(A) + (B - A) * (f(C) - f(A)) / (C - A)$

This last value is the linear interpolant between the points $(A, f(A))$ and $(C, f(C))$ at $x=B$. Figure 9.1.2 gives the program after appropriate modification.

9.2 Built-in Debugging Tools

Some language processors have built-in trace and debug options. These can be very useful in well-trained hands. Unfortunately, we have found few that are easy to use because of the learning cost and the volume of output produced.

The benefits that trace and debug options may bring, depending on implementation, are:

- Automatic output of all variables, or else of user-selected variables;
- Record of program flow;
- Single statement execution so that the user may execute the program one statement at a time;
- Array dimension checking;
- Checking for undefined variables or array elements.

The big disadvantage lies in the effort to learn how to use them. If one is using several different computational tools, it is easier to use printouts of a few key variables, which can be a trivial task when the language processor is an interpreter, e.g., MATLAB, **Stata**, and many BASICs. We may even be able to display variable contents while execution is stopped. Compilers require slightly more tedious steps to be taken, in that the program source code must be altered and then recompiled, linked and loaded. However, much of the tedium can be overcome, either by working within a suitable program development environment such as Borland's Turbo Pascal Integrated Development Environment, by using a macro editor that provides similar features, e.g., BRIEF, or by using BATch command scripts or similar

Figure 9.1.1 Partially completed program to find the minimum of a function of one variable by quadratic approximation.

Note that a quadratic function (line 510) is used to test that the formulas were correctly implemented. This example does ***not*** include steps to ensure stability of the computation of the approximating parabola, and for the three abscissa $x = -1, 0, +1$, an incorrect approximation results.

```
10 PRINT "QUADRATIC APPROXIMATION TO A FUNCTION MINIMUM"
15 DIM X(3),Y(3)
20 REM SUBROUTINE AT LINE 500 PUTS F(Z) IN F
30 PRINT "INPUT 3 ARGUMENTS OF FUNCTION"
40 INPUT X(1),X(2),X(3)
50 FOR I=1 TO 3
60 LET Z=X(I) : GOSUB 500
62 PRINT " F(";Z;")=";F
70 LET Y(I)=F
80 NEXT I
300 REM QUADRATIC APPROXIMATION
310 REM DENOMINATOR FOR COEFF 1 OF PARABOLA
320 LET K4=(X(1)-X(2))*(X(2)-X(3))*(X(1)-X(3))
330 REM COEFF 1
340 LET C=((Y(1)-Y(2))*(X(2)-X(3))-(Y(2)-Y(3))*(X(1)-X(2)))/K4
350 REM COEFF 2
360 LET B=(Y(1)-Y(2))/(X(1)-X(2))-C*(X(1)+X(2))
370 REM THIRD COEFF
380 LET A=Y(1)-X(1)*(C*X(1)+B)
390 PRINT "PARABOLA IS ";A;"+ (";B;
400 PRINT ")*X+(";C;")*X^2"
410 LET Z=-B*0.5/C
420 GOSUB 500
430 PRINT "FN VALUE=";F;" AT ";Z
440 STOP
500 REM FN
510 LET F=(Z*Z-4)*Z^4: REM QUARTIC TEST FUNCTION
520 RETURN
```

tools. The goal is to avoid many keystrokes. We confess to largely ignoring the debugging tools built into the programming environments we use because of learning cost.

We should not forget the error reporting that is always a part of any language processor or package. It is an unfortunate reality that the error reporting may be limited to one of a few very cryptic messages. We consider error reports that list only an error number to be ***unacceptable***. Fortunately, most such unfriendly products are now obsolete.

Figure 9.1.2 Partially completed program to find the minimum of a function of one variable by quadratic approximation.

This version incorporates a test for the proper arrangement of the three points used to calculate the approximating parabola. Note that several other changes would be needed to make this a reliable program. (See for example, Nash, 1990d, Algorithm 17. In the first edition of this book there is a typographical error in step 15, which should read "goto step 18" instead of "goto step 20".)

```
10 PRINT "QUADRATIC APPROXIMATION TO FUNCTION MINIMUM"
15 DIM X(3),Y(3)
20 REM SUBROUTINE AT 500 PUTS F(Z) IN F
30 PRINT "INPUT 3 ARGUMENTS OF FUNCTION"
40 INPUT X(1),X(2),X(3)
50 FOR I=1 TO 3
60 LET Z=X(I) : GOSUB 500
62 PRINT " F(";Z;")=";F
70 LET Y(I)=F
80 NEXT I
90 REM AT THIS POINT TEST VALUES
100 FOR I=1 TO 2 : REM BEGIN BY ORDERING THE ARGUMENTS
110 FOR J=1+I TO 3
120 IF X(I)<X(J) THEN 180
130 IF X(I)=X(J) THEN STOP : REM EQUAL ARGUMENTS CAUSE
135 REM FAILURE IN CALCULATION OF APPROXIMATING PARABOLA
140 LET T=X(I):LET X(I)=X(J):LET X(J)=T
150 LET T=Y(I):LET Y(I)=Y(J):LET Y(J)=T
180 NEXT J
190 NEXT I
200 LET Y2=(X(2)-X(1))*(Y(3)-Y(1))/(X(3)-X(1))+Y(1)
205 REM Y2 IS LINEAR APPROXIMATION TO Y(2) FROM Y(1),Y(3)
210 IF Y2>Y(2) THEN 300
220 PRINT "POINTS OUT OF ORDER; ENTER NEW C=";
230 INPUT X(3)
260 GOTO 50
300 REM QUADRATIC APPROXIMATION
310 REM DENOMINATOR FOR COEFF 1 OF PARABOLA
320 LET K4=(X(1)-X(2))*(X(2)-X(3))*(X(1)-X(3))
330 REM COEFF 1
340 LET C=((Y(1)-Y(2))*(X(2)-X(3))-(Y(2)-Y(3))*(X(1)-X(2)))/K4
350 REM COEFF 2
360 LET B=(Y(1)-Y(2))/(X(1)-X(2))-C*(X(1)+X(2))
370 REM THIRD COEFF
380 LET A=Y(1)-X(1)*(C*X(1)+B)
390 PRINT "PARABOLA IS ";A;"+ (";B;
400 PRINT ")*X+(";C;")*X^2"
410 LET Z=-B*.5/C
420 GOSUB 500
430 PRINT "FN VALUE=";F;" AT ";Z
440 STOP
500 REM FN
510 LET F=(Z*Z-4)*Z^4
515 REM LET F=1+Z*(2+3*Z) : REM TEST FUNCTION (PARABOLA)
520 RETURN
```

9.3 Listings and Listing Tools

As mentioned in Section 5.4, a crude but often effective backup mechanism is a hard copy listing of file contents. They are also a first line of attack in finding errors. Given that we all tend to read what we think is present rather than what is actually written on the page, it is usually necessary to mark the listing to find errors. Lines and arrows can be used to show program flow, brackets can be used to mark loops and a small example can be hand-worked beside each statement. Data files can be annotated to note which program statements will work on which parts of the data.

It is helpful if listing tools "print" a program source code file in a way that renders it easy for humans to comprehend the program content and structure. That is, we want to split multi-statement lines, ensure that there are blanks between keywords and variables, indent loops, lay out comments or remarks clearly, allow subroutines to be separated, with pagination and titling (under the user's control), for neatness of presentation. We believe that it is also useful if the program can list sets of files in a batch without the need for operator attention, add time / date stamps of the file and the time of listing, cope with differing page and font sizes, number the lines on the listing, provide a cross-reference of variables and sub-programs to these line numbers along with target destination line numbers for any transfers of control, and finally permit this listing to be output to a file for inclusion in documents.

Satisfying these desiderata is a time-consuming and arduous task. Many details must be kept in mind, such as the line and page size, and dialect differences in programming languages. Some source programs may be SAVEd in a ***tokenized*** form where common keywords such as PRINT are replaced with a single special character. We have found, especially in our earlier work in BASIC where variables are global, that listing tools are among the more heavily used programs in our repertoire. For other programming languages the availability of proper sub-program structures allows us to segment and localize variable names. Still, clean or "pretty" listings do help in the detection and correction of errors, for example, unbalanced comment delimiters. If new language elements are introduced, for example, the object-oriented facilities in Turbo Pascal versions 5.5 and later, then listing program(s) will require alteration.

While commercial program listing tools exist, we have found it useful to have access to the source code of the listing tool itself. On several occasions we have modified such programs to adjust for different printers or to send output to a file. Our BASIC cross-reference lister XREF.BAS (Section 6.2) can be obtained via electronic mail; send requests to jcnash@acadvm1.uottawa.ca. We also mentioned the PASCAL program TXREF (Roberts, 1986). For FORTRAN code, POLISH (Dorrenbacher et al., 1979) was written at the University of Colorado by computer science students under the direction of Lloyd Fosdick.

9.4 Sub-tests

When building a large program ourselves or trying to dissect one created by another programmer, it is obviously useful to know that each segment of the program is performing exactly as intended. The key word here is "exactly". It is difficult to find and correct errors when the program "mostly" or "almost always" does what we want it to do.

In divide-and-conquer fashion, we can often break up a program into small segments of code and test each part separately before assembling or reassembling the entire program. In FORTRAN and other languages with facilities for separate compilation of sub-programs, this is a natural consequence of the language constructs. In interpreted languages with global variable names, such as BASIC, APL or some special-purpose packages like **Stata** or MATLAB, we must be more careful about variable and array names, but the process is the same.

There are two ways to be sure a program is correct: ***prove*** it is correct, or ***test*** all the possibilities. Proofs of program correctness are important in theoretical computer science and in certain applications demanding the security that a program will always do what it should do. The proof process encompasses a careful examination of all the possible execution paths of the program no matter what the input. As such, it corresponds to testing all the possibilities. Most users, we included, are too eager to get on with the job of running the program to think of all the possible and bizarre combinations of input data that may at some point be presented to our program code. However, in the event that an error does occur, one may have to carry out such a test. The following questions may help in building a test data set and adjusting the program code.

- What inputs are acceptable to this program or program segment? The allowed possible values of all variables used by the program must be specified. If necessary, the program should test to see if the inputs are acceptable and provide for reporting of prohibited input data.

- Is there a unique (or at least well-defined) result for each valid set of input data? If not, is there a suitable error exit from the program?
- Can sets of data be prepared that easily show the processes in the two preceding points?
- Can every path through the program segment be traced to show that it performs the desired functions?

As an example, consider the code in Figure 6.2.1 to calculate the cube root of a number by Newton's iteration. The process is designed to find a solution or root of

(9.4.1) $f(x) = x^3 - b = 0$

where b is the number for which a cube root is desired. The Newton iteration uses

(9.4.2) $x_{new} = x_{old} - f(x_{old})/f'(x_{old})$

where $f'(x)$ is the first derivative of f(x), that is,

(9.4.3) $f'(x) = 3x^2$

Note that $x=0$ causes a ***zero-divide*** unless we are careful. Our test data set should include zero and near-zero numbers to examine the behavior of the program in this region. It should also include negative numbers so the correct sign of cube roots can be verified. Very large numbers in the data set test upper limits on sizes of inputs that may be accepted.

9.5 Test and Example Data

When the parts of a program are put together, the ensemble may still not perform correctly even if each subunit meets its specifications precisely. This may be a result of inconsistent design specifications for different parts of the program, but is more likely a consequence of their being incomplete. Users are often the first to discover such errors.

Whatever the deficiency, be it in design or coding or even some failure of the machine or programming language to perform as expected, a form of test is needed to ensure the program is working properly. Very few programs are complemented by a set of test data that fully exercises the program. A proper test data set is difficult to devise for most programs. It should:

- Contain data for ***normal*** cases for which exact or very precise results are known;
- Contain data sets that are ***extreme*** in that they force the program or the method to the limit of its capabilities;
- Contain data sets that ensure every ***control path*** within the program to be executed at least once;
- Contain data sets that generate ***error messages*** from the program.

Each control switch (e.g., IF statement) in a program gives two control directions, so the number of possible paths will likely be too large to test. It is rare that we can ensure that every path is tested. However, it is not difficult to think of data sets that test each line of code at least once, thus ensuring that all the error traps we have built into the program work.

Programs to be employed by users of diverse sophistication must be robust in handling input that may be totally inappropriate. That is, the program should not lose control when given the wrong type of information but should allow for some manner of recovery. This robustness is frequently left out of scientific programs, because the programmer must look after functions that are usually in the operating system or programming language. For example, on typewriters a letter I or lower-case letter L might be used for numeral 1 (one), or letter O (oh) for digit 0 (zero). Such letters as input for numbers will usually cause programs to fail. We devised a program to use "O" and "l" and accept commas in numbers, but the

code is nearly two pages long even for such "obvious" cases. In a batch processing environment, simple failure of the program with a proper error message may be acceptable. For interactive computing, robustness is more important since an error near the end of a long input phase is very frustrating to the user. A robust program will detect errors and allow for correction or reentry of the data.

Programmers can help users avoid errors initiated by incorrect input. Programs can be set up so that a carriage return is a suitable response to most requests for input. Programmers using "sensible defaults" should be careful how default choices are established for file names. Using the name of file that already exists may overwrite that file, destroying data.

Choosing defaults, command names and command structures is a time-consuming task, requiring many hours of effort and many more of testing and refinement. It is complicated by hypertext-style interfaces (e.g., Nash J C 1990b, Nash J C 1993b).

The use of menus or selection boxes is also helpful to users, but can be overdone. We recommend it for permitting user selection of one file from several or for "checkoff" of options. A mouse or other pointing device could be used, but programming with character position cursor controls or even numerical or letter selections is easier and almost as effective. The simpler approach also lends itself easily to saving screen output via a console image file as discussed in Section 9.6.

When a filename has to be supplied to a program, it is helpful if a program displays a list of available files (of an appropriate type or naming convention). This helps us supply the right data to programs. Ideally, users should be able to check the contents of files, disks or disk directories from within a program, or be able to escape to the operating system to do this, then resume program execution. Techniques exist on most computers for such "shelling", but they are not standardized across operating systems, so if used, reduce the portability of programs.

A final function of example data is to show the uses of a program. Such examples also allow a user to edit his/her own data in the place of the sample data, rather than working from instructions. In our experience, this is much more efficient than a prescription of what to do in user documentation. We like example data to be accompanied by some form of the results to be expected. Few scientific programs we have encountered do a very good job of providing the output.

9.6 Scripts and Documentation

While not yet common practice, we believe it should be possible to put comments in ***input*** files. Nash J C (1991a) describes a program where data file lines beginning with an exclamation mark (!) are simply displayed on the screen and copied to the console image file. A better choice would be to allow comments anywhere in the input file, {for example, delimited by curly braces as in Pascal code and this phrase}. This allows example data for the program to be commented. The programming needed for the simple method above (using "!") is trivial, yet it saves time and effort by providing the necessary reminders about bad measurements, troublesome calculations, people to be thanked, and other ideas.

In our own programs, we try to save a copy of screen output in what we call a ***console image file***. The tactic is generally simple; we repeat every screen output command but direct the information to a file. This file may be set to NUL if no output is wanted. Clearly, this only works for sequential output. This is a severe hindrance if one wishes to design a program that uses pop-up menus and graphical interaction (mouse or pointer input). Fortunately, few scientific programs truly need such input/output. Moreover, it is much more demanding to program, so except where absolutely needed, we would recommend the simpler approach. This still allows one to provide menus and to output graphics, although a text-only console image file will have messages replacing graphics, or the names of files saving the graphic screens. The console image file can be incorporated directly into reports.

Scripts of commands to programs avoid the risk that users type the wrong instructions. They show how to invoke a program's features and can be edited to save effort and avoid mistakes. In practice, such

scripts, along with a console image file, are also vital to program ***development***. Developers can automate a sequence of such tests (called "regression tests") to verify that new versions of software are free of "bugs" that have afflicted earlier editions.

For UNIX and MS-DOS PCs, the operating system provides facilities for supplying scripts to programs via input-output redirection. There are also operating system BATch command files within these operating systems. In graphical operating environments such as Microsoft Windows, OS/2 or the Macintosh Finder, one loses a good deal of this capability. This may explain some of our diffidence concerning such environments. We do not like the unproductive wait for (possibly slow) processes to finish. We prefer to prepare a set of commands for several tasks and let the machine do the work while we have coffee or do something else.

A form of "batching" used in some programs allows users to see and select all or many options available ***before*** execution begins, either using a point-and-click mechanism or menu selection. Clearly, the value of this approach will depend on the context of the computations at hand and the experience and knowledge of the users. Nevertheless, it is another method to reduce the amount of time users spend waiting to provide the next piece of input data.

All these tactics serve to document what the program does. They should, of course, be complemented by appropriate documentation, though we are tempted to agree with a dissatisfied user who returned a popular statistical package with the complaint "I don't want it if I need to read the documentation to run it". One trend is to make "help" available within programs. Another (Nash J C 1993b) is to have hypertext documentation as the framework from which software is operated. Separate paper documentation is likely to diminish in popularity, in part because it rapidly becomes obsolete and cannot easily be corrected in case of errors.

9.7 Resilience to I/O Failure and Disk Problems

In the previous sections we wanted to avoid program failure caused by incorrect user action, e.g., by entering invalid data. Now we presume that the user behaves appropriately, but the computer system itself suffers an "Unrecoverable Application Error (UAE)", i.e., fails. Such untoward events often concern peripheral devices — disks, printers, modems, instruments. Some memory systems also have error checking (usually parity bit checking). Input/output handlers may perform various tests on the data received or sent to a peripheral. Parity checks are very common. So are extra bytes of redundant information sent each block of data that we can verify. Cyclic redundancy checks or check sums are almost universally used for data transfer and storage.

Errors detected via these techniques usually suggest a problem that cannot be fixed under the program's control. Still, we would like to have programs come to a controlled halt, as opposed to stopping or "hanging" so that only the reset button or power switch have any effect. Many collapses of our computations are unavoidable. Others require an understanding of processes within the operating and language software that are usually inaccessible to the programmer. When the application demands, however, we must wade into the manuals and work out actions to maintain control of our calculations. Some suggestions follow.

- ***Disk or file out of space***: Programs may try to write more data than files will hold because of a lack of physical space or operating system limits. Mechanisms resembling the disk directory facility (Section 5.3) may help find out space available. Sometimes logical limitations may be overcome, but physical constraints mean we must provide more storage capacity in some way. If we expect capacity shortages, then we could arrange that data is segmented across a set of files or storage units. The segments may later be combined if ways exist to store the combined file; special tools may be needed to do this.
- ***Input/output device errors***: To trap data transfer errors (e.g., parity) or control conditions (e.g., paper out) for peripherals, we will again need to interact with the operating system. Some compilers have

special functions to allow detection of conditions within a program.

- ***Output to files:*** To avoid direct control of peripherals, we could write all output to one or more files. Following successful completion of our program, we can COPY the output files to the relevant devices. This also saves paper when our program fails just before completion.
- ***Suppression of user interrupts:*** For some applications, we wish to be sure that the "user" cannot carry out functions other than those intended. To do this, we must examine all input from the keyboard or pointer device and "trap" unwanted control commands. Sounds can be made to inform the user that such input is invalid.

In our experience, producing a code that carries out a desired calculation represents only 10% of the human effort needed to produce a fully functional, bug-free, piece of software with a friendly, documented interface and example data sets. While "only 10%" may appear to devalue the role of the researcher, we refer here to effort and perspiration rather than genius and inspiration.

9.8 Tests of Language Translators

Previous sections of this chapter concern user error or hardware, generally peripheral, malfunction. We turn now to programs through which the user may learn about the language processor or its interaction with his/her system. That is, we will attempt to discover the properties of our computing machinery by means of programs that run on that machinery. We have highlighted the topics below.

Floating-point arithmetic: Several authors (Malcolm, 1972; Nash J C 1981b, 1981c, 1981h; Cody and Waite, 1980; Karpinski, 1985) have suggested ways in which the floating-point arithmetic properties may in part be discovered. We presume a model for each floating-point number in the form of n "digits"

(Sign) (Exponent) (Radix point) Digit_1 Digit_2 . . . Digit_n

Generally the most important pieces of information are the value of the radix (or base) of the arithmetic and the number of radix digits used (*n*). Prof. W. Kahan, in "A paranoid program to diagnose floating-point arithmetic" (informally distributed), shows what can be done with imaginative programming in BASIC to learn many features of the machine arithmetic used. Others have prepared PARANOIA programs in C, FORTRAN, PASCAL and other languages (Karpinski, 1985).

PARANOIA attempts to find out such information as:

- The ***machine precision***, *eps*, that is, the smallest positive real number such that $(1.0 + eps)$ exceeds 1.0. (Some authors use a slightly different definition.)
- The ***floating-point ceiling***, *ceil*, that is, the largest positive real number that can be stored and used
- The ***floating-point floor***, *ffloor*, that is, the smallest positive real number that can be stored and used.

The character set: It is possible in most language processors to convert an integer (in an appropriate range) into a character in the character set of the machine. A simple loop over the allowed integers gives the ***collating sequence*** of the characters, that is, the order into which characters are sorted. This is extremely important for many applications such as name lists, indexes, catalogs etc. One fault of the ASCII character set (ISO Standard 646, 1973) is that the upper and lower case letters are not in the usual "dictionary" collating sequence, so that sorting programs must be carefully devised to avoid placing "a" after "Z".

For those of us who work in bilingual or multi-lingual environments, accented characters present further complications. "Standard" character sets exist such as the IBM PC set, ISO sets, and those used by Hewlett-Packard and Apple, but the multiplicity of choices means we must be very careful in any situation where we must manipulate, search or sort data that use such characters. We note that the correct display or printing of accented upper case characters requires wide interline spacing. The lack of standardization is troublesome. Personally we prefer to drop the accents, but this may be undiplomatic.

To display or print characters, simple programs can be devised that fill a character variable with appropriate bits (i.e., a number). For example, in BASIC, we could use

```
10 FOR I=1 TO 127
20 PRINT I;TAB(10);CHR$(I)
30 NEXT I
40 STOP
```

Similarly, input characters may be altered because programmers of compilers or operating software have not provided for them. However, many peripheral devices such as printers and modems use special control characters to control special features, such as fonts or transmission speeds. One way to send such controls is to enter them into a character string from the keyboard, a process thwarted if software masks or traps such characters. We can easily check this by running a program such as the following BASIC code.

```
10 DIM X$(2)
20 INPUT "ENTER CHARACTER THEN (CR):",X$
30 PRINT "CHARACTER NUMBER =",ASC(X$(1))
40 GOTO 20
```

Special functions: The logarithmic, power, exponential and trigonometric functions are a part of most scientific computing languages. They are unfortunately often very weakly programmed (Battiste, 1981). The user may carry out tests to protect against some errors that may occur, but the very large number of possible arguments for these functions usually precludes exhaustive checking. For example, any representable floating-point number could be an allowed input to the SIN function. Even if we restrict ourselves to a reasonable range, the magnitude of the testing task is great. Usually, we content ourselves with some specific tests near commonly troublesome arguments. Cody and Waite (1980) give some other examples and produced the ELEFUNT set of FORTRAN tests.

- For trigonometric functions, evaluation is usually accomplished by rational approximation (a ratio of two power series) using an argument reduced to a small range. The range reduction is performed using trigonometric identities such as

(9.8.1) $sin\ (x + 2*n*\pi) = sin\ (x)$ where $n=1, 2, \ldots,$

Clearly, if n is very large, the representation of the number

(9.8.2) $(x + 2*n*\pi)$

is the same for many different values of x because of digit loss on rounding. That is, if we have two numbers x and y that give different values for $sin(x)$ and $sin(y)$, there is not necessarily any difference between the machine-stored numbers

(9.8.3) $(x + 2*\pi*n)$ and $(y + 2*\pi*n)$

nor, obviously, between their trigonometric functions. Another test is to add or subtract one bit at a time to the representation of π and examine the sine, cosine or tangent functions for correct values.

- The logarithm function is often poorly approximated near 1.0. It is quite easy to evaluate an approximation of $log\ (1 + x)$ using the McLaurin series for $x^2 < 1$ (or some more economical one)

(9.8.4) $log(1 + x) = x - (1/2)x^2 + (1/3)x^3 - (1/4)x^4 + \ldots$

  This can be compared against the approximation produced by LOG( ) or LN( ) in the programming language.

- The power function x^y is frequently abused by programmers to form simple integer powers of numbers such as squares and cubes. These are usually more safely and rapidly calculated by multiplication. The power function should really be reserved for powers that are not integer or integer/2 (i.e., using square root). Language processors may treat all negative arguments y as invalid, even when they are mathematically admissible. Users should check these cases as needed. It has been

noted that some versions of the popular spreadsheet Lotus 1-2-3 have an error in the power function (Nash, 1989b). The errors can be brought to light by computing very small powers of numbers between 1 and 2.

Comparisons: Comparisons are made to decide which control path to follow in a program (IF statements). It has become part of the folklore of computing that comparisons for equality between floating-point (REAL) numbers should not be made, because of the rounding errors made in a sequence of computations. However, a statement such as

(9.8.5) *if ((abs(x) + 10.0) = 10.0) do ...*

should work as a test for x being zero ***relative to*** 10.0. Clearly one can check if the test works, for example in PASCAL with:

```
x:=1.0; i:=1;
repeat
    x:=x/10.0; writeln(i,'   ',x); i:=i+1;
until ((abs(x) + 10.0) = 10.0) ;
```

Compiler writers attempt to optimize execution by removing common elements on both sides of a test. Here such an alteration in the instructions is a disaster. Such a failure occurred in a program we were helping to prepare with the Microsoft C compiler (Version 6.0 for MS-DOS) that effectively removed the "10.0" on either side of a test similar to that in (9.8.5) above, although such optimization was supposedly "turned off". Our code failed because iterations never terminated.

Tests for "smallness" as above are important in ***termination criteria*** in iterative algorithms (Nash J C, 1987d; Nash J C and Walker-Smith, 1989b). Note that we avoid the term "convergence tests". Convergence is a property of an algorithm, that is, of the mathematical process under study. Termination, on the other hand, could involve checks on false inputs, hardware or software failure, user or other interruption of execution, file or storage capacity exceeded, and many other factors beside the mathematical steps that make up the iteration.

A rarer complication is the use of a "fuzzy" comparison. Floating-point numbers within some FUZZ are treated as equal in such comparisons. The Tektronix 4051 BASIC had such a feature (Nash, 1978b). Our opinion is that such "features" are offensive.

Data structures: Sometimes restrictions exist on the size of declared arrays or strings, or on the number of dimensions allowed. It is relatively easy to test these possibilities, as we have done in Section 7.1. Often variable dimensions are not allowed, for example, in BASIC

```
10 INPUT "NUMBER OF ROWS IN MATRIX=";M
20 INPUT "NUMBER OF COLUMS = ";N
30 DIM A(M,N)
```

Loop control: A common cause of confusion for students of programming arises in the study of looping mechanisms. We need to be sure whether loop control calculations are carried out at the beginning or the end of the loop. It is easy to devise short programs that verify loop operation by printing out the loop control variable each time the loop is executed. We also note that there may be restrictions on the types of variables that can be used in loop control, so that apparently trivial changes in declarations in one part of a program may have untoward consequences elsewhere. An example concerns Turbo Pascal, where type ***longint*** (long integer) is not permitted in ***for*** loops.

Chapter 10

Utilities — a desirable set

10.1 Editors
10.2 File view, move, copy, archive and backup
10.3 File display, conversion and print
10.4 File comparison
10.5 Directories and catalogs
10.6 Fixup programs
10.7 Sorting

We have mentioned utility programs often in this book. Now we suggest the contents of a useful set. While some utility functions come with operating system software, they may be incomplete or poorly suited to our needs. The acquisition and tailoring of utilities to our needs take time and effort. When we need a utility program to use the computer, we will spend effort or money to acquire it. When a utility improves our ability to use the PC, we must decide if the new program is worth obtaining and installing.

10.1 Editors

Editors are probably the most used programs on PCs if we include word processing software under the "editor" heading. Editors are important in computing applications: programs need changing, data must be altered and output requires formatting for presentation (as in this book).

Every editor has roughly similar functions. The differences lie in the ways we control them and in special features. The main functions of an editor are to allow data to be added, changed or deleted. Other features include copying or moving data, assembling or breaking up files, or performing certain translations or display functions so that we can note the presence of control characters not normally printable. Because of both similarities and differences, those who must use more than two or three editors soon find themselves giving the wrong commands. It is helpful if we can use just one editor.

This goal may be frustrated by the ways in which data is stored. Programs may use tokenized keywords or include formatting information for greater readability. With increasing memory capacities, the incentive for tokenizing source code has declined, but recent versions of the Microsoft BASIC interpreters for MS-DOS PCs still default to a tokenized form of storage. We can force the SAVE command to store our program in text (ASCII) form by using the syntax

```
SAVE "PROG",A
```

To reduce editing problems, we recommend that program source codes ***always*** be saved in text mode wherever possible.

Desirable features of a text editor are simplicity, power and flexibility. Unfortunately most products on the market today fail to meet one or more of these desiderata. Too many special features clutter manuals and render an editor awkward to learn. Which editor one uses may be a matter of taste. Some users swear by reliable but pedestrian line-oriented editors, but most editors now use full screen capabilities, where text displayed on the screen is modified before our eyes.

Note that word-processing editors often present the user with a picture of the (probable) form of the printed documents. Useful for producing attractive text, such "what you see is what you get" (WYSIWYG) programs can be a great nuisance if we wish to adjust the exact content of a file, since they may

automatically insert codes for spacing, tabs, underlining, etc. Most word processors with retrieve and save simple text, but default storage modes generally include formatting codes.

Many screen.oriented editors present the user with a lot of information at once. Besides the text, there may be tab positions, ruler, current page size, cursor position, file in use, mode of operation and other details. If, like ourselves and Jerry Pournelle (1983) you only want to see your own text on the screen, this can be most annoying.

Many programming environments (e.g., Turbo PASCAL, *True BASIC*, Microsoft Quick BASIC and Quick C) provide their own editor. Don't expect that it will have the familiar commands of your favorite text editor. Some programming editors, e.g., BRIEF, allow the user to edit, compile and run programs easily in various programming languages from a single, powerful editing environment. Because of the power and richness of features, BRIEF strains the "simplicity" criterion.
For making complex changes to text files, a ***macro editor*** (Section 2.6) is helpful. It allows sequences of commands to be executed from a script. We find such a tool invaluable for adjusting the layout of data or output files. On the negative side, macro editors may be more awkward to use. One keystroke can do a lot of work — or damage! The macro editor we use in our own work is SEE, for which we purchased and modified the C source code some time ago. It has a limited but useful macro facility and a line ***wrap*** feature helpful in adjusting text file widths for display and printing. Unfortunately, SEE's producers have not replied to our letter. BRIEF, mentioned above, is also a macro editor.

Editors are also used for viewing files. It is critical that one have at least one editor that can handle very large files reliably. Many editors try to hold the entire file of text in memory, so are limited either by memory size or memory addressing. This includes our own freeware NED (Nash J C 1990a), but not its commercial counterpart.

We regard word processing and desktop publishing as applications rather than utilities (Chapter 2). Section 10.3 discusses their use in data file reformatting.

10.2 File Move, Copy, Archive and Backup

A single utility for viewing, moving and copying files has yet to appear on our machines. The features we want exist in separate utilities. User interfaces vary. Some use commands with switches, some a "tag and go" approach, while still others employ the "click and drag" mechanism made popular by the Apple Macintosh. Our preference is to tag files then issue a command for an operation to be made on these tagged files. While "tagging", it is helpful to be able to view or edit the files, at least if they are plain text. We want to do all this with a minimum of keystrokes.

Several utilities in public collections allow almost the functionality just described, but a separate utility must be used to move whole directories. Macintosh's "click and drag" allows this, but it fails to allow easy use of ***wildcards***, that is, the specification of a group of files by giving a filename having some characters replaced by place holders for regular characters. The MS-DOS operating system uses a "?" to replace any regular character and "*" to replace any characters to the end of the main filename or the filename extension. Thus the filename specification FILE????.C* can refer to FILECOPY.COM FILELIST.CMD or FILEDUMP.C but not FILEDEL.COM or FILECOPY.EXE.

We use special utilities to copy or move files only if the source version is more recent than the target. Copying "old" over "new" is a common and annoying source of data loss.
While we continue to watch for a file manipulation utility that is ideal from our own perspective, there are many good programs available and operating system facilities are improving. Windowed environments have built-in facilities many users find satisfactory (we find them a little slow and awkward to use). Some hypertext processors allow users to develop their own "utility" by gluing together a set of existing programs and launching them under control of a hypertext script.

A utility that in some ways comes close to what we would like is the Laplink transfer utility intended for

movement of data between portable and stationary PCs. For users of notebook PCs a utility of this type that can transfer data easily via serial or parallel ports is almost essential. Macintosh machines have a form of networking built in, so do not have quite the same needs.

Compressed archives can be a nuisance to move and copy, since we cannot move files in and out of them as we would with directories. In Section 5.5 we have discussed the merits of compression and archiving. We recommend that users select just one such tool to use regularly. Since others may package software using a variety of archiving tools, it is helpful to have the "unpacking" part of several tools. It is easy to write BATch command files that unpack from different compressed forms and repack into the form on which we have standardized.

Backup was discussed in Section 5.5. Users should standardize on a single backup tool, preferably one that allows all backup to be carried out at a single workstation PC with a minimum of human effort. We strongly recommend testing the recovery of files from the backup medium; also the development of policies and practices for the safe storage of the backup media.

For making copies of disks we find a utility that does requires us to swap disks just once helpful. We use DCOPY by Scott Abramowitz when we need to make a security copy of new software disks or when we want to make disks to distribute our work.

10.3 File Display, Conversion and Print

Files often need to be printed, but various types of files may need to be treated differently. Some important possibilities are:

- Program listings (Assembly code, BASIC, FORTRAN, PASCAL, MATLAB, **Stata**, SAS, C, DBASE);
- Data files (binary numeric files, text numeric or mixed numeric/string data, text processing files with formatting commands, spreadsheet files, database files, hypertexts);
- Graphics (drawing or CAD files, various graphic output format files, scanned images or faxes, PostScript files for printing).

Program listings require some formatting. We may want indenting of loops, separation of statements in multi-statement lines, positioning of comments, and general cleanup of the presentation. Tabs may have been used for indenting program statements. Assembly listings need the labels (if any), instructions, operands, and comments lined up in appropriate columns for ease of reading. Extra functionality may allow formatting commands to be included, such as setting tab positions, pagination, titling, forced page throw, and special character sets.

Data files for particular applications may need highly specific listing programs. For example, a file of random digits could store two digits per byte in binary-coded decimal form. To list such a file, each byte must be read, split into two digits, each digit converted to its character form, and the character form of each digit printed.

Text files are easier to list, except that at the end of each line the PC must perform a carriage return and line feed. This can be signalled by a carriage return character in the file. More sophisticated lists can use the "carriage return" character as an end of paragraph marker, with automatic line splitting to some specified maximum line length. Note that UNIX text files have line feed rather than carriage return characters (Nash J C, 1993a).

Files of unknown origin may require a viewer that can display the data in various translations of the binary data, for instance as text, as hexadecimal digits, or perhaps even as binary bits.

Mixed data types create difficulties since each file configuration will need its own lister. The Macintosh FINDER overcomes this by loading the appropriate application program when a file of a given type is selected. This fails if the application is not available on the present Macintosh. We also find that it can be annoyingly slow for "large" applications that take time to load.

Beyond display, we may need to be able to convert one form of file to another, preferably in a way that is reversible. From the standpoint of automating the conversion tasks, it is helpful to have standalone utility programs to do such conversions, for then the commands can be put into a batch file and executed while we do something else. We have found a few such utility programs, though some are less than perfectly reliable. We chose DBMS COPY for converting statistical and database formats.

Some file management utility programs claim to be able to display a variety of file types, and to do so automatically. Because they are trying to be encyclopedic, such programs have a tendency to need a lot of program code to cover all the file types. We prefer to manage our way around this problem. That is, we try to select just a few different formats with which we will work. Our choices at the time of writing are as follows.

- Data files are kept in ***text form***, preferably with commentary if the application programs allow this. We also keep memos, letters and outgoing faxes in plain text form if possible.
- Reports, formal letters, manuscripts, etc. are kept in the format of WordPerfect 5.1, which was used to write this book. We are not great fans of WordPerfect, but the mass of users in our community of colleagues makes it a sensible choice. This standardizes our word processing / report preparation format.
- Graphics files are kept in a form that can be imported reliably into the chosen word processor. (The GRAPHCNV program for WordPerfect can be used in batch command files.) The formats we have found most helpful are HPGL (Hewlett-Packard's graphic language) and Lotus PIC files, with a poor second choice being various files in the PCX format. The PCX form is a bitmap, so images lack the crispness allowed by the other formats when graphics are scaled to fit into reports. Bitmaps arise when images are scanned optically or captured from a screen (see examples in Chapter 19).
- Our own program codes are kept only in source code form along with scripts for their compilation unless we are running the programs daily. This saves much space and allows us to view the contents of the program.

Note that conversion of files between types can to some extent be accomplished using import and export facilities within application programs. By restricting the formats we use, we can reduce the number of conversion tools needed and ensure their reliability.

10.4 File Comparison

A file comparison utility is essential when we wish to determine if two files are identical, such as in verifying disks for transmission to other users, ensuring all copies of similarly named files are the same, or checking the read / write hardware or disk media.

File comparison may be awkward if end-of-file markers are used. For example, text files in MS-DOS are frequently ended with a Control-Z character (ASCII 26). Comparison should stop when the end-of-file mark is detected in one of the files being compared. Everything works well if files are of the same length and are identical, byte for byte. The file comparison may give confusing output if it is not following the "end of file" convention and compares "data" in the unused space beyond the marker. Another problem may be that one application program puts in the marker, while another relies on the file length held in the directory.

We use a shareware COMPARE program for quick looks at differences between two files, but use the MS-DOS utility FC for a serious comparison of differences between text files. The MS-DOS COMP utility is helpful for comparing two sets of files or two directories, for instance, in checking if there are changes

(and in which files they are located) between two ostensibly different releases of a set of files.

10.5 Directories and Catalogs

A file catalog utility (Section 5.3) is most helpful for workers who have large collections of exchangeable disks or tapes and who need a global listing of the files.

Others may be able to manage their collection of files by segmenting the files into appropriate directories, with these directories localized on specific drives and machines on a network. If duplicate directory structures are used on unconnected machines, there ***must*** be procedures for maintaining equivalence of the files. Users must assiduously practice the discipline such procedures impose. In our own experience, this is next to impossible.

All operating systems provide facilities for listing the names of files in a directory. File specifications with wildcards (Section 10.2) let us focus on particular names. There are also many utility programs that allow enhanced directory listings to be prepared. We use one of anonymous authorship that allows us to display a compact list of files sorted by name and giving the file size. Other display formats are chosen by command switches. A feature we use frequently lets us list the filenames to a file that we can edit to create a batch file to perform operations on the files.

One reason we are less comfortable with Windowed operating environments (such as the Macintosh FINDER or Microsoft Windows) is that we have not found easy-to-use tools for arranging for actions to be carried out by a script that we have prepared. No doubt enterprising software developers will fill this gap.

10.6 Fix-up Programs

Frequently, errors in programs, failures in electronic or mechanical components or mistakes by operators leave some aspect of our system or its files in an improper state.

- Interrupting a program after it has written data to a file but before the file is properly closed may leave the file unreadable to programs.
- Occurrence of a scratch or bad spot on magnetic media will always cause some data loss, but we will want to be able to recover most of our data. We may subsequently instruct our PC to avoid writing to or reading from the offending block of storage.
- Accidental change to or deletion of a file, e.g., by giving the name of an existing file to store program output, may cause an end-of-file marker to be written at the beginning of the space occupied by the file.

The correction of these problems requires their diagnosis and a tool to fix them. Some difficulties are commonplace enough that there are operating system or other utilities available to help. An example is an "UNDELETE" program; these use the fact that deletions usually only alter the filename in the directory, so that clever software can put the right name back and recover the file. Such programs generally refuse to operate on networked drives. For fixing files, we generally must do much more work. The expert's tool of choice is the ***sector editor*** that allows access to the raw binary data on a disk. We can do much damage quickly if not careful.

When the directory is corrupted by some error, access to files is no longer reliable. Operating systems provide some mechanisms for verifying the integrity of the directory structures, e.g., MS-DOS CHKDSK. More comprehensive tools automatically check and "fix" a variety of disk problems, e.g., Norton Disk Doctor. Some provide a certain level of preventive maintenance in refreshing the disk format without data loss, e.g., SPINRITE.

Defragmentation of files may also be considered as preventive maintenance, since contiguous data is straightforward to recover, particularly if it is in text form (Section 8.4).

Over the years, users develop small utilities to repair file deficiencies. We quite frequently find that an application program cannot cope with a text data file stored with "carriage returns" (ASCII character 13) at the end of each line, instead needing a "carriage return / line feed" (ASCII 13, ASCII 10) sequence as marker. We wrote a very simple BASIC program to do the fix-up called CRTOCRLF.BAS, but a variety of such tools exist (J C Nash, 1993a). Sometimes it is enough to read a file into a text editor and saving it again. Similarly, programs may be devised to display and work with special characters, e.g., in names of files, where they cause trouble. For example, it is not possible to delete a file that has a space in the middle of its name using the MS-DOS command ERASE; the command interpreter takes the material after the space to be a second parameter to the command.

Other utilities we have written ourselves include a small program to strip blank characters from the right hand end of text lines (RBLANK) and LINES, which counts the lines in a text file and lists the five longest. These are used when we want to send text data to a printer or electronic mail where overlength lines cause misalignments or lost data.

Users who do not wish to program may have difficulty in finding sources of good fixup programs. Unfortunately, the descriptions of the kinds of errors that may occur can be long enough to discourage their inclusion in advertisements. We recommend keeping in touch with a local PC users' group or bulletin board where advice may be sought from others.

A common cleanup (rather than fixup) problem occurs when disks contain obsolete information and we want to recover them for reuse. Reformatting may take up to two minutes per disk, and generally ties up our machine. We have had limited success with background formatting, which allows formatting to proceed while we are doing other work. We prefer to use a very quick reformatting program that simply blanks out the disk control sectors and directories (QDR, The Quick Diskette Reformatter Version 3.3c, Vernon D. Buerg 1988). Note that if the disk is exposed to magnetic fields, it should be formatted using the tools supplied with the operating system.

Finally in the category of fixup programs we will mention computer virus control programs. These fall into three categories: ***scanning programs*** that look for specific code segments peculiar to different viruses, ***behavior monitors*** that watch for unusual disk or memory activity, and ***bait programs*** that watch for changes in their own structure. Viruses, which is the term we will use as a catchall for all intentionally destructive software (see Denning, 1990, for more details), require some code to be executed in order to gain a foothold in a computer. Once executing, they seek an opportunity to propagate. Clearly they cannot infect read-only devices. Unfortunately, small segments of code are executed when most disks are read, so even simple DIR commands may result in infection. We recommend running a simple scanning program against any disks received. Removing viruses requires that we have good backup copies of our files. As the operating system is a favorite target of viruses, we may have to reinstall it.

10.7 Sorting

Frequently we need to sort data so as to use it effectively. Address lists are an obvious example, especially if we need to reorganize them so they are in postal code order. Similar tasks occur in scientific data analysis if we wish to look for spatial relationships.

Sorting text files is trivial if the files are small. In MS-DOS there is even a SORT utility provided. Alternatively, we can use sorting functions in a spreadsheet. Large files give more troubles. If a database management program is available, then it may be used. Many shareware programs exist. For example, QSORTL by Ben Baker allows large files, long line lengths, multiple sort keys and a lexicographic sort, that is, capital and lower case letters are not separated as they are by the ASCII collating sequence. We urge special attention to the collating sequence if lower case letters are present, or if special or accented characters appear.

Numeric data may be sorted using features within a statistical or database package. Alternatively, conversion to text and use of a text sorter is possible. However, we need to ensure that the data is correctly aligned by column position or we will get 10 following 1 and 22 following 2. The same problem occurs in ordering the lines in a BASIC program. We generally load or merge files within a BASIC interpreter to sort the lines automatically, but have had occasion to write a program to do this so we could consolidate segments of code automatically using a batch file. Note that the interpreter allows us to ***renumber*** program lines. We must remember to SAVE the program, of course, and to do so as text.

Chapter 11

Looking after the Baby: Hardware and Operating Practice

11.1 Cleanliness and a decent physical environment
11.2 Bad habits — smoke, sticky fingers, games, pets
11.3 Magnetic disks and their care
11.4 Tapes, CDs and other storage media
11.5 Power considerations
11.6 Interference and radio frequency shielding
11.7 Servicing and spare parts
11.8 Configuration maintenance

In this chapter we consider ways in which the environment of the PC and the manner in which it is handled can minimize the incidence of "glitches" or breakdowns. Most of the measures suggested are simple to set up. They arise out of a common sense approach to the PC. Like any human or machine, a PC will give better service if it is well-treated.

11.1 Cleanliness and a Decent Physical Environment

Some hazards that a home or office presents to a PC, apart from those associated with the power socket, are:

- Dust and dirt;
- Heat or cold;
- Humidity or dryness leading to static electricity.

In many respects, the treatments for these problems are highly interrelated, but the various steps will be considered one at a time.

Keep the PC and its area clean and tidy

Usually, simple dusting with a slightly damp (***not*** wet) cloth is sufficient for exterior cleaning of PC equipment. We avoid the use of any chemical cleaning agents for fear of contaminating switches, keys, circuit connectors or magnetic recording surfaces. Where grease or grime are present, a mild cleaning material such as dish washing liquid may be used. Spray-on chemical cleaners should be avoided unless they are specifically designed for cleaning of electronic equipment. As most ordinary household cleaners contain sodium hydroxide (caustic soda), care should be taken so no cleaner gets inside the equipment or on sensitive surfaces such as monitor screens.

Since dust can be a problem inside equipment (especially printers), it is helpful to have good filters or air cleaners for the heating or air conditioning of the office. This is not always under our control. We have in the past resorted to making our own filters from rigid domestic forced air furnace filter material. Such filters were held in place by plastic U-channel (normally used as kitchen shelf edging), though Velcro would do. We arranged that the cooling fan sucked air through the filter, but are aware that this is not easy to do on all machines.

Reduce clutter

Keep wires off the floor and out of the way. Make sure the PC is on a steady surface, otherwise banging or wobbling of the surface may cause disks to go out of alignment.

Adjust ventilation or add fans

The cooling of PCs is often not given a very high priority. Fans may be poorly positioned in the case. Floating-point hardware uses power to obtain the required speed. You can easily get a mild (thermal!) burn by touching a floating-point "chip" while it is processing. In a recent software demonstration, the PC had its case off and a desk fan blowing over a floating-point co-processor. The presenters complained that without the fan, the unit was overheating, resulting in intermittent failure of the whole system. The co-processor itself may not have been failing; the fault could be in nearby chips, or come from thermal stress on connectors or solder joints on the circuit board(s).

Keep the PC room comfortable

If the PC room is hot or cold, dry or sticky, it is not only the user who suffers. Overheating is a greater danger than cold, since it is rare that PCs live in rooms where the temperature is even approaching the freezing point. Once the power is on, the PC will generate some heat. If the room is dry, static electricity may be a problem. High humidity may give condensation on components and cause short circuits.

Control static

Static electric discharges from the user against the keyboard or other ungrounded parts of the equipment can have serious consequences by altering memory contents or burning out integrated circuits. In our own experience, we have rarely needed to take special measures such as anti-static carpet. Some users install a grounded button or wire that they touch before touching any other part of the equipment. Such a button is not needed if a grounded conductor is available, such as the metal casing (unpainted) of the PC. However, it is important to verify that the casing is grounded and to remember to touch it before touching the keyboard. High voltage discharges to the casing may still cause troubles. Therefore, if one notices that static electricity has reached the level of sparks, it is time to take other measures such as anti-static carpets and humidification.

Clean the PC

Even with dust filters on PC air intakes, some dust will get inside. Therefore, once a year or so, it is a good idea to check the interior of the equipment and clean if necessary. This implies some disassembly of the PC and removal of circuit boards. We use a vacuum cleaner with a gentle brush nozzle to remove dust from the circuit boards and the chassis. It is important to ensure that the PC can be reassembled correctly and that circuit boards are kept grounded during cleaning to avoid static electricity damage.

Video display screens of CRT type attract dust and may need more frequent cleaning. Be careful if you have a fabric anti-glare surface. Keyboards get grimy from ink, sweat, and general hand-dirt, and they have many places to attract hair and dust. Vacuum gently and wipe with a damp cloth when the PC is turned off.

11.2 Bad Habits — Smoke, Sticky Fingers, Games, Pets

The glossy advertisements for PCs show them everywhere — in the office, in the kitchen, in the family room, in the car. Unfortunately, many areas of human habitation are quite hostile to most PCs.

Many work and home environments have tobacco smoke and ashes in the air. Disregarding the health arguments, it is wise to keep any magnetic recording surface out of smoky air. Ashes can settle on the

surfaces and scratch them, causing loss of data. Worse, the smoke can dissolve the binders of the magnetic recording medium, resulting in data loss. Though there is some dispute as to the necessity of avoiding smoke, we have personally observed a reduction in magnetic media data errors after smoke was eliminated from a machine room. Food and drink near PCs is also unwise, so forgo a PC recipe database on the kitchen counter.

PCs also survive poorly in the company of unsupervised or ill-behaved children. If children are allowed to use the PC, they should be trained to operate it with due care and attention. Toddlers may copy older siblings — we know of one who was taught that only diskettes go in floppy disk drives after he fed in a grilled cheese sandwich. Learning fast, his next computer session involved feeding multiple diskettes at once in the same drive! The use of the PC for games encourages rough treatment of the keyboard in particular, with excited players pounding keys. It is surprising PCs survive as well as they do, given the way they are made. Joysticks and mice also get mistreated, but most can be replaced for only a few dollars. Games are often traded, and are a main avenue for transmission of computer viruses. We have purged most games from our machines.

Some parents use access control mechanisms — locks, passwords, etc. — to limit how children may use the PC. For example, parental files may be in a separate disk partition hidden unless a password is given. Our own SnoopGuard has been used in this way (Nash J C and Nash M M, 1993).

Pets often have hair and feathers to get in the works or on disks. Some pets also like marking their territory. We know of a tomcat who scored a hit on the inside of a floppy disk drive!

11.3 Disks and Their Care

In this section we consider some practical ways of minimizing difficulties with disks of various types.

- When disks have protective envelopes (5.25") or cases (CD-ROM), use them to reduce the chances of contaminating the surface.
- Store disks in an orderly way, maintaining disk catalogs if large disk sets are used. This reduces disk handling and saves time as well.
- For archival information, use disk write-protect features (notch or slider) to avoid deletion or overwriting.
- Handle disks gently.
- Use reinforced mailers when shipping disks.
- Drive doors or levers should be closed slowly so the user can note any resistance suggesting the disk is poorly positioned, which could cause read/write errors. About 5% of the time that we load 5.25" disks we feel sufficient resistance to stop, joggle the disk in the drive and try again. Gentle handling also saves wear and tear on the drive, reducing the chance of misalignment. 3.5" disks and CD-ROMs are less problematic; the Macintosh does most of the work for us.
- Keep disks away from wires, tools or other electromagnetic fields. A magnet of any sort can cause trouble with magnetic recording media. Paperclips, often stored in magnetic holders, are a common hazard. There are magnetic coils inside most display screens. Students we know have managed to erase whole boxes of disks by placing them next to the screen in the computer lab.
- Do not leave disks lying around to be dropped, bent or otherwise mishandled. Use a disk box, a simple rack made by sawing slots in a block of wood or by folding and stapling paper (Figure 11.3.1).
- If a diskette appears to be unreadable, it may help to try reading it on another machine. If successful, copy data to another disk. Alignment of the heads on the writing and reading drives may not be exactly the same. Even if both drives are within specification, they may still be different enough to cause errors.

- Heavy-handed diskette insertion, vibration from keyboards or from impact printers may be transmitted to fixed disk read-write heads, causing mispositioning or else physical contact with the spinning disk. We try to keep mechanical vibration isolated from disks, so our dot matrix printers live on small separate tables made from sawhorses with a plywood top. Some commercial PC furniture has poor design from the point of view of vibration and physical access to printers for paper and ribbon adjustment or clearing jams.
- The disk may not be initialized or formatted in the correct way. MS-DOS and Macintosh machines use very different formats for 3.5 inch disks. 3.5 inch High Density (1.44MB capacity) disks may appear unreadable if formatted at 720K. By covering the hole that distinguishes the formats, these disks may be made readable again.
- 5.25 inch diskettes on MS-DOS machines generally store either 360K or 1200K of data. The higher capacity is achieved by closer track-to- track spacing, which requires that the read-write head use a narrow magnetic track. Errors may occur when a diskette formatted on a 360K drive (with "wide" tracks) is overwritten on a 1.2 Megabyte drive. The new track does not completely obliterate the edges of the old, so that subsequent attempts to read the disk on a 360K drive may fail. Occurrences of this type of error can be minimized by writing low-capacity disks on 360K drives only. That is, we only read them on the high capacity drives. In practice, we have found quite low error rates, and that some diskettes seem more prone to the problem than others.

11.4 Tapes, CDs and Other Storage Media

Most of the above comments about cleanliness and gentle handling apply equally to all forms of storage. Similarly, we want to maintain adequate labelling and documentation so that we do not mix up different volumes of data. This is particularly important for tapes, since they are used mostly for backup purposes, so represent our "insurance" against disaster. We recommend developing a set of simple procedures to carry out backups, following suggestions from the manufacturer of the tape drive and the developer of the backup software for handling tapes. CD-ROMs are usually well-labelled by their producer. The only problems we have noted are read-errors, probably caused by dust.

Other storage media will generally have a proprietary physical form. However, there are some seemingly standard disk drives that use nonstandard format disks of a regular physical size to achieve high capacity. Some of these drives may also be able to handle standard formats, but in any event, users should take care to distinguish the "special" disks from the regular ones.

11.5 Power Considerations

The quality of power supplied to electronic equipment is important in preventing damage to the parts or errors in programs and data. Alternating current supplied to households or offices has specified voltage and frequency. Circuits drawn from such mains supply are rated for specific maximum current (amperage) or power (wattage). In North America typical ratings are 115 Volts, 60 Hz (or cycles/second), 15 Amps, while in the UK and Europe we would see 240 Volts, 50 Hz, 13 Amps.

The supplied electrical energy may, however, fail to meet specifications:

- It may be below voltage, even to the extent of a "brownout";
- It may be over-voltage, so lights burn very brightly or fail; or
- The frequency may be unsteady (this usually precedes a blackout).

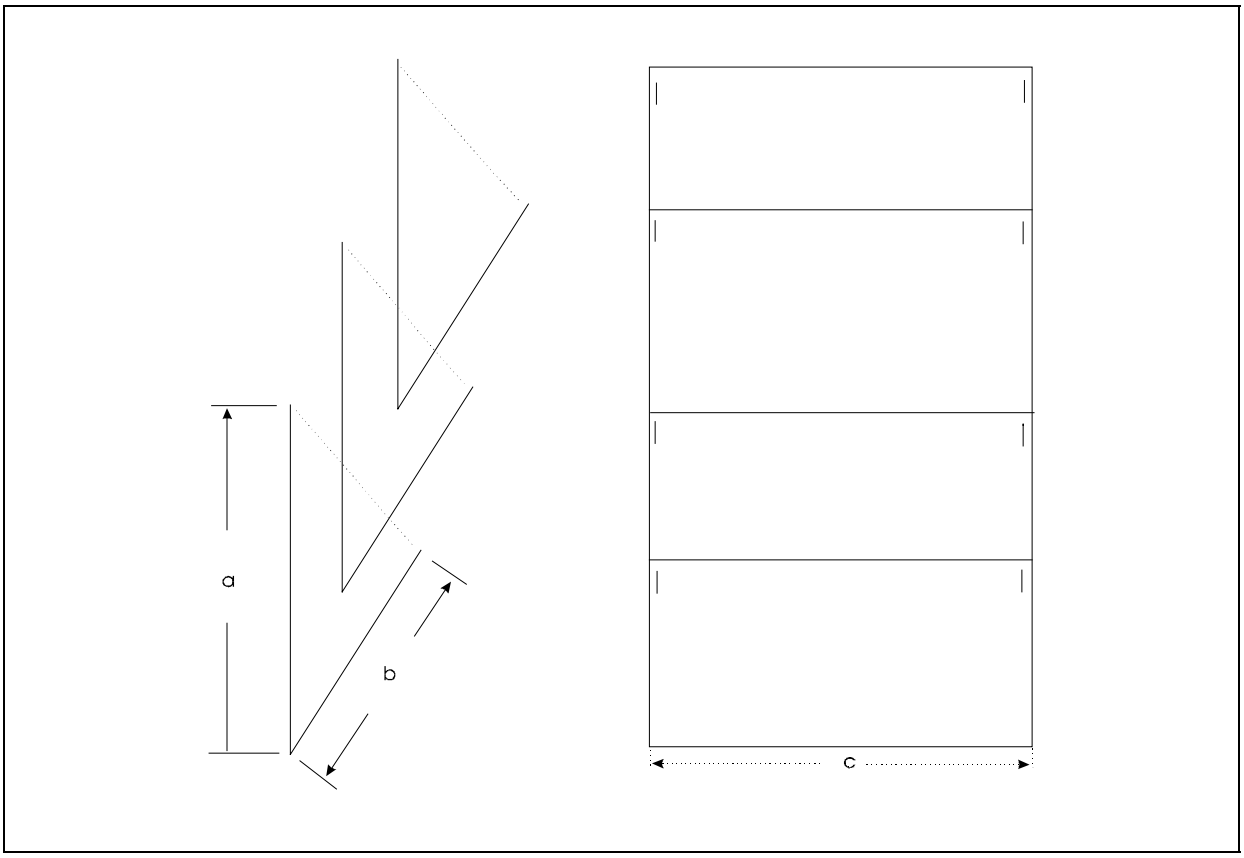
Furthermore, the electrical grid serves many users and is a dynamic system. Just as one may experience changing water pressure when someone flushes a toilet, so power supplied to a given wall outlet may fluctuate. Such fluctuation may be due to high voltage DC pulses like lightning, temporary voltage dips

due to heavy demand suddenly placed on the system such as a furnace motor switching on, or high frequency transients that are superimposed on the AC power from equipment switching or from interactions between devices connected to the system.

The PC and peripherals are equipped to handle some of these conditions, but we may wish to add extra protection with commercially available line filters, isolation transformers, or uninterruptable power supplies. Our own practice has been to use inexpensive surge-protected power bars. These offer only modest protection from the hazards above, but they cost little more than conventional power bars. We also use a telephone line protector on our modem line.

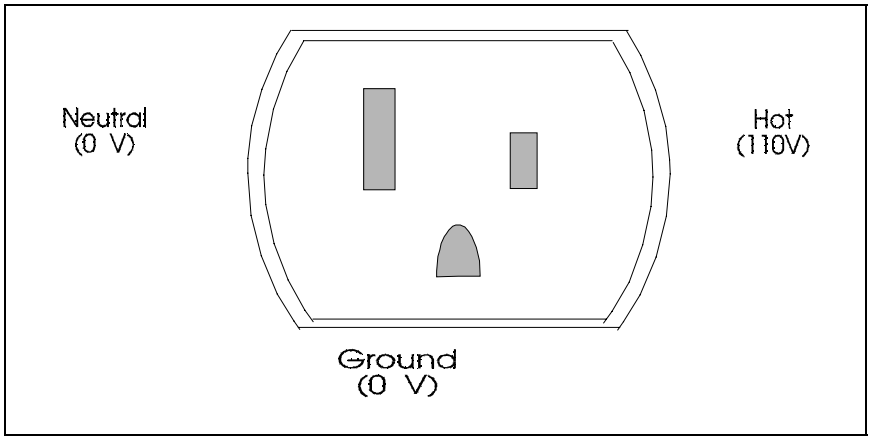
When power difficulties are suspected, one has the choice of buying or renting expensive monitoring equipment or installing protective devices. No device used between the AC line and PC offers total protection. One choice is a battery powered machine. We have seen our own notebook run through a blackout without a hiccup (we were running it off the mains as we charged the battery). The conventional wisdom with Ni-Cad rechargeable batteries is to run equipment to complete discharge then recharge to avoid the "memory" of this type of battery.

Figure 11.3.1 Disk holder made from single sheet paper. *b* should be 3.5" for 5.25" disks; 2.5" for 3.5" disks.



Apart from the electricity coming from it, the wall outlet needs to be considered in other ways. Wall outlets should have three holes; a live (or hot) connection, a neutral and a ground or earth. Figure 11.5.1 shows a typical North American configuration. Unfortunately, it is very easy to wire a socket incorrectly; it may still seem to work, but the ground may not be connected and/or the hot and neutral may be reversed. The user can verify the socket by means of commercial devices (e.g., Leviton Circuit Tester, Model 49662, Cable Electrical Products Inc., Providence, RI) or by ***carefully*** checking voltages. Correct wiring implies: Live - Neutral 115 V AC; Live - Ground 115 V AC; Neutral - Ground 0 V AC. Circuits should have a correctly rated fuse or circuit breaker.

Figure 11.5.1 North American 110-115 Volt AC wall outlet



On the subject of fuses, users should be aware of the locations and ratings of fuses in equipment. Fuses are the first place to look when a failure occurs. Simple replacement of a fuse rarely solves a problem. Fuses blow for a reason, for example, a jam in a printer. However, by knowing which fuse has failed, we may quickly localize the trouble.

11.6 Interference and Radio Frequency Shielding

The two issues here are the interference with the PC and the emanation of radiative energy from the PC. It is difficult to identify cases where radiation from outside the PC has upset its operation. There have been concerns that the very low charge used to store data in modern memory chips could be altered by particle radiation from the decay of radio isotopes in the chip substrate or packaging. Cosmic rays are presumably another menace. Man-made radiation, for example, over-limit CB radio transmissions or static from unfiltered automotive engines, is a potential source of trouble because it can be clearly registered on stereos and television receivers. However, well-documented cases of such interference with PCs appear to be lacking.

The only clear cases of interference come from the modem — the link between the PC and the telephone network. Here line noises from whatever cause are a common source of data transmission errors.

We may divide emanations from the PC into three parts:

- Ionizing radiation (ultra-violet or X-rays);
- Radio frequency radiation;
- Glare, noise or other stress inducing factors.

From available evidence (Treurniet, 1982, and similar reports since), it does not appear that PCs or video-display terminals emit ionizing radiation in significant amounts. This does not mean that long-term human health anxieties should be disparaged. However, it does appear that ionizing radiation is not a hazard of PC equipment.

Radio frequency (RF) radiation from PCs and related equipment is another matter. This can be detected with an ordinary radio or television as audible or visible "noise" received at broadcast frequencies. Such RF energy may have health implications for operators of PC equipment. However, since all kinds of radio transmitters, both public and private, are pumping a great deal of electromagnetic energy into our environment, avoiding such energy requires a metal suit.

Governments have made regulations concerning RF emanations from PCs. In particular, the United States Federal Communications Commission requires manufacturers to conform to strict tests and to provide shielding. Cables running between PC components may serve as an antenna to broadcast RF signals from within a PC case. Shielding cables is troublesome. Some military applications require no signal leakage, as enemy detectors could then fix the position of equipment quite easily. The TEMPEST shielding technologies developed for such applications will come to the consumer product area when the cost of complying with stricter RF emanation rules makes them worthwhile.

Stress induced by glare and noise also receive attention. There are special anti-glare filters to place in front of the screen. Impact printers have acoustic covers to muffle the noise of the print head. Fans have aerodynamic blades to keep them quiet. Such trends are complementary to ergonomically designed equipment intended to aid user productivity and acceptance of the new technology.

11.7 Servicing and Spare Parts

Every PC will fail from time to time, so users must be prepared for "down time" and repairs. The user's response to hardware failure will depend on his or her ability to repair things, on the type of use to which

the equipment is subjected, on the relative availability or suitability of different types of servicing, and on the urgency with which the PC must be restored to operation.

Many users buy service contracts with repair companies or PC makers. The contracts vary, but generally the user pays a certain sum per year to a service company that agrees to repair the PC when it goes wrong. The contract details cover points such as speed of response to a request for service, where service will be carried out (on site, at a service depot or in the factory) and who pays for transport, what service and parts are covered, what the user must do to keep the service contract in force and how any dispute over any of the above points may be resolved.

Typical equipment service contracts cost about 1% of the original purchase price for each month of service. Rates may be reduced if the user agrees to "carry in" the equipment to a service depot. Costs are higher for contracts involving round-the-clock response to service calls or for installations in hard-to-reach locations.

We prefer to repair our equipment as failures occur. We see PCs under service contracts receiving heavy-handed use, kept in hostile conditions, or attached to unsuitable power outlets. A service contract is designed to make money under average conditions of treatment of the equipment. Our experience has been that the money costs for repairs are much less than half the costs of service contracts, especially for well-treated PCs.

A "cost" that is often forgotten is that of arranging for the service call. Waiting for a technician to arrive is costly, either in lost productivity or salaries. Many PCs are installed in places where the service technician cannot enter unless someone is specifically waiting. Moreover, a minimum time charge may apply. This is especially frustrating for intermittent faults. We once paid a 2-hour minimum charge for a technician to conclude "The output shows a definite printer fault, but it's working fine now." We eventually fixed it ourselves.

If you are "handy", some do-it-yourself servicing is possible by:

- Careful recording of symptoms;
- Verification, if possible, of hardware operation by self-tests of system or components, or by use of diagnostic software;
- Location and repair of fault by cleaning, adjustment, or component exchange, where possible. We do not recommend repairs to parts that are not easily exchangeable unless you are adept at soldering.

If one has several similar machines, it is possible to maintain a modest selection of components. The Faculty of Administration computer labs do not carry a service contract on PCs. Instead a stock of a few keyboards, screens, disk drives, and circuit boards is kept to swap into machines as needed. This has turned out to be several times cheaper than a service contract, even given the heavy usage of these PCs.

The exchange of circuit boards is straightforward. ***First, turn off the power!*** Label any cables and connectors before disassembly so they can be reassembled correctly. We use sticky labels, marking pens or typewriter correction fluid to do this. We mark connectors for orientation that may be critical, e.g., for disk control cables. Take care in removing or replacing retaining screws so that such small parts and their washers do not drop into awkward places or get lost. Removal or insertion of boards should be done gently but firmly, pulling or pushing the board so connector pins are straight. It is easy to put sideways stress on pins or connectors that can break soldered joints or mechanical supports.

Note the position of any switches, jumpers or headers on our board, as these are critical for the ***configuration*** of such boards. Ignore such settings at your peril. We usually check that socketed integrated circuits are well-seated by pressing each gently but firmly. Inspection with a magnifying glass under a strong light may reveal that the pins of such circuits are bent double under the "chip". Contact may still be made with the socket most of the time, giving unfortunate intermittent faults. We have twice seen such

problems on our own machines. They are extremely difficult to diagnose. We suspect such "bent pin" faults may be a major source of motherboard (the main PC circuit board) replacements.

To fix bent pins, we proceed as if we were exchanging the integrated circuit. That is, gently remove the circuit by prying it up a little at a time, first from one end, then the other, until it is free of the socket. Special tools are available to "pull" circuits, but it can be done easily by loosening the chip with a jeweller's screwdriver. Once the chip is out, it should be placed on a grounded conductive surface to avoid static damage. Then use fine point pliers to gently straighten the pin. Breaking the pin means getting a new chip. Carefully reposition the chip, ensuring correct orientation and that each pin is directed to the proper socket position. A gentle but firm push will seat the chip.

Cables are a frequent source of problems. It is easy to accidentally pull them in a way that puts a great deal of mechanical stress on plugs and connectors. Where provided, screws or clips that give mechanical support to a connection should be used. However, we feel manufacturers do not always provide enough bracing for these. To see just how little support there is, try giving a well-secured cable a small sideways pull. Watch the flexing of the circuit board to which it is attached! On most PCs, the keyboard connection is a circular DIN plug with no extra mechanical support, even though keyboards get moved a lot in use. We use foldback clips or similar clamps as a cable strain relief. This serves to attach the cable firmly to either the PC case or to furniture so that there is no stress on the connector to the PC itself. After all, a keyboard is a lot cheaper than a motherboard, and we can replace it without technical assistance.

Apart from computer viruses, strange or intermittent effects are often caused by:

- Dust, dirt, or loose parts causing short circuits;
- Overheating of some components due to poor ventilation;
- Memory failure.

Dust and dirt can be dealt with by cleaning. Overheating requires that we ensure adequate ventilation of all components. Memory failure, which is usually in a single chip or bank of chips, can be fixed by replacing the offending parts. Finding which chips to replace may be possible using special diagnostic software. Sometimes this is supplied with a computer. If not, we recommend contacting a local users' group and asking the software librarian or similar member about such diagnostic programs.

Diagnostic software can also help in improving the configuration of our PC. That is, we can adjust various settings of both hardware and software to improve performance or make our PC simpler to use. This is a continually changing field, and we will not mention any products by name here.

A servicing task that users may need to carry out from time to time is the reformatting of fixed disks. The tracks that carry the magnetization recording our data are laid down either in the disk factory or the computer supplier's store by special programs. Over time, temperature and mechanical stress may cause the read-write mechanism to drift off-specification or the tracks to lose some magnetization. In either case, we may be unable to persuade the PC to read our data. Assuming we have a backup, the main issue is to restore the disk to working condition. This requires a low-level reformatting, a task requiring special software. Users' groups or a friendly computer store probably can supply this. (Many vendors seem to believe users should not be trusted with such programs.) Software also exists that will "renew" the low-level format and test a disk simultaneously, e.g., SpinRite.

Clocks commonly need battery replacement every couple of years. Some PCs use a rechargeable battery that can lose charge if the PC is switched off for extended periods of time. Usually the configuration memory is also lost and must be restored. See Section 11.8.

11.8 Configuration Maintenance

Many problems arise due to the different ways in which personal computers may be configured.

Recommendations made by one user may be totally inappropriate for another. To a large extent, these differences show up in the ***configuration*** of the PC. In the configuration we include the set of physical devices that make up the PC system, the connections and interfaces to outside devices and networks, the physical installation, the partitioning of disk and memory storage, the structure of directories on fixed disk storage, the optional choices that are set for all operational hardware and software, and the selection of and order of loading of any resident software.

Many important aspects of the configuration of MS-DOS PCs are embedded in three particular places:

- The continuous configuration memory (often called CMOS memory) of the computer that holds physical startup information;
- The CONFIG.SYS file in the startup directory (root directory of the "bootup" disk) of the PC contains instructions that set the maximum number of files allowed, the number of buffers, the partitioning of memory for different uses, and the loading of device drivers for special disks (including compression of the existing disk), tapes, keyboard features, or other tasks;
- The AUTOEXEC.BAT file that is executed when the operating system command processor is active and that loads memory resident software, sets the command environment, file path and command prompts, and that launches programs we want active immediately, for example, a windowing environment, word processing shell, or integrated programming environment.

Change to one configuration component may affect others, forcing us to test all regularly used software after significant changes. For example, during the writing of this book, we needed a mouse with a 9-pin connector for our notebook computer. The only one available was on our 80386 tower machine, which could take either a 9-pin or 25-pin connector. We "borrowed" a different mouse from our old XT machine where it was little used, then had to change the configuration files of the tower machine to use the correct software associated with this different mouse. The AUTOEXEC.BAT file, Microsoft Windows and several other programs had to be "set up" again. Unfortunately, after several uneventful weeks, we found the editor BRIEF was unable to use the "new" mouse driver, and we had to reverse all our efforts.

Updated programs require installation steps that also affect the configuration. Indeed, version numbers of programs in use form a part of the configuration information. Unfortunately, upgrades that affect operating software or features may make the user memory too small to run our favorite programs. Many packages are now very memory-hungry. We have seen systems employing overlays appear to "run" after a configuration change, then fail due to lack of memory when a menu choice is made. This is poor software design, since the main routine should perform memory checks to allow us to avoid a "crash".

Keeping a record of the configuration is essential if we need to restore a PC after a failure or disastrous user error, such as accidental reformatting of a fixed disk. Programs exist that can save the contents of the CMOS memory, though it is generally possible to edit this information at startup time if one has a ***listing*** of the appropriate settings. Otherwise, if the PC can be started from a diskette, this is what we do. Data is then copied from the diskette to the fixed disk and CMOS. We also have to load backup software so we can restore software and data from backup volumes.

On 80386 and later MS-DOS machines, the configuration files, especially CONFIG.SYS, allow options that can markedly alter the amount of user-accessible memory for programs. Setting the correct options for maximum memory is not a trivial task, especially if there are several special drivers for CD-ROM, network or other functions as well as a set of resident programs to load. Overcoming perverse interactions between different functions we want to include can waste many hours of our time.

A corollary to our configuration is the set of manuals describing the software and hardware we use. We have three "collections": the hardware manuals, the software manuals we use regularly, and the less used or obsolete software manuals that we may refer to occasionally. In the hardware manuals we try to keep pencil notes of switch settings or other important information. Discard manuals that you will never use again.

While we have talked here of MS-DOS PCs, Macintosh configurations have entirely equivalent functions, but the mechanisms are different. Configuration information is held in the ***system folder***. The user may select ***preferences*** for the operating environment; some of these may be changed for each folder. Selected programs may be made rapidly available for execution, and others may be made permanently active. An overly "busy" configuration is detrimental to performance. Serious pruning may give better performance.

The configuration is important to ***how*** we work with our PC. Vanilla configurations can be very tiresome. A "travelling disk" of everyday utilities can save time when visiting colleagues. We can set up a directory for temporary use and invoke familiar tools that aid productivity. Before leaving, the temporary directory should be purged.

We always configure our machines with a RAM disk, since we find it important to have a fast area of scratch space on "disk". Print buffers, which are built into most networks, avoid waits for printing to complete. There are occasional difficulties with such buffers if a PC is interrupted in the middle of printing or a printer is not ready and data is lost.

If we have more than one computer type, the potential configuration problems multiply, especially if we must share data or peripherals between the different platforms. With some care to standardize on disk formats, printer interfaces and characters sets (e.g., PostScript), we may be able to reduce the level of annoyance. It is useful to localize certain tasks on one platform or another. In our own case, for example, we use an IBM mainframe almost exclusively for electronic mail, and IBM RS /6000 for Internet connections, a Macintosh to help edit a professional journal and MS-DOS machines for everything else.

Part III: The problem and its solution method

This part of the book presents our viewpoint on the actual solution of problems in scientific computation with PCs. In previous parts of the book we have dealt with the machinery and the software, with their attendant difficulties and details. Now we will look at problems and how their solution. First we will look at formulation, then consider some cases, simplified for expository purposes. Throughout we stress empiricism — if something works, use it! If it doesn't, find out why.

Chapter 12

Steps in Problem Solving

12.1 Problem formulation example
12.2 Algorithm choice
12.3 Algorithm implementation — programming
12.4 Documentation
12.5 Testing — data entry
12.6 Testing — sub-programs
12.7 Testing — complete programs
12.8 Production runs
12.9 Modifications and improvements

Faced with a computational problem, one explicitly or implicitly follows a sequence of steps in passing from the statement of the problem to the number, set of numbers, formula or graph that provides a solution.

This chapter outlines these steps and partially illustrates them with an example of linear least squares fitting of data to a model. This problem arises throughout the physical, biological and social sciences, in applications ranging from chemical kinetics to real estate valuation. Readers with experience in least squares modelling may disagree with some choices made at various phases of the problem solution.

Let us consider the steps in developing a solution. The steps are not necessarily sequential, though some naturally precede others.

1. Problem formulation or statement;
2. Mathematical formulation or restatement;
3. Choice of technique or method;
4. Choice of algorithm;
5. Selection of computing environment, namely computing system and programming language or application package;

6. Coding of program;
7. Testing of program;
8. Documentation of program;
9. Revision and modification, with retesting;
10. Further documentation of program;
11. Regular or "production" use of program.
12. Repeat as necessary!

12.1 Problem Formulation Example

There is rarely a unique formulation to a problem. Without considerable practical experience, we are unlikely to have a good appreciation of the relative merits of different formulations. A correct formulation of a problem is vital to the choice and development of a satisfactory solution method. Moreover, the problem statement may not show the formulation. For example, we could be asked:

> *Find the relationship between the earnings of computer programmers and their formal education and experience.*

This problem presupposes a ***relationship***, but does not give a ***form*** to it. Thus, our first choice is the form of the model. We will simply propose a model in the form:

(12.1.1) $$Earnings = r * Education + s * Experience + t$$

This form, a linear model, is well-known and widely used. Before, we can apply it however, we need appropriate data for the variables *Earnings*, *Education* and *Experience*.

Earnings could be measured by gross annual salaries, *Experience* by years of paid employment as a programmer. For *Education* we propose years of post-secondary education in a computer-related subject, though this ignores other post-secondary studies that may have some impact on earnings. Our task is therefore to estimate r, s, and t, the three linear coefficients in this model. In certain circumstances we may also be required to provide measures of precision of these coefficients.

Mathematically, it is convenient to rewrite the problem in a more compact way. Let us suppose we have m observations, that is, we have asked m computer programmers how much they earn, and how many years of education and experience they have. The number of observations m may be 10 or 10000; this is immaterial now, but it will become important later.

We rename *Earnings* as variable y. The i'th observation of y will be y_i. The variables *Education* and *Experience* can be renamed. However, instead of separate names, we will let *Education* be the first column of a matrix X and *Experience* be its second column. To complete the matrix, its third column of X will be a column of ones.

(12.1.2) $$y_i = \sum_{j=1}^{3} X_{ij} b_j + e_i$$

where $r=b(1)$, $s=b(2)$ and $t=b(3)$, and e_i is the "error" in the i'th observation. The whole ensemble of observations has a matrix product form (using boldface for vectors)

(12.1.3) $$\boldsymbol{y} = X \boldsymbol{b} + \boldsymbol{e}$$

The fitting of the model now has the obvious interpretation that the three coefficients b_j, $j=1, 2, 3$ must be chosen to make the elements e_i, $i=1, 2,..., m$ small in some way. The most common measure for the size of the "errors" is the sum of squares

(12.1.4) $$S(\boldsymbol{b}) = \boldsymbol{e}^T \boldsymbol{e} = \sum_{i=1}^{m} e_i^2$$

This norm for the vector $\boldsymbol{e}$ produces a least squares estimation of the model. The superscript ^{T} denotes matrix transposition.

Having decided that we have a linear least squares problem, our formulation could be considered complete. However, the problem may arrive in disguise, for example, as a function minimization.

(12.1.5) Minimize $S(\boldsymbol{b})$ with respect to $\boldsymbol{b}$

Or we may be asked to solve the linear equations

(12.1.6) $$X^T X \boldsymbol{b} = X^T \boldsymbol{y}$$

for $\boldsymbol{b}$. These are the ***normal equations*** for solving the linear least squares problem. We can classify the tasks as either linear least squares, function minimization or linear equations. Clearly, the different classifications will direct us toward different methods for solution of the problem.

12.2 Algorithm Choice

In our example, we already have formulations as linear equations, function minimization and linear least squares. Once our general approach is settled, we must look at the various features of our problem to choose an appropriate algorithm — a recipe for calculating the desired solution. Different algorithms may have advantages if we must solve many similar problems. To illustrate the choices, let us consider possibilities for the least squares problem in some detail.

First, traditional treatments form the normal equations (Nash J C, 1990d, p. 22). Letting

(12.2.1) $$A = X^T X$$
(12.2.2) $$\boldsymbol{v} = X^T \boldsymbol{y}$$

we can rewrite the normal equations as

(12.2.3) $$A \boldsymbol{b} = \boldsymbol{v}$$

Many algorithms exist for solving n equations in n unknowns. (In our case n=3). As n is small it may even be reasonable to use Cramer's rule (See Dahlquist and Björck, 1974, p. 138) to find the solution. It is more likely that a variation on a general technique such as Gaussian elimination (Nash J C, 1990d, Section 6.2) is appropriate. Since A is symmetric and non-negative definite (Nash J C, 1990d, Chapter 7), we could also use the Cholesky decomposition or a symmetric Gauss-Jordan reduction (Nash J C, 1990d, Chapter 8). We could even use general QR or singular value decomposition algorithms to solve the normal equations.

Note that a formal solution of the normal equations is obtained by inverting the sum of squares and cross-products matrix A and multiplying the inverse times the vector $\boldsymbol{v}$. The inversion and matrix multiplication introduce unnecessary work, but there are numerous Gauss-Jordan flavor programs of mongrel parentage for performing this task. Unfortunately, stepwise regression is also very easily programmed using this approach, but risks numerical instability unless care is taken.

The least squares problem can also be solved by direct decomposition of the data matrix X. In the ***QR decomposition***, we find the product of an orthogonal matrix Q and an upper triangular matrix R such that

(12.2.4) $X = Q\ R$

where

(12.2.5) $Q^T\ Q = 1_n$

the identity or order n, and

(12.2.6) $R_{ij} = 0$ if $i > j$

We can show that the simple solution of the ***triangular*** equations

(12.2.7) $R\ \boldsymbol{b} = Q^T\ \boldsymbol{y}$

is a solution to the normal equations, since

(12.2.8) $X^T\ X\ \boldsymbol{b} = R^T\ Q^T\ Q\ R\ \boldsymbol{b} = R^T\ Q^T\ \boldsymbol{y} = X^T\ \boldsymbol{y}$

and we know R is non-singular if it has no zero diagonal elements.

There are several good methods for computing a QR decomposition. The ***Gram-Schmidt orthogonalization*** is one of the oldest. Rice (1966) showed that a modified form of this method has superior numerical properties to the conventional algorithm. The Gram-Schmidt method builds the R matrix row by row, or column by column, by orthogonalizing the columns of matrix X with respect to each other. By thinking instead of a process that transforms X to an upper triangular matrix via multiplication by elementary orthogonal matrices, one arrives at the ***Givens and Householder decompositions*** (Nash J C, 1990d, Chapter 4). Clearly, one has plenty of choice in carrying out the QR decomposition of X.

The ***singular value decomposition*** (svd) offers yet another approach to solving the least squares problem. The svd decomposes the matrix X into a product of three matrices U, S, and V in the form:

(12.2.9) $X = U\ S\ V^T$

In the svd, the matrix S is diagonal and its elements are non-negative. That is,

(12.2.10) $S_{ij} = 0$ for $i \neq j$

(12.2.11) $S_{ii} \geq 0$ for $i = j$

The matrices U and V have the following orthogonality properties (U is m by n, V is n by n)

(12.2.12) $U^T\ U = 1_n$

(12.2.13) $V^T\ V = V\ V^T = 1_n$

where 1_n is the identity matrix of order n.

There are two main algorithm families for the svd for sequential computers. The first is due to Golub and Reinsch (1971) with variants published by Businger and Golub (1969) and Tony Chan (1982) and is derived from the QR algorithm applied to matrix eigenvalue problems (Stoer and Bulirsch 1980, page 377). The other algorithm family for the svd is based on the Jacobi method for eigenvalue problems (Nash J C, 1975; Nash J C and Lefkovitch, 1976; Nash J C, 1990d, Algorithms 1 & 4; Nash J C and Schlien, 1987; Luk, 1980). Providing certain simple steps are taken during the calculations, the Jacobi algorithms will order the singular values S_{ii} so that

(12.2.14) $S_{11} \geq S_{22} \geq \ldots \geq S_{nn} \geq 0$

Jacobi-type methods have surprisingly few steps, and with the property of ordering the singular values, they are good candidates for use in situations where code length must be short. It has also been of interest for users of computers with unusual architectures (Luk 1980).

With so much information about different algorithms, the user has a considerable analysis to perform to

decide which algorithm to implement. The comparisons can be made under three main categories: features, size/complexity and efficiency.

The ***features*** of an algorithm include:

- The classes of problems solved in terms of type (e.g., linear equations, least squares) and size (m and n).
- The "extras" offered by the algorithm. For example, in linear least squares modelling we may want standard errors for the estimates of the model coefficients. These are easily calculated from information in the matrices that comprise the svd, which also leads to a natural method for performing the principal components regression variant of linear least squares modelling (Nash J C, 1979b).
- The reliability and accuracy of the algorithm in terms of its ability to compute the correct solution. Certain least squares methods based on the normal equations and the Gauss-Jordan reduction will usually give accurate estimates for the coefficients b_j , $j = 1, 2, . . ., n$ (often more accurate than the svd approach). Unfortunately, one can devise cases where they generate very poor answers. Under similar circumstances the svd remains stable and provides good estimates of the coefficients, with diagnostic information on their lack of precision.
- The robustness of the algorithm (or program resulting from it) to exceptional cases, for example a least squares problem with only one observation or variable.

Without presenting the subject of computational ***complexity***, we can still discuss and compare algorithms in terms of the number of calculations required (e.g., additions, multiplications), the working storage required in terms of variables and arrays, and the structure of the algorithms such as the number of branches and decision points and number of special cases to be handled.

The last area of comparison concerns speed, effort and cost under the overall heading of ***efficiency***. Thus the run time to compute a solution may be important. If we have to compile programs, the compile and linkage time may be important. The amount of time and effort the user or programmer need to implement and install a working program is another measure of efficiency. The acquisition or license costs of any programs must be totalled. This may be exchanged for user time and effort if we write our own codes. Availability of freeware programs is a factor to consider here. A last, but extremely important, measure of efficiency is user happiness; while difficult to measure, user attitudes to an algorithm color effective use of it. These attitudes should be considered when choosing an algorithm for a particular task.

12.3 Algorithm Implementation - Programming

For most problems, we will estimate linear models in an application program and never need to program, but we will continue our example as if it were a less common task. This section concerns traditional programming rather than the writing of scripts for packages. The programming step in solving a numerical problem is straightforward if the method and algorithm are clearly stated and well understood, but ambiguities and unstated conditions must be clarified and resolved, and errors avoided.

Step one is to decide the programming language(s) to be used. This depends on the programming tools available, the language features needed, our ability to use the tools, and our preferences. Special conditions may alter our choice. For example, if we must solve problems in a microprocessor-based controller, we need a language that can be compiled to the appropriate machine code. If we want portability across computing platforms, we must choose a language for which standardized compilers exist on all target machines.

Whatever language is available, we want to avoid over-sophisticated coding, the use of special language dialects or undocumented features, or inclusion of unverified source code in our final program. Some examples of such poor practices follow.

To save program length, programming tricks may be used that accomplish several algorithmic tasks at once. At times such techniques can be useful, but they complicate our work and can cause grief when debugging. Programs that rely on the system (hardware or software) to initialize variables or seed pseudo-random number sequences save us the code and memory needed to perform the initialization but may give unpredictable results with any change in the system configuration or a move to another computer. The use of constructs like

```
DIMENSION A(1)
```

in FORTRAN to permit variable dimensioning of arrays, while used in early programs, should be avoided. The use of single subscripts for two dimensional arrays as in the early IBM System/360 Scientific Subroutine Package (Manual 360-CM-03X) had the same goal, but is notorious for its preoccupation with saving index calculation time. The resulting codes are difficult to follow and alter. Similarly, the brilliant and tiny Bauer-Reinsch (1971) Gauss-Jordan inversion of a positive definite symmetric matrix is difficult to follow and understand (Nash, J C, 1990d, Chapter 8).

Programmers may also use tricks to access data via pointers. We urge directness and simplicity. Older FORTRAN programs sometimes used EQUIVALENCE to access data in some unusual way. For example, data read in by an A4 format to a single-precision array could be used 8 characters at a time via a double precision array EQUIVALENCED to the same location. This fails if the single and double precision data types do not match up perfectly. An example on Page 1 of Kernighan and Plauger (1974) shows how ***not*** to set a matrix to the identity.

If it is imperative that we use programming constructs that support special features of a particular computer, we should identify non-standard program code to make modification for other compilers or machines easier. We may be the ones to make the changes.

We should proof-read a program at some point to see that it makes sense, even if test results seem correct. There are still possibilities for grave errors due to paths through the program that the test cases do not exercise. See Kernighan and Plauger (1974) for a short, readable, and valuable guide to reasonable programming style.

When programming, we want to avoid being diverted from the task of finding an adequate solution for the real problem in the search for a perfect method for the mathematical one. Remember the original task! We are confirmed (and somewhat unrepentant) sinners in this regard, since it is very satisfying to find a better, faster or more accurate methods for a particular problem. For academics, there are articles in numerical analysis or computing journals, the opportunity to show off programming virtuosity to colleagues and the inner warmth of cracking a challenging puzzle. However, unless the new method has wide production use, the solution of the real problem is the one that buys the groceries.

12.4 Documentation

Documentation is a permanent headache in all spheres of programming. Ideally, the documentation exists before the program is written. This is possible to the extent that the algorithm is expressed in detail in some pseudo-code such as a step-and-description form. What must be added is information on the order and format of data that is needed for a successful computation. This information must also be kept current as the program is applied to new problems or moved to different computers.

The main reason documentation is forever incomplete, out of date or contains errors, is that documenting today's work only helps us tomorrow, while the rewards or brickbats are earned for results now, so writing documentation is easily postponed. The only remedy is continuous discipline and good programming habits, but no programmer maintains a perfect record in this regard.

Some workers like to have all their documentation stored in the computer, as comments within the program or in a text or hypertext file that can be called up by the program. We must still ensure that the

comments are correct and up to date. In interpretive environments, comments may also slow down the execution of the program.

The importance of documentation is to clarify information that is not obvious from the program code. Thus, comments of the form

```
100 FOR I = 1 TO N: REM LOOP ON I
```

are a waste of time, whereas

```
100 FOR I = I TO N: REM LOOP OVER ALL PRODUCT CODES
```

tells the reader something about the use of the program code.

Full documentation should describe the following aspects of a program:

- How the program is invoked, that is, a step-by-step set of instructions to using it;
- A data dictionary (Section 6.2) describing the function of each variable array, string or other data structure in the program;
- The author of the program, date of writing or date of last alteration;
- The files used by the program, their size, type and format;
- Any special requirements and all devices used by the program. For example, the program may assume a 24 X 80 video output format, a 120 character per line printer or clock accessible via some I/O port.
- Any non-standard or unusual programming language constructs;
- The mechanisms used in any of the algorithm steps, or a reference to sources where this information may be found.

Despite all the above, documentation should be as succinct as possible. To this end, summary cards are very useful, containing all the information needed to operate the program in a small, portable reference.

12.5 Testing — Data Entry

The first level at which a program may fail is where the user must enter data into the program. For example, let us consider the entry of the order of a square matrix, which must not be bigger than 50 X 50, its maximum dimensions. This number will be an integer. Consider the following examples, where [cr] denotes the "carriage return", (ASCII 13, OD Hex):

4[cr] 65[cr] [cr] A[cr] 4J[cr] 4,5[cr] 4.5[cr]

Only the first entry is acceptable. The second is too large for the maximum dimensions of the matrix. The third is null, and some programs may take the entry to be zero, especially if the carriage return is preceded by blanks. The fourth entry is the letter A, the fifth has a letter J after a number. The sixth is either wrong in having a comma or uses the European form for the decimal point and, like the final example, is not an integer.

Catering to the needs of users who may employ either commas or periods for decimal points may be quite difficult. We may have to read numbers as character strings that are then converted to numerical values under control of our program, rather than use the operating system or language processor (Section 9.5).

It is unfortunate that truly robust programs require such drastic steps. The input handlers associated with the operating system, programming environment, linkage or run-time libraries or packaged computing environments are rarely documented enough that we can know in advance which error conditions they will detect. Even learning the behavior of a specific input handler sufficiently well to rely on it requires considerable effort. Worse, the behavior of the input handler may change from version to version of the

product in which it is embedded. We found three ***different*** input routines in different parts of one database program.

For reading text data, various errors may arise relating to the length of the string or to special characters that cannot be entered. To enter such special characters or nulls, we may have to alter our input mechanism. Typical approaches use some form of ***escape character*** that tell our program that a special character is coming. For example, we could specify accents by using an escape character "\" (back-slash) then the letter of the alphabet, then a character defining an accent, such as \e' to define é. Such tactics are needed for entering characters that might stop execution.

Of course, we sometimes have to halt our programs. For example, when a program prompts for a number, we may realize we need to look it up in a reference book, so wish to abort the run. This can sometimes be impossible, short of switching the PC off. A good input routine has some mechanism for stopping a program. However, the choices made by system implementors are not uniform. One interesting choice was that of Sinclair Research in the Sinclair ZX81 and Timex Sinclair 1000. The BASIC interpreter in these very small machines assumed all input was to be interpreted just like a program so the handler would accept

```
EXP ( -PI/4)
```

as a valid numerical entry. To stop a program when it was prompting for data, the STOP keyword was needed rather than the BREAK key (Nash J C and Nash M M, 1982, 1983b).

We strongly advocate (Nash J C, 1990b, 1990d, 1992) allowing programs to be controlled from a file, which we will call a script. We can build various test scripts that include error conditions. We like to be able to include comments in input scripts (Section 9.6). We also insist (Section 9.6) that programs should be able to copying all output to a file for later review. This is critical if we want to run programs in batch mode, but it simplifies verification of results.

12.6 Testing — Sub-programs

A well-defined sub-program makes testing easier, since we can focus on a smaller segment of code. We need to know all the possible inputs to a sub-program and the correct response to those inputs. We must also be sure all required exits from the sub-program are correctly included.

To test a sub-program, we can employ a dummy driver program that calls the sub-program with known input information and reports on the correctness of returned results. The biggest task, as in data entry, is to provide all possible cases. Users will eventually produce cases that match a given permutation of conditions, however unlikely. If our program prevents certain options, we do not have to test the sub-program for these. For example, in a subroutine to find the eigenvalues and eigenvectors of a real symmetric matrix, we may ***choose*** not to verify symmetry if other program components guarantee this property. However, if the subroutine becomes part of a general library of mathematical software, a symmetry test or a warning should be included.

Structuring sub-programs (Sections 6.4 and 6.5) so that they have only one entry and one exit helps to control the amount of testing required. However, we sometimes need failure exits from sub-programs. In program libraries, handling errors is a major headache. There may be sophisticated mechanisms to carry out the task of reporting errors and stopping the program. In a PC one can be much less fancy. A simple PRINT "message" and STOP suffices. The general library must allow the user program to regain control after an error has been detected. If we are writing both driver and sub-program, our decisions can be made at the most convenient point in the program. We do not have to return to the driver program information as to where, when and how the program failed, and pass this back through two or three levels of sub-programs to our driver program.

As an example, suppose we are trying to calculate the so-called square root of a matrix A. We shall assume A is real symmetric and positive definite, so that we can form an eigenvalue/eigenvector

decomposition

(12.6.1) $A = V D V^T$

where V is the matrix of eigenvectors and D is the diagonal matrix of eigenvalues. The square root of A is then

(12.6.2) $H = V S V^T$

where

(12.6.3) $S_{ii} = \sqrt{D_{ii}} = (D_{ii})^{1/2}$ for $i = 1, 2, . . ., n$

as can be seen by forming

(12.6.4) $H H = V S V^T V S V^T = V S^2 V^T = V D V^T = A$

and using the fact that the eigenvectors of a real symmetric matrix are orthonormal. Suppose we have a subroutine to compute the square root of a matrix. If, unknown to us, A has negative eigenvalues, execution may halt when the square root of a negative number is attempted in a sub-program at least two calls below the driver program. Preferably, our "matrix square root" subroutine will instead return to the main program with a flag variable set to indicate A is not positive definite.

12.7 Testing — Complete Programs

Testing a complete program is an extension of the ideas in the previous two sections. We must find all the possible routes through the program and make sure all of them are valid and properly executed. Clearly it is worth keeping the control structure of the program simple.

If we develop the main programs and sub-programs simultaneously, a top-down approach to testing may be useful (Howden, 1982, p. 224). Program units under development are replaced by dummy routines that merely return the right results using sample inputs and outputs. This allows the calling program to be tested independent of the sub-program. Once the sub-program is verified correct, we may substitute it for the dummy routine. Expensive calculations may be avoided if we preserve the dummy program for testing purposes.

Test data sets and certified test results are valuable and difficult to come by. Such collections are not frequently published, yet they form an important tool for building reliable and correct software. Programmers should carefully document and preserve such data sets.

Examples of input and output help users of programs (Nash J C, 1992). In particular, prepared scripts can be used as a template for the user to develop the input data for a new problem.

12.8 Production runs

Even a properly implemented, fully tested program does not lead automatically to a correct solution of a given problem. "Large" problems may not fit in the memory available despite our best efforts. More annoying may be the very slow progress of calculations, particularly if the solution method is iterative in nature. Elapsed times of several hours are not uncommon when using PCs for difficult numerical problems. If such a computation has been running for some time and another use for the PC arises, we must decide whether to abandon the calculation in favor of the new task, thereby wasting the effort so far expended.

By modifying a program to save appropriate information at some point in the calculation, we can arrange for it to be restarted without losing all the work done so far. This is worthwhile for "long" calculations.

We run multiple calculations of a similar nature using a command script, either as a set of instructions to the program or else a batch command file for the operating system that runs our program with different data sets. In one case, we performed 6000 nonlinear least squares problems for a client in one week. The output data filled all the available fixed disk space on our machines several times. We moved this output onto diskettes in compressed form, automatically generating summary data for our client, and were able to continue computations from the next case in the script.

For one-off problems, we have found it most convenient to use packages that give us a high level computing environment, such as **Stata** or MATLAB. However, we like to use a command script to carry out the solution because we can store the script or incorporate it in our working documentation. It is too easy to forget the details of how we accomplished a solution. Although the script is only "used" once, it can be referred to often. Truthfully, we cannot remember a computation that remained "one-off".

12.9 Modifications and Improvements

After a program has been used to solve problems, deficiencies will almost certainly become apparent. The input methods may be clumsy or error-prone. Users may always choose the same settings or tolerances or not make use of special feature of the program. Output may not be set up in a way that allows it to be easily transferred to reports.

If the program has been well designed and documented, suitable modifications and improvements should be easily incorporated. If design or documentation is poor, then we should consider restarting the problem solution process from the beginning. Can we salvage any of the existing program code? Can we estimate the costs of rebuilding versus repairing? Such estimates may be very difficult to provide, especially if we are trying to make them for programmers other than ourselves.

A common modification of a program is its adaptation to a new system. Here we may change hardware, operating software or programming language dialect. Generally, this is a difficult task unless the programmer has kept portability in mind when designing the program. The difficulties come about because effective modifications can only be made if one has a very good working knowledge of both source and destination systems. In the realm of calculation, we may be further burdened by poor documentation concerning number representations and floating-point arithmetic or function approximation properties. The function and sub-program libraries of different compilers and interpreters may differ. This is beyond the usual problems of language syntax changes and I/O and file conventions. Following programming language standards as much as possible will reduce the work of transporting programs between computing systems.

We have noted a specific difficulty in transferring linear algebraic calculations to C from FORTRAN, PASCAL or BASIC. C generally indexes a 1-dimensional array of n elements from 0 to (n-1) rather than from 1 to n. This makes some algorithms, in particular the Cholesky codes of Chapter 16, more difficult to translate to C than to the other common programming languages. Conversion software exists that automates at least some translation from FORTRAN or PASCAL to C. The translators appear to do a good job of the bulk of the conversion, but programmer effort is needed to tidy the resulting code.

Because of these difficulties, it is worth considering the use of an application package with compatible versions on different platforms. For example, **Stata** and MATLAB use the same files and scripts across platforms, with documented local specializations.

Chapter 13

Problem formulation

13.1 Importance of correct formulation
13.2 Mathematical versus real-world problems
13.3 Using a standard approach
13.4 Help from others
13.5 Sources of software
13.6 Verifying results
13.7 Using known techniques on unknown problems

This chapter is a guide to formulating problems so that they can be solved. We wish to translate a collection of statements or conditions given in words into a matching set of mathematical equations or inequalities.

13.1 Importance of Correct Formulation

The goal in formulating problems is the right answer. If we fail to generate a proper mathematical statement of our problem, the chances of getting even approximately correct answers are small. However, what makes up a proper mathematical statement of a real world problem is difficult to define objectively. Like Stephen Leacock's Mr. Juggins (Leacock, 1945), we can continue to add new details and refinements and never get close to producing an answer. Equally, in a headlong rush to print out numbers, we can overlook subtle but crucial features of the problem. Eschewing the extremes, let us consider the middle road. Thus, our mathematical formulation should:

- Contain the most simple and direct statement, in equations and inequalities, of the key points of the real problem;
- Note any unusual features in the real problem;
- Avoid unnecessary detail.

This easy to say but more difficult to accomplish, especially when the real or mathematical problems fall outside our regular experience. When dealing with the unknown or unfamiliar we may add:

- Be ready to start again!

A good formulation allows the choice of the right tools for its solution. Many real-world problems have several correct mathematical statements as we have seen in the example in Section 12.1. Some formulations are practically useless for computational purposes, while others lead to calculations of dubious stability. A mathematical formulation leading to a sequence of ***approximate*** results by stable methods may be more useful than a totally correct set of equations for which solution methods are unstable. By "stable" we mean that the method does not magnify any errors present in the data input for the problem. An "unstable" method may find results far from a solution even when given data of adequate accuracy to find a good approximation to a solution of the problem.

A proper formulation of the problem should allow particular features of the real-world situation to be incorporated. This flexibility allows us to require, for example, that prices remain positive, that a storage bin must not exceed two meters high and one meter wide, or that building temperatures be between 15 and 28 degrees Celsius. However, formulations that are too restrictive may make it difficult to find a

satisfactory solution.

The conditions that a solution must satisfy help us to categorize the problem and to select appropriate solution methods. Positivity or negativity conditions on solution values are common. Similarly, we often find upper or lower bounds on quantities. In some problems, parameters must be integers since equipment such as vehicles, railway junctions, cranes, etc., is measured in whole numbers. In other situations, parameters may have sums or linear combinations that are constrained e.g., the total energy value of an animal's feed must be at least a certain level of calories. We may want to require parameter sequences to obey some condition such as monotonicity (always increasing or decreasing): the number of animals still alive in a drug toxicity test must be non-increasing. Combinatoric constraints, e.g., that a student pass one course before taking a related one, may also be formulated.

Researchers have developed special methods to handle constraints in many common problems. These techniques, such as bounded least squares estimation (Gill and Murray, 1976), have gradually found their way into the numerical methods literature. However, situations exist where methods for incorporating constraints efficiently remain elusive.

It is unfortunate that in many problems, constraint conditions may remain unstated or unrecognized until the results of calculations are presented. The consequent adjustments that have to be made in the solution method, algorithm and program can prove inconvenient and time-wasting. We may, however, ***choose*** to ignore constraints when solving problems. Methods for determining free (unconstrained) parameters are more commonly available, so that the effort to incorporate conditions explicitly may be uneconomic. We can try such methods. However, the conditions on the parameters should still be written down ***first***. The try-it-and-see use of unconstrained methods is then a ***conscious*** step in seeking a solution. We get answers quickly and cheaply if they satisfy the conditions imposed.

By keeping our initial mathematical statement of the problem simple and direct, we allow related mathematical formulations to be explored. A least squares problem may be transformed into an equations problem for minima, maxima or saddle points by setting first derivatives of the sum of squares function to zero. Alternate formulations are useful because they may be easier to solve or provide checks on the chosen method. Comparisons may show that the problem has multiple solutions or is inherently very unstable.

"Clients" of any consultant will have their own formulations of problems that are often several steps removed from the original, real-world problem. The true problem may not surface until later. See, for example, Watts and Penner (1991). It is important to obtain a statement of the original problem along with its context rather than the processed (and altered) problem sometimes presented. The original problem with its possibly critical side conditions allows us the maximum range of formulations.

A proper mathematical formulation may allow us to decompose the mathematical problem. ***Decomposition*** is a practical and important principle in the solution of mathematical problems. Each sub-problem is in some way "smaller" and more likely to be solvable with more limited computational resources. We can use known techniques on these partial problems and verify our progress at every stage.

Good formulations allow general methods to be applied to problems. This may sacrifice machine time to human convenience, and fail to give an acceptable solution, but the nature of the problem may be better revealed. Applying a general function minimizing program to a linear least squares problem can indicate the shape of the sum of squares surface.

A hindrance to progress may be the traditional or historical approaches taken to solve problems. We have come to regard some "usual" methods that are popular in many scientific fields as confirming ***Nash's axiom***:

The user (almost) always chooses the least stable mathematical formulation for his problem.

Several examples spring to mind. The use of the determinant of a matrix via Cramer's Rule is rarely the correct approach to solving linear equations. The roots of a polynomial resulting from secular equations

generally lead to unstable methods for finding parameters in orbit or structural vibration problems. In fact, the original eigenproblem is usually more stable; good methods for polynomial roots use eigenproblem ideas. Similarly, general rootfinding methods applied over a restricted range work more efficiently for the internal rate of return problem (Chapter 14) than polynomial rootfinders. Newton's method, the basis for many methods for solving nonlinear equations and minimizing functions, often does not work well directly. In our experience, better progress is usually possible using the ideas within a different framework, for example, quasi-Newton, truncated Newton and conjugate gradient methods. Similarly, the steepest descents method for minimization, despite its name, is slow.

13.2 Mathematical versus Real-World Problems

Perhaps the toughest part of any problem solving job is deciding what kind of mathematical problem best fits the real world problem. This part of the job is often mired in the mud of tradition and unoriginal thinking.

Consider econometric modelling. Despite the obvious flaws that observations on all the variables are to some extent in error, that there may be a systematic bias in figures that is much larger than random fluctuations and that occasional deviations from the true values may be extreme, econometricians continue to use ordinary least squares (OLS) estimation as a primary work-horse of their trade. There is no unchallengeable reason why the square of the error (L2 loss function) should be more suitable than the absolute value (L1) or even the minimum maximum error (L-infinity). However, OLS and its extensions for the simultaneous estimation of several equations (Johnson, 1972) do provide measures of precision of the estimates if one is prepared to believe that a set of fairly strong assumptions are obeyed.

The least squares criterion and its relations result in ***mathematical*** problems that can be solved by linear algebraic tools such as matrix decompositions. The L1 and L-infinity criteria, however, result in mathematical programming problems that are, in general, tedious to set up and solve, particularly on a PC. While derivative-free function minimization methods such as the Nelder-Mead polytope (or Simplex) method (Nash J C 1990d, Algorithm 20) or the Hooke and Jeeves Pattern Search (Nash J C 1982c; Nash J C 1990d, Algorithm 27; Kowalik and Osborne, 1968) could be used, they are not recommended for more than a few parameters and may be extremely slow to converge for such econometric problems. Worse, they may not converge at all to correct solutions (Torczon, 1991). The choice of model of the real world in these econometric problems is driven, at least in part, by the availability of methods to solve the mathematical problem ***representing*** the real world.

Mathematical representations of real problems may have solutions that are not solutions to the real problem. A simple example is finding the length of the side of a square whose surface area is 100 square centimeters. Clearly the answer is 10 cm. But the mathematical problem

(13.2.1) $S^2 = 100$

has solutions $S = +10$ and $S = -10$. A length of -10 cm. has no reality for us. Here the task of discarding such artifacts of the representation is obvious, but in complicated problems it may be difficult to distinguish the desired solution from the inadmissible ones.

The point of this section is that we should remain aware of the different possibilities for mathematically formulating real-world problems. Traditional formulations may be the most suitable, but there are always occasions when a new approach is useful (Mangel, 1982).

13.3 Using a Standard Approach

Proper formulation of our problem permits us to take advantage of work already reported by others. We can use known methods for which the properties are (hopefully) well understood. These "known" methods

may, unfortunately, not be familiar to us. We must find them, and they must be usable on our particular computing environment. Useful pieces of software may not be indexed or listed under the headings users expect. Correct formulation helps the creator of software provide index keywords for which users are likely to search.

To find "known" methods, we can try several routes. First, we may have a very good idea of the traditional solution methods, especially if the problem is a common one in our field of work. There will be textbooks, review articles, and computer programs or packages already available for the task. These may or may not be suitable to our particular problem and computing environment, but for all their faults and weaknesses, methods that are widely used carry with them the benefit of the accumulated experience of their users. In particular, methods and computer programs in widespread use are like a trail that is well-trodden. There will be signs for dangers either built into programs or documented in manuals, newsletters, or reviews. Guidance may be obtained from other users and possibly from consultants. For very popular methods, there may be books to explain their intricacies or foibles in comprehensible language.

PC users originally had few choices of packages for numerical problems (Battiste and Nash J C, 1983), often having to write our own programs. A different job now faces users. Sometimes there are too many possible programs to allow a thorough investigation of each. When there are too few or too many choices, we should use programs we already know.

A common dilemma for users is the awkward balance between familiarity and experience with a well-known computational method and the lack of suitability of that method for the task at hand. As an extreme example, we may have a simple and effective general function minimizer, such as the Hooke and Jeeves Pattern Search (Nash J C 1990d). This can solve a least squares fitting problem by minimizing the objective function 12.1.4 with respect to the parameters b_j, $j=1, 2, \ldots, n$. However, as we have already seen in Sections 12.1 and 12.2, a method for solving linear least squares problems is "better": starting values for the parameters b are not needed, nor is possible false convergence of the program a worry. On the other hand, it is very easy to add constraints to the Hooke and Jeeves objective function by use of simple barrier functions. That is, whenever a constraint is violated, the program is given a very large number instead of the value S defined by Equation 12.1.4. Again, one may need to be concerned with false convergence, but the modifications to the method and computer program are almost trivial. The price paid may be very large execution times to achieve a solution.

13.4 Help from Others

Colleagues can aid in the search for methods. Asking questions of co-workers may seem a haphazard train of clues to a good solution method, but rarely a waste of time. Talking to colleagues will frequently suggest alternate views of the problem we wish to solve. This opens up new terms, keywords and possible formulations for our consideration. Sometimes we know program librarians and scientific programmers whose job it is to help others in their calculations, though it is rare to find such information resources outside large government, industrial or academic institutions. How can we find free advice and assistance from such sources?

Knowing what we want to do — that is, having a correct problem formulation — allows us to seek help and advice intelligently, so a good attempt should be made in this direction first. Keep requests as short as possible. Nobody likes to have their time occupied unnecessarily. Offer what you can in return. Most workers who try to develop software are interested in test problems, so giving the data in return for advice may be a fair exchange. Other aids to the advice-giver are timing and performance information for the solutions obtained. Organize your requests. Many questions that arise do not concern the problem but the PC and can be answered by those upon whom the user has a legitimate claim for assistance.

If you are going to make money with the result, some financial consideration for the assistance is due. Payment of another kind is ***always*** due, and that is an acknowledgement of the assistance. "Thank you"

notes, clear mention in any written reports, or comments during a presentation, recognize those who have given time and effort. Most workers can benefit either directly or indirectly from such appreciation in promoting their careers or businesses, and this is one way "free" advice can be repaid. Journal editors never delete such acknowledgements.

13.5 Sources of Software

A difficult task for any author or consultant in the personal computer field is recommending sources of software. It is easy to list names of software packages, but difficult to be sure of the quality of programs, level of support, and business practices of suppliers. Many vendors of excellent products are no longer in the software business, while poor products continue in widespread use despite their deficiencies. This section will concentrate on long-term "sources", those that are likely to remain useful for some years to come, even if they do not provide software that is perfectly adapted to the user's needs.

For mathematical software, the Collected Algorithms of the Association for Computing Machinery (ACM) is a solid mine of information. New programs and methods are described (but ***not*** listed completely) in the ACM Transactions on Mathematical Software. Unfortunately the ACM algorithms are presented primarily in FORTRAN, though some earlier contributions are in Algol 60 and more recent entries sometimes in C. The major target has been large machines. The programs usually have very rudimentary user interfaces. Most programs are available on the NETLIB facility described below. It seems likely that CALGO, as the Collection is referred to, will become a purely electronic product in the future.

Most scientific subroutine libraries are aimed at the large machine market. International Mathematical and Statistical Libraries Inc. (IMSL) and the Numerical Algorithms Group Inc. (NAG) have been primarily FORTRAN subroutine libraries targeted to users in centers with at least one scientific programming advisor. Subsets are marketed, however (Nash J C 1986c, 1986d). One collection of quality mathematical software for PCs is the Scientific Desk from C. Abaci Inc., P.O.Box 5715, Raleigh NC 27650, (919) 832-4847. The product is aimed at FORTRAN users.

Statistical packages are far too numerous to mentions in detail. Over the years there have been several catalogs and attempts at reviews of packages. In 1987/88, when the Boston Computer Society attempted to review as many statistical packages for MS-DOS machines as possible in a study led by Dr. Richard Goldstein. There were over 200 products considered. A review of selected statistical and forecasting software by PC Magazine in their 1989 issue considered several dozen products, of which we had a hand in reviewing three (Nash J C and Walker-Smith, 1989a). The American Statistician regularly publishes reviews of statistical software (e.g., J C Nash, 1992). The Current Index to Statistics may be useful in finding such reviews.

Our own use of statistical packages has not always been driven by scientific considerations. We use MINITAB for teaching purposes because the University of Ottawa has a site license for this product and a student version has been available at a modest price. Moreover, its time series tools — rare in student packages — help us teach forecasting.

For research purposes, we like **Stata** for easy-to-control but powerful graphical and data manipulation functions, along with an interpreted command language that extends functionality. Other users may prefer a fully menu-driven package. For forecasting applications, an example is MESOSAUR (thanks to Dr. MaryAnn Hill, SYSTAT Technical Director, for review copies of MESOSAUR and SYSTAT).

As a general numerical package, we use MATLAB. Originally designed for teaching, it has become a professional product, then returned to its roots with a new student version. In the sphere of symbolic mathematics as well as computation and graphics, there seems to be healthy competition from **Maple** and *Mathematica*, with ***DERIVE*** occupying an interesting niche (Nash, 1995).

Quality software of a scientific nature for specific problems is much more difficult to recommend. There

are many products — far too many to analyze in any detail — and these often have a very small base of user experience on which to judge user satisfaction. Nevertheless, it is possible to guide users to sources of information about software products in their own subject area.

First, as already mentioned, other users with similar needs can point out their success or failure in finding or using software, thereby saving us the time and trouble to duplicate their effort. This is very much the "networking" approach to gathering information. It works. Some researchers have started distributing regular newsletters by electronic mail. One of the more successful has been the NANET Newsletter (for Numerical Analysis NETwork). There are similar electronic exchanges (or ***list servers***) for other subjects.

Second, computer magazines or professional trade publications may have occasional reviews of products. We have already mentioned the reviews of statistical software (Nash J C and Walker-Smith, 1989a) and Lotus 1-2-3 add-ins (Nash J C, 1991b) in PC Magazine.

Third, journals on the subject of the application of interest may publish announcements and reviews of products. In the area of statistics, the American Statistician and AMSTAT News have been useful to the authors for keeping up with the marketplace.

Fourth, scientific conferences often have product demonstration exhibits. These can be a very useful source of information, since the developers are usually on hand and can respond to detailed questions.

Fifth, public database services, such as the Knowledge Index (from DIALOG Information Services Inc.) and BRS After Dark, allow the user to search bibliographic abstracts for reviews of software. The art of efficiently selecting wanted references and avoiding others takes some experience. Some libraries and information companies such as our own will carry out searches for a fee, which may be less costly for inexperienced searchers. Some database services also support computer conferences between like-minded users. Without a moderator we believe these to be of little value. Similarly, we do not often use bulletin boards.

A different form of database is beginning to appear using the academic and commercial electronic mail networks. There are several mechanisms for access and file transfer. One of the most useful has been NETLIB (Dongarra and Grosse, 1987) which contains codes and data relating to numerical mathematics. More recently similar services in other subjects have begun operations. The academic networks also support several file transfer mechanisms that are beginning to have a role in the distribution of reports and software. Related developments include list servers and various network search aids such as GOPHER and ARCHIE (Krol, 1992).

Finally, books are published that contain programs for diverse applications, both general and particular. Some, including two of our own works (Nash J C and Walker-Smith, 1987; Nash J C 1990d) and one by a relative (Kahaner, Moler and Nash S G 1989) include diskettes. We feel that published software directories are a waste of good paper. They are out of date too quickly and at best provide only a partial list of potentially interesting software. The effort to reduce this list of possibilities to a workable small set is not, we think, worth expending.

We find computer stores and agencies poorly informed about scientific software. With the trend to sealed packages, they will rarely offer demonstrations. Mail-order sources limit the time to ask for refunds. We may lose shipping costs, customs duties, or "restocking fees". Worse, we spend time trying to get recalcitrant programs to work as claimed.

Exhausting all of the above routes to "known" methods does not mean that they do not exist. We must decide how much time and effort to spend in finding existing methods before we begin to develop our own. Or we may make do with a "poor" method until something better is available, e.g., using a function minimizer like Hooke and Jeeves for least squares problems as in Section 13.1.

Even if we find a source of some software, we need to know that it will work with our PC configuration and our problem, and we still have to get it. There may be delays or no response to our order. Our usual

practice is to make enquiries for information first to gauge the speed with which an order is likely to be filled. Unless we are convinced a supplier is reliable, we will not order software.

13.6 Verifying Results

Good formulation for a problem lets us more easily verify that the results we obtain are correct. For "standard" problems, many tests are available, so the sub-problem solution method(s) can be checked ***before*** we go to a full solution. Since many sub-problems are well known, the dangers and characteristics are discussed in documentation and other literature, so there is less danger of building a program of rotten blocks.

Also, we may be able to obtain subroutines already written for the sub-problems, or use a package like MATLAB where the blocks are available as simple commands. Even if we cannot simply get machine-readable code ready-made for our PC, the break-up of the problem into well-defined parts will usually be a help to getting correct answers. Results obtained by different approaches can be compared. By formulating a problem two different ways, we have a natural check on results. Even if a method is too slow for production use, it may still be a valuable tool for comparison purposes.

It may seem obvious that answers should, where possible, be tested, but users may not know what tests may be appropriate. We need to ask how well the proposed solution satisfies the mathematical problem representing the real problem. Are there subsidiary conditions or identities that must be satisfied by the answers? What results are expected from experience? By users? By alternative solution methods? Where possible, it is a good idea to draw pictures, that is, to graph the results. We must also be aware of the possibility of multiple solutions.

The rest of this section includes some suggestions of tests that may be applied in specific areas.

Approximation of functions

Cody and Waite (1980) give several identity and comparison tests for the common special functions. From a less computational point of view, Abramowitz and Stegun (1965) provide a wealth of tables and formulas.

Linear equations $A\,\boldsymbol{x} = \boldsymbol{b}$

For these equations, we can compute the residuals $\boldsymbol{r} = \boldsymbol{b} - A\,\boldsymbol{x}$. The condition number of A can be estimated to provide a measure of the likely precision of the computed solution (Forsythe, Malcolm and Moler, 1977, p. 42ff., Kahaner, Moler and Nash S G, 1989, p. 68).

Linear least squares approximation $A\,\boldsymbol{x} \approx \boldsymbol{b}$

Residuals $\boldsymbol{r} = \boldsymbol{b} - A\,\boldsymbol{x}$ should always be calculated. Methods which compute solutions via the singular value decomposition (Nash, 1990d) or eigenvalue methods provide a measure of collinearity in the columns of Belsley, Kuh and Welsch (1980) have aptly titled their book Regression Diagnostics.

Algebraic eigenvalue problem $A\,\boldsymbol{x} = e\,\boldsymbol{x}$

This problem yields so many identities that there is no excuse for not testing output from an algebraic eigenvalue calculation (Wilkinson, 1965).

Differential equations

We can check the adherence of a solution to the original problem by approximating derivatives. This

should be a part of any ODE package. We recommend graphing the solutions. As with quadrature, we will want to learn as much as possible about the problem. Partial differential equations and integro-differential equations bring additional difficulties, and we have too little direct experience of these to comment on their solution or its testing.

Quadrature

The most difficult aspect of quadrature is that there may be singularities or other irregularities in the function that pass undetected at the evaluation points of the function. Comparison of several quadrature methods may be a partial aid, but the best approach is to learn as much as possible about the problem and its solution. Symbolic integration tools let us carry out parts of the problem analytically.

Function minimization

Restart(s) of the minimization process at random points near the supposed minimum allow for possible detection of a false convergence. Furthermore, it is possible to compute the approximate curvature of the surface to verify the minimum conditions on the gradient and Hessian (second derivative matrix).

13.7 Using Known Techniques on Unknown Problems

Sometimes, the world presents a computational problem for which no adequate method exists. The PC practitioner must then be inventive and devise some way to approximate a solution. This is the way in which all existing methods were devised.

First, it is worth some effort to write down all the conditions (as in Section 13.1) and pose the possible solvable problems that arise as one or more conditions are relaxed. One can then "try it and see" or attempt some forcing mechanism or transformation that ensures the relaxed condition is met. Second, graphical or handwaving "solutions" may be used as models leading to a mix or extension of existing methods. Third, many mathematical problems are solvable in terms of some minimum principle, so that a function minimization program may be a route to a crude solution. Fourth, simulation techniques may provide a mechanism to explore aspects of the problem.

Only when all else fails should one consider developing a new technique. In such cases, a very thorough search should be made to determine if someone else has already considered the problem.

Part IV: Examples

The next four chapters present examples to illustrate the ideas we have been developing so far. We follow these examples with a timing study showing how minor differences in program code may alter running time and other program characteristics, underlining our recommendation to time and test programs. We conclude our illustrations with a case study in the use of graphical tools for analyzing program performance. This achieves two goals — we illustrate how to analyze performance while demonstrating some graphical tools to assist in the analysis.

Chapter 14

The Internal Rate of Return Problem

14.1 Problem statement
14.2 Formulations
14.3 Methods and Algorithms
14.4 Programs or Packages
14.5 Some solutions
14.6 Assessment

This chapter presents the internal rate of return (IRR) problem as a case study of problem formulation and solution.

14.1 Problem Statement

A common calculation to help measure the value of investments is the ***internal rate of return***. While not directly a scientific computation, it illustrates many characteristics of computational problems but has easily understood origins. We invest various amounts $I(t)$ in different time periods $t= 0, 1, 2, \ldots ,n$ and these investments (or costs) return revenues $R(t)$ in the corresponding time periods. The net revenue in each period is then

(14.1.1) $N(t) = R(t) - I(t)$ for $t = 0,1,2, \ldots ,n.$

The "zero'th" period allows for initial investments. The net value of the investment is the sum of the net revenues, but to take account of the time value of money, we discount each net revenue appropriately. The later the net revenue is received, the less it is worth. Given a discount rate r, we create Table 14.1.1.

Table 14.1.1Schematic layout of costs and revenues for the internal rate of return problem.

Period	Investment	Revenue	Net Revenue	Discounted
0	*I(0)*	*R(0)*	*N(0)=R(0)-I(0)*	*N(0)*
1	*I(1)*	*R(1)*	*N(1)=R(1)-I(1)*	*N(1)/(1+r)*
2	*I(2)*	*R(2)*	*N(2)=R(2)-I(2)*	$N(2)/(1+r)^2$
t	*I(t)*	*R(t)*	*N(t)=R(t)-I(t)*	$N(t)/(1+r)^{(t-1)}$

The sum of the discounted net revenues, or cash flows, is called the ***net present value*** (NPV) of the investment at the beginning of the investment sequence. The IRR is the value of r such that this NPV is zero. This rate can be compared with interest rates offered by other investments. Uncertainties imply that high precision is not needed in our calculation.

14.2 Formulations

The mathematical formulation of the IRR problem is:

Find the discount rate, r, such that the NPV of the revenue stream $N(t)$, $t=0, 1, 2, \ldots, n$ is zero.

(14.2.1) $$NPV(r) = 0 = \sum_{t=0}^{n} (R(t)-I(t)) / (1+r)^{t}$$

Letting $1/(1+r) = x$, we have

(14.2.2) $$\sum_{t=0}^{n} (R(t)-I(t)) x^{t} = \sum_{t=0}^{n} N(t) x^{t} = 0$$

This is the polynomial root finding problem, since the last summation simply defines a polynomial. A polynomial with n coefficients $N(t)$ is said to be of degree $(n-1)$ and has $(n-1)$ roots. Not all the roots of the polynomial need to be real; complex-conjugate pairs are possible. However, the answers for the rate of return must be real. We don't have imaginary deposit rates! It is useful in some approaches to multiply (14.1.3) by $(1+r)^n$,

(14.2.3) $$\sum_{t=0}^{n} N(t) (1+r)^{(n-t)} = 0$$

The problem can be simplified if we look for just one root between reasonable limits. Clearly a NPV that is negative when $r=0$ means that the investment is a poor one. It is losing money even when there is no "interest" on the investment. So $r=0$ may be chosen as a lower limit to the root. A 50% return per annum ($r=0.5$) is generally considered extremely good, so would be a ***reasonable*** upper limit. If the return is less than 50%, then $NPV(0.5)$ should be negative — revenues late in the sequence of cash flows don't count as much. However, it is possible that there are multiple roots that arise to confuse the whole situation.

It is wise to calculate and plot the NPV for several likely values of r. This gives us a picture of the NPV at various discount rates and errors in a purely automatic solution. Such graphical checks of calculations should always be performed if possible.

We can perform tests other than a plot of the function. A positive return on the investment, means $NPV(0) > 0$, as mentioned. If we are to have just one root, NPV to decline with increasing r, so the first derivative of $NPV(r)$ with respect to r should be negative at $r=0$. This is easily calculated. We use the chain rule to find:

$$(14.2.4) \qquad d\ NPV(r) / dr = - \sum_{t=1}^{n} N(t)\ t / (1+r)^{(t+1)}$$

For illustrative purposes, we will use two sets of cash flows. Figure 14.2.1a presents a straightforward problem; data in Figure 14.2.1b includes some of the potentially tricky features mentioned above.

As suggested in Chapters 12 and 13, we have formulated our problem in two main ways, and have listed some side conditions on the problem and some reality checks for suggested solutions. Our two formulations are:

- Find all the roots of a polynomial and select the one that is appropriate;
- Search for just one root in a restricted range with tests on the applicability of the search.

Figure 14.2.1 Two cash flow streams for the IRR problem;
a. a straightforward problem, b. a problem with multiple roots.

```
Problem IRR2A --
a straightforward problem with
a simple root (discount rate)

Period  Invest  Revenue  Cash Flow
======  ======  =======  =========
  0       600        0      -600
  1         0      300       300
  2         0      250       250
  3         0      600       600
  4      2000        0     -2000
  5         0        0         0
  6         0      455       455
  7         0      666       666
```

```
 IRR3 --
 problem with
 multiple roots

Period   Cash Flow
======   =========
   0      -64000
   1      275200
   2     -299520
   3     -189696
   4      419136
   5       41376
   6     -218528
   7      -23056
```

14.3 Methods and algorithms

The main formulations suggest that we need either

- A method for finding all the roots (or zeros) of a polynomial, or
- A general root-finding technique for one root in a specified interval.

Both methods can be found in the literature. Many methods exist for the polynomial roots problem. See Ralston, 1965, Chapter 8 for a historical overview. Unfortunately, most methods have weaknesses, and few will compute all the roots. The method of Jenkins and Traub (Jenkins, 1975) is considered by many workers to be definitive. An alternative approach is to compute the eigenvalues of the companion matrix of the polynomial (Mathworks, 1992, p. 394ff). A general method for solving a single nonlinear equation (one real root of a function) is easier to find (Kahaner, Moler and Nash S G, 1989, Chapter 7; Nash J C, 1990d, Algorithm 18). An advantage is that we can work entirely in real arithmetic.

14.4 Programs or Packages

We now need to decide how to implement our solution method. If we decide to compute all the roots of the polynomial, we need a tool that can compute these. Since the Jenkins (1975) program is part of the ACM Transactions on Mathematical Software collection available through NETLIB we could get this by

electronic mail or a file transfer method. We would then have to write a driver program, compile it and supply the polynomial coefficients.

MATLAB uses the companion matrix approach and has a function **roots()** built in. A useful adjunct to this is the **poly()** function that lets us rebuild the polynomial from its roots as a check on the computations. We note that ***DERIVE*** will ***symbolically*** solve for real roots of some nonlinear equations. It is designed to find exact or symbolic solutions, so we cannot be certain it will be of use. There are many choices of general rootfinder software. In addition to the references above, we can use codes from Press et al. (1986) and subsequent volumes. There are also rootfinders in a number of public software collections e.g., NETLIB.

Using spreadsheets we can easily plot $NPV(r)$ for a reasonable range of discount rates r. Some spreadsheets now offer to find roots of functions (solve equations), though student versions on our shelf of Lotus, Quattro and Excel did not have this capability. They have a built-in IRR and NPV functions that we do not think are worth using, as will become clear. It is possible to "program" in the macro language of spreadsheets, and root finding could be carried out this way.

Lotus allows other software to be attached to it. Of these "add-in" programs, What-If Solver (Nash J C, 1991b) provides a capability to find roots of general nonlinear equations, so could be applied here.

14.5 Some Solutions

Our software choice for solving rate-of-return problems would be a straightforward spreadsheet package ***without*** special additions to compute roots of equations. That is, we forgo the mathematical satisfaction of finding the complete set of roots of the polynomial equation (14.2.2). Because the rate of return is used as a guide to investment management, it is not important to find a very accurate approximation to any single root. Instead, we suggest plotting the NPV against discount rate r and observing where zeros are located. It is easy to add to the table used for plotting and verify NPV for good "guesses" of r. However, we suggest that IRR and NPV functions built into many spreadsheets ***not*** be used for reasons we give below.

Figure 14.5.1 shows the data and expressions for the straightforward problem defined in Figure 14.2.1a. Figure 14.5.2 shows the graph of $NPV(r)$ versus r, the discount rate. Calculations were carried out with Lotus 1-2-3; Quattro Pro gives equivalent results. Readers should note that the @NPV() function within spreadsheets does ***not*** give us $NPV(r)$ as defined in Equation 14.2.1 without some modifications. If in the spreadsheet our net revenues N(1) ... N(9) are stored in cells C11 to C19, with the initial net revenue (i.e., the investment) N(0) in C10, the correct expression for the NPV for time $t=0$ at a rate stored in cell B10 is

```
+C10+@NPV(B11,C11..C19)
```

Since the IRR is a built-in function of many spreadsheet packages, it is tempting to use this function. In Figure 14.5.1 this works correctly. DO NOT trust such functions. They will not always work for problems with multiple roots, such as that defined by the net revenues in Figure 14.2.1b. From the graph in Figure 14.5.3 we see that there are solutions near 10%, 50% and -150% and these are confirmed by the worksheet. The @IRR function determines this latter root at -143.857% from starting guesses at 0, 0.5, and -1.5, even though the correct value is very close to -143%. It fails (gives ERR as the result) from several other trial starting values. In an attempt to overcome the difficulty, we changed the sign of all net revenues. This should not change the position of the root, but it caused all our attempted @IRR calculations to give an ERR result. The NPV at -143.857 as calculated by the @NPV function and by direct spreadsheet statements are different. This is probably because the elements of the sum are quite large and digit cancellation is occurring. Note @IRR does not find the root at 10% that is likely to be of interest.

We can also program our own solution by rootfinding. In 1980 we built a rate-of-return program in BASIC using character graphics to plot NPV versus r and the rootfinder of Algorithm 18 in Nash J C (1990d).

Figure 14.5.1 Data and expressions for a straightforward internal rate of return problem using a Lotus 1-2-3 spreadsheet.

```
IRR2a.WK1 -- Internal rate of return  =   7.827 %

Time period:       0    1    2    3     4    5    6    7    8
Investments -->  600    0    0    0  2000    0
Revenues       -->       0   300   250   600        0       0   455   666   777
=========================================================
Combined    --> -600  300  250  600 -2000    0  455  666  777
Contribution to -600  278  215  479 -1479    0  289  393  425
NPV at r= 7.8275  == Summed NPV contributions =    0.002

NPV (r from @IRR = 7.8275) --> -2E-14
    == check on calculated IRR using = -600 + NPV(t=1..t=8)
```

We would not recommend programming this problem now unless it is to be embedded inside some heavily-used investment analysis package.

Using the "all roots" formulation, we can quite in quite straightforward fashion acquire and install the Jenkins (1975) program. This took one of us about an hour to do, including getting the code from NETLIB by electronic mail, downloading it by telephone to our PC, writing and testing a driver program, and then running our problem. A nuisance was finding the right values to use for the radix, number of digits, smallest and largest real numbers that the program needs. These are particular to compiler and computer used; we eventually spent over half a day investigating the possibilities, as illustrated in Figure 14.5.4.

A further difficulty comes in deciding whether roots are admissible. The **roots()** function of MATLAB gives (1+r) values at 1.10, 1.50 and -0.5 having small non-zero imaginary parts. Initial results from the Jenkins program did not seem to match. Using a smaller "machine precision" value, though the arithmetic is unchanged, gave results in closer agreement to MATLAB. Using MATLAB, we reconstruct the polynomial, scale it appropriately, and find the deviation from the original sequence of cash flows. Such an exercise showed that the roots computed by MATLAB indeed gave us back the original problem. We tried the same reconstruction with results from the Jenkins code, varying the tolerance used to judge "small" numbers. In the case of the simple-root problem (data of Figure 14.2.1a) the deviations decreased as the tolerance was decreased. For the multiple-root problem, however, Figure 14.5.4 shows that the solutions vary in quality as the tolerance for zero is made smaller. For both problems, a very small tolerance caused a failure flag to be set. The behaviour of results using three different compilers (Lahey F77L 5.01a, Microsoft Professional Fortran 5, Watcom Fortran 9) were similar but far from identical.

Figure 14.5.5a shows the very simple steps to use the SOLVE capability of the symbolic mathematics package ***DERIVE***. We get just three reported roots (***DERIVE*** makes no attempt to assess multiplicity). In this case we can SOLVE. This did not give a solution for the more straightforward problem of Figure 14.2.1a, though we note that a good approximation to roots can be found by plotting NPV(r), since ***DERIVE***'s graphs have a user-controllable cross-hair for which the position is displayed as well as a ZOOM facility that lets us locate a root as accurately as we like. Alternatively, as shown in Figure 14.5.5b, we can set up a Newton iteration in ***DERIVE***, but must remember to set the arithmetic as approximate to get numerical answers. If we leave arithmetic as exact, the iteration fills memory as it takes a great deal of time to "compute" roots.

Figure 14.5.2 Graphical solution of the problem of Figure 14.5.1.

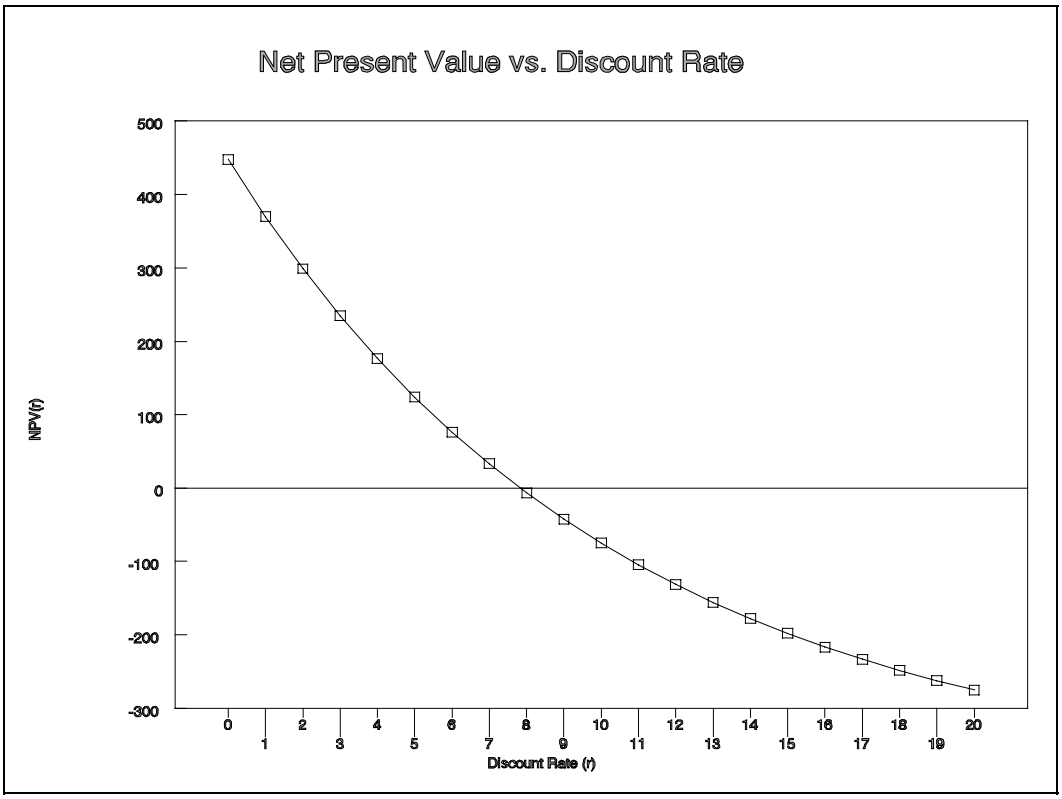


Figure 14.5.3 Graphical solution of the problem of Figure 14.2.1b. The graph is truncated when off-scale.

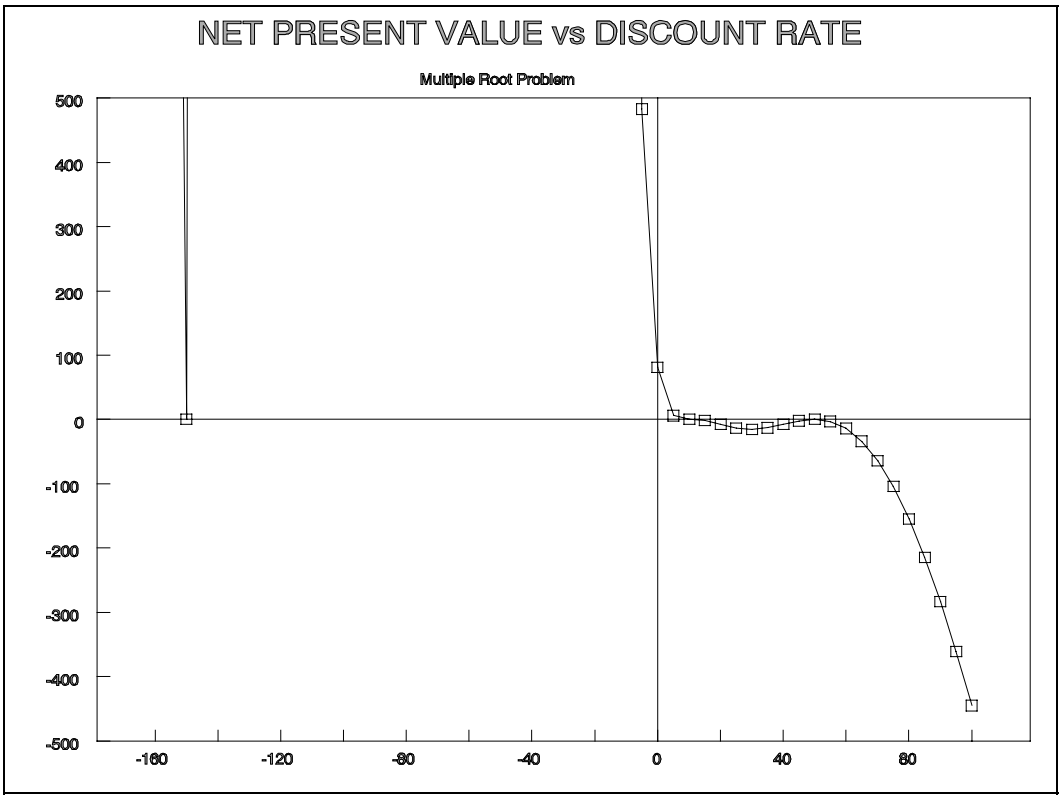


Figure 14.5.4 Graph of the log of the sum of squares of the deviations between the cash flow coefficients and their reconstructions from the computed polynomial roots for the problem described in Figure 14.2.1b.

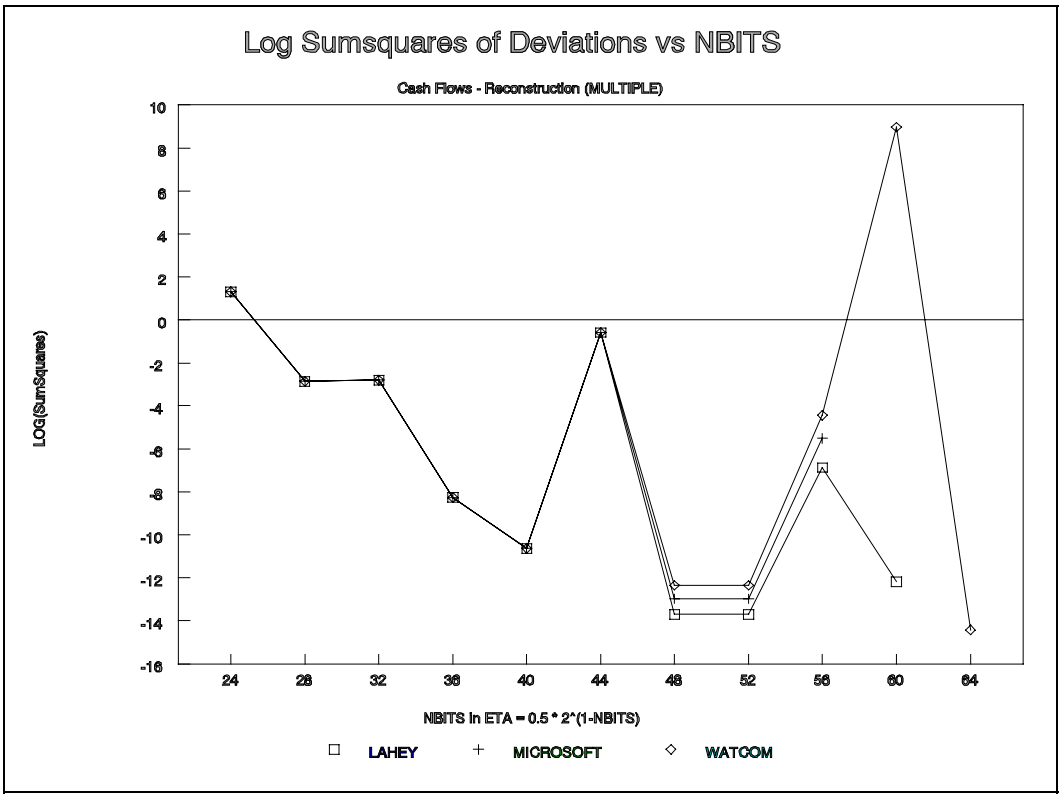


Figure 14.5.5 a) Solution of the internal rate of return problem 14.2.1b by the SOLVE function of ***DERIVE***.

```
c:=[-64000,275200,-299520,-189696,419136,41376,-218528,-23056,47190,11979]

ply:=SUM(ELEMENT(c,i)*(1+r)^(1-i),i,1,10)

(275200*r^8+1902080*r^7+5419264*r^6+8402240*r^5+8072416*r^4~
 +5272416*r^3+2331216*r^2+573462*r+64081) / (r+1)^9-64000

r=1 / 10

r=1 / 2

r=-3 / 2
```

Figure 14.5.5 b) Solution of the internal rate of return problem 14.2.1a by a Newton iteration defined in ***DERIVE***. Approximate arithmetic is used.

```
c:=[-600,300,250,600,-2000,0,455,666,777]

ply:=SUM(ELEMENT(c,i)*(1+r)^(1-i),i,1,9)

NEWTON(u,x,x0,n):=ITERATES(x-u / DIF(u,x),x,x0,n)

NEWTON(ply,r,0)

[0,0.0545808,0.0757515,0.078245,0.0782755,0.0782755]
```

14.6 Assessment

The mathematically obvious solution of the IRR problem in terms of polynomial roots led us to annoying detail both in assessing the validity and admissibility of roots and providing appropriate machine constants for our compiler. If one wants to know all the roots, MATLAB or a similar tool seems a better choice. ***DERIVE*** seems to win the contest on simplicity, though it will not always compute all the roots.

Of course, when we draw a graph of NPV versus discount rate, our eyes only pick out distinct roots. We can confirm these roots by computing the NPV directly in a spreadsheet or with ***DERIVE***. ***DERIVE*** also has the Newton iteration if we want very precise roots.

If IRR values must be supplied automatically, a rootfinder that computes a single root in a given interval is our choice. We would not recommend programming this in the macro language of a spreadsheet. Having tried this, we believe it is too easy to make small but damaging errors placing data in the spreadsheet so the macros can work on it. Instead, we would choose a FORTRAN version of Nash J C (1990d) Algorithm 18 and graphs drawn with VG (Kahaner and Anderson, 1990) so only a reasonably small driver program must be coded.

In solving the example problems here, we brought to light some deficiencies of built-in functions in spreadsheets. Users should run check calculations of functions in any package — errors can and do creep in, so we must protect ourselves as best we can.

Chapter 15

Data Fitting and Modelling

15.1 Problem Statement
15.2 Formulations
15.3 Methods and Algorithms
15.4 Programs or Packages
15.5 Some solutions
15.6 Assessment

This case study concerns fitting or modelling of data by single equation models. This topic encompasses a large class of practical scientific and statistical calculations. For example, we use weed infestation to illustrate growth function modelling, but the same techniques are used for market penetration, bacterial infection or similar data modelling problems.

15.1 Problem Statement

We consider several data fitting problems of different types. They result in similar formulations but no single solution method is appropriate to all. We looked briefly at modelling data with a linear model in Section 12.1 under a least squares criterion of fit. We now allow more general forms of model that can approximate data for which "straight line" functions are inappropriate. Let us consider several examples:

- An attempt to relate farm incomes to the use of phosphate fertilizer and petroleum products (Nash J C, 1990d, p. 46);
- The refinement of land survey height differences between different surface locations on a piece of land (Nash J C, 1990d, p. 240);
- The approximation of the number of weeds per square meter measured each year for 12 years by a growth curve function.

These general statements have to be cast into mathematical form. Data is given in Table 15.1.1.

Table 15.1.1 Data for three data fitting problems.
a) Data for relating farm income with phosphate and petroleum use
b) Height differences between benchmarks
c) Growth data recorded at yearly intervals

a) Indices for phosphate use, petroleum use and farm income

phosphate	petroleum	income
262	221	305
291	222	342
294	221	331
302	218	339
320	217	354
350	218	369
386	218	378
401	225	368
446	228	405
492	230	438
510	237	438
534	235	451
559	236	485

b) Measured height differences in meters between 4 benchmark locations.

```
Height 1 - Height 2 = -99.99
Height 2 - Height 3 = -21.03
Height 3 - Height 4 =  24.98
Height 1 - Height 3 =-121.02
Height 2 - Height 4 =   3.99
```

c) Hobbs data for the logistic growth function problem (weeds/sq.m)

```
5.308
7.24
9.638
12.866
17.069
23.192
31.443
38.558
50.156
62.948
75.995
91.972
```

15.2 Formulations

We write our set of data

(15.2.1) $\{ y_i, X_{i1}, X_{i2}, \ldots X_{ik} \}$ for $i = 1, 2, \ldots, m$

where $\boldsymbol{y}$ is the vector of data we wish to "explain" or fit and the matrix X holds in its columns data for the variables that we anticipate will help to predict $\boldsymbol{y}$. Then suppose we wish to approximate $\boldsymbol{y}$ by a function g of the data X and parameters $\boldsymbol{b}$ to give a residual vector $\boldsymbol{r}$ having elements (note that these are functions of $\boldsymbol{b}$ as well as the data y, X)

(15.2.2) $r_i = g(\boldsymbol{b}, \boldsymbol{x}_{iT}) - y_i$

where

(15.2.3) $\boldsymbol{x}_i^T = (X_{i1}, X_{i2}, \ldots, X_{ik})$

That is, we have a matrix X of data holding k variables in its columns. Thus X is m by k. The i'th row of X will be called $\boldsymbol{x}_i^T$. The function $g()$ is our ***model***. To adjust the parameters $\boldsymbol{b}$ to fit the model to the data, we need a criterion of fit or ***loss function*** that allows us to decide if one set of parameters is better than another. The ***least squares*** fit is found by finding the parameters b_j , $j = 1, 2, \ldots, n$ that minimize the loss function

(15.2.4) $$S(\boldsymbol{b}) = S(b_1, b_2, \ldots, b_n) = \sum_{i=1}^{m} r_i(b)^2$$

Here we use functions $r_i(\boldsymbol{b})$, $i = 1, 2, \ldots, m$, that all have the same algebraic form, that of a residual, though we have used a "model - data" form that is the negative of common statistical practice. We do this so the derivatives of $\boldsymbol{r}$ with respect to $\boldsymbol{b}$ are the same as those of $\boldsymbol{g}$. In general, we need not have the same definitions for all the functions. They could even be algorithmic expressions.

There are other choices than least squares for the measure of how good the "fit" is between the modelling function and the data. ***Weighted least squares*** minimizes the sum

(15.2.5) $$S(\boldsymbol{b}) = \sum_{i=1}^{m} w_i \; r_i(b)^2$$

where the vector $\boldsymbol{w}$ defines the weights. These weights are larger for data values y_i we are sure of and smaller for those we consider uncertain. ***Maximum likelihood*** estimation depends on our knowing the probability distribution or density function for the residuals. If the probability we observe a given residual is $P(r_i(\boldsymbol{b}))$, then the probability or likelihood we observe all the residuals simultaneously is

(15.2.6) $$L(\boldsymbol{b}) = \prod_{i=1}^{m} P(r_i(\boldsymbol{b}))$$

Our loss function is then $-L$, or more usually $-log(L)$, the negative of the ***log likelihood***.

Some workers have reasoned that occasional very large residuals are generally the result of ***outliers***. We should not give these observations the same weight as the rest. Such ideas produce special ***loss functions*** that look like least squares for small residuals but use a constant penalty for all "large" residuals (Goodall, 1983). The results are considered ***robust*** to the presence of outliers.

The notation $\boldsymbol{y}$, X and $\boldsymbol{b}$ corresponds to that most commonly used by statisticians. However, it should be mentioned that it is common to set all elements of one of the columns of X to 1 (the constant) and to consider the $(k - 1) = p$ other columns as the ***variables***. Different notations are used in other branches

of science. While "trivial" in the mathematical sense, they cause users much annoyance. In particular, for ***linear models***, the p variables $X_{.1}$, $X_{.2}$, . . . $X_{.p}$ give rise to $(p+1)$ parameters to be determined. The farm income problem is like this, but the height difference data is not, as we shall see below. Models without a constant (intercept) term are uncommon in statistical applications. In both cases we can write,

(15.2.7) $$\boldsymbol{g(b)} = X\,\boldsymbol{b}$$

Using a matrix notation and writing the residual vector in its usual form

(15.2.8) $$\boldsymbol{r} = \boldsymbol{y} - X\,\boldsymbol{b}$$

the sum of squares loss function can be written compactly as

(15.2.9) $$S = S(\boldsymbol{b}) = \boldsymbol{r}^T\,\boldsymbol{r}$$

Note that this is equivalent to substituting (15.2.7) in (15.2.2).

For the height difference problem, we have a matrix X

(15.2.10)
```
 1   -1    0    0
 0    1   -1    0
 0    0    1   -1
 1    0   -1    0
 0    1    0   -1
```

Note that this has not constant column, and that one combination of benchmarks is missing. We could also have replicated measurements. More important for finding an appropriate method, however, is the realization that we can set an arbitrary level as our "zero" or "sea-level" of height. That is, any constant can be added to all the b_i and not change the height differences. This indeterminacy in the solutions will show up as singularity of the matrix X and may cause software to fail in mid-calculation. Because one of the heights is arbitrary, we can set one of them to zero. For example, setting b_4 zero lets us use the triangular structure of the first 3 rows of X to get initial estimates of the heights. There are then two other rows of information to be reconciled with these estimates. It is this reconciliation that is the core of this problem.

The model suggested for the weed growth data is called a ***logistic growth function***, an S shaped curve. This variant uses three parameters b_1, b_2, and b_3 to approximate the weeds per square meter in year i as

(15.2.11) $$g(i) = b_1 /(1 + b_2\, exp(-b_3\, i))$$

For our proposed logistic growth function, we put the time (years) in column 1 of matrix X and the corresponding weed densities in y, writing the residual for the logistic function as

(15.2.12) $$r_i = b_1 /(1 + b_2\, exp(-b_3\, X_{i1}\,)) - y_i$$

Thus, function (15.2.11) could be rewritten

(15.2.13) $$g_i\,(\boldsymbol{b},X) = b_1 /(1 + b_2\, exp(-b_3\, X_{i1}\,))$$

Since our problems are stated as a minimization, they can be solved in this way. For the growth curve problem with any loss function or for linear models using some robust or maximum likelihood loss functions, this is often a reasonable formulation. However, it is not an efficient way to solve for the parameters $\boldsymbol{b}$ for linear least squares problems. The growth curve problem is usually formulated as a ***nonlinear least squares*** problem.

Note that we could apply calculus minimization techniques to $S(\boldsymbol{b})$. That is, solve the equations that arise when we set the derivatives to zero. Here we want to find the root(s) $\boldsymbol{b}^*$ of the equations

(15.2.9) $$\boldsymbol{grad}\ S(\boldsymbol{b}) = \boldsymbol{0}$$

where ***grad*** is the gradient operator that forms the vector of first derivatives of $S(\mathbf{b})$ with respect to $\mathbf{b}$.

Subtle changes in the specifications can radically alter the formulation. For example, simple constraints on the parameters, such as the requirement that they are positive, may hamper use of traditional techniques. We have not here specified any extra conditions on our problems. For instance, we could note that all the growth data must be positive, and further insist that models be monotone increasing. The first condition forces b_1 to be positive, the second that b_2 and b_3 have the same sign. At this stage of the work, we should already have plotted the data to see if it a growth function is appropriate. To save space, we refer the reader to Figure 15.5.2 later in the chapter.

15.3 Methods and Algorithms

The criteria for fit discussed in Section 15.2, namely, least squares, weighted least squares, maximum likelihood or robust loss functions, all result in either a minimization or maximization mathematical problem. Therefore, we first seek function minimization methods. (Converting maximization to minimization is accomplished by multiplying the objective by -1.) There are many choices available.

First, we may look for nonlinear least squares methods, since our linear problems are special cases. In a statistical context, this may be indexed under the more general topic of ***nonlinear regression***. We may even find that growth modelling is explicitly indexed.

More generally, function minimization or minimization of a function of several variables is a topic covered in many works on numerical methods. Often minimization is considered a sub-topic of ***optimization***, particularly unconstrained optimization. For regular solution of problems of one type, we are likely to want algorithms that are both reliable and efficient. Minimization methods vary widely in their motivations and detail, giving rise to a very large literature. Nash J C and Walker-Smith (1987) includes a large bibliography. In general, considering only function minimization tools, we may distinguish methods as (see Table 7.7.1):

- Direct search — not requiring derivative information;
- Gradient methods — requiring the user to supply first derivative information; and
- Newton-type methods — requiring second derivative information to be supplied. This category may be broken down further to include the Gauss-Newton family of methods for loss function that are sums of squared terms, including the Marquardt variants.

Usually methods become more efficient as we supply more information, but there can be some nasty surprises. Sadly, the computation of derivatives is non-trivial. It requires attention to detail and generates quite lengthy program code. About 90% of the "failures" of minimization codes in our experience result from errors in the derivative code. To avoid such errors, we may turn to symbolic manipulation packages (e.g., **Maple**, ***DERIVE***) that allow output in the form of program code. Automatic differentiation tools such as AUTODIF (Fournier, 1991) or ADIFOR (Griewank, 1992) essentially differentiate our program source code for the objective function rather than a mathematical expression. Another choice is to use numerical approximation of derivatives, with possible consequences of "poor" approximations.

For the linear least squares problems, we can clearly do better. We have already seen some options in Sections 12.1 and 12.2 so will not repeat that discussion here. There is no shortage of methods for our problems. The work will be to select among the possibilities.

15.4 Programs and Packages

Since the growth curve problem (Table 15.1.1c) is the most general, we will start there. A first software option is statistical packages that include nonlinear regression modules. This is clearly sensible if we are

familiar with the package ***and*** it gives us the results we want. Operational details can get in the way. Nonlinear estimation usually requires the user to specify the model, starting values for parameters, and sometimes the loss function to be used. Also needed may be settings for convergence tolerances and numbers of iterations. Users should understand the actions these control. The advantages of a package — in terms of additional output, graphics, and integration with related computations — are worthwhile if the learning cost is acceptable.

Packages may employ inappropriate algorithms; they may fail to give correct answers or may fail to converge. SYSTAT uses a Gauss-Newton nonlinear least squares method, with derivatives computed automatically, but this information came from the developer rather than documentation.

A second approach is to use programs or systems specific to nonlinear estimation or optimization. Subroutine libraries remain useful for building a special-purpose program when many problems of one type are to be solved over an extended period. The user must prepare a driver program as well as routines to tell the subroutine the nature of the minimization, possibly including derivative information. If good examples exist, the coding task may be straightforward. In our own work (Nash J C 1990d), we have tried to provide moderately detailed examples, but the practice is by no means universal.

Special systems exist for nonlinear estimation (Ross, 1990; Nash J C and Walker-Smith, 1987). Different problems benefit from different algorithms. To simplify bringing together problem specifications and minimizers Nash and Walker-Smith use program builder with a one-line command:

NL (name of method) (name of problem)

Menu-driven and hypertext variants of this program builder have been created (Nash J C and Walker-Smith, 1989b; Nash J C, 1993b). We provide a variety of examples that can be edited by users so they do not have to prepare problem specification files from scratch. Special systems may have particular features we need: the Nash and Walker-Smith codes allow parameters to be made subject to upper and lower bounds or to be temporarily fixed (masked). A "not computable" flag can be used in the function specification to avoid calculating the model or the loss function when parameters have unsuitable values.

An "add-on" that is especially useful is graphics. If only very simple graphs can be produced (as in Nash J C and Walker-Smith, 1987), an easy way to move data and results to other software for presentation must be found. For this book we used **Stata** to graph the original data and fitted line in Figure 15.5.2.

For spreadsheet users, the Lotus 1-2-3 "add-in" What-If Solver (Nash J C, 1991b) could be used, but the specification of the objective function and data are the responsibility of the user. These are entered into regular spreadsheet cells using the spreadsheet functions. Traditional datasets are less easily used since they must be imported carefully into the appropriate spreadsheet locations. There are similar "solvers" for other spreadsheet packages.

A fourth approach is provided by general math / calculation tools. MATLAB is our example here. This offers toolkits of procedures, e.g., for optimization problems. A variety of additional calculations or graphs may be prepared. The problem specification must be "programmed", but even the Student MATLAB includes a Nelder-Mead minimization and we can also program other algorithms. These may use derivative information or be specialized to functions that are sums of squares. To learn about the present growth curve problem, we computed residuals, their sum of squares, the gradient, the Jacobian matrix (partial derivatives of the residuals) and the Hessian (second derivative matrix of the loss function) and its eigenvalues.

For the farm income problem (Table 15.1.1a), we specify as our explanatory variables the two data columns labelled *phosphate* and *petrol*. The column *income* is $\boldsymbol{y}$. The linear least squares problem is contained within the linear regression problem of statistics, with a vast array of software available for its solution. From software already installed on just one of our PCs, we can choose among the general statistical packages MINITAB, SYSTAT (and its offspring MYSTAT), and **Stata**, a special-purpose ridge

regression package RXRIDGE (Obenchain, 1991), our own algorithms from Nash J C (1990d) and Nash J C and Walker-Smith (1987), and simple expressions in MATLAB. Several other packages were on our shelves but not installed (they use up disk space!). We could also think of solving this problem in a spreadsheet package such as QUATTRO (our version of Lotus 123 does not offer multiple regression).

Statistical packages offer extra output relating to the variability of the estimated parameters $\boldsymbol{b}$ as standard errors and t-statistics, along with measures of fit and (optional) graphical checks on how well the model works. For purposes of illustration, we include a MINITAB output in Figure 15.5.5. Note that this was created by "executing" a file of commands prepared with a text editor. Moreover, the output was saved by instructing MINITAB to save a console image (or log) file.

The height difference problem is less straightforward. We can attempt to apply MINITAB, using a NOCONSTANT sub-command because X does not have a column of 1s. However, we do not know if the software will cope with the indeterminacy in the heights (the "sea-level" issue). We can also use MATLAB's capability to generate a generalized inverse of X. Data refinement problems like this one often arise in large scale land survey and geodesy calculations. We know of a problem where X was 600,000 by 400,000. The structure of matrix X is very simple and the essential data for each height difference is just a row index, a column index, and an observed height difference. We do not need to store the matrix itself. If the problem were large, a sparse matrix method is appropriate. A simple one is the conjugate gradient method (Nash J C, 1990d, Algorithm 24), though better methods could be found.

15.5 Some Solutions

This section presents some results mentioned above. For the weed growth problem, Figure 15.5.1 shows output from SYSTAT as well as the command file the user must supply to run this problem. Figure 15.5.3 gives the output of the Nash and Walker-Smith MRT code. Figure 15.5.2 is a graph of the data and the fitted model from the latter solution. We see from this, that the sigmoid shape of the logistic function is not evident. This explains some of our difficulties. These are made clear in Figure 15.5.4, which gives the Hessian and its eigenvalues at a point "near" the solution.

A useful feature of the Marquardt (1963) method (Figure 15.5.3) is that it allows us to attach quite detailed ***post-solution analysis*** to the program to compute approximations to standard errors and correlations of the estimated parameters. The user, in the problem specification, is also permitted in the Nash and Walker-Smith codes to include a ***results analysis*** that pertains to the application. For example, we may wish to scale the parameters so the results are expressed in units familiar to other workers in the area.

Figure 15.5.1 Weed growth curve model using SYSTAT.

a) Input command file

```
NONLIN
OUTPUT E:SSTTHOBB
PRINT = LONG
USE HOBBS
MODEL VAR = 100*U/(1+10*V*EXP(-0.1*W*T))
ESTIMATE / START=2,5,3
```

b) Screen output saved to a file

```
ITERATION    LOSS      PARAMETER VALUES
    0      .1582D+03 .2000D+01 .5000D+01 .3000D+01
    1      .2889D+01 .2056D+01 .4985D+01 .3077D+01
. . .
    8      .2587D+01 .1962D+01 .4909D+01 .3136D+01

 DEPENDENT VARIABLE IS      VAR

    SOURCE   SUM-OF-SQUARES    DF  MEAN-SQUARE

  REGRESSION      24353.213     3     8117.738
    RESIDUAL          2.587     9        0.287
       TOTAL      24355.783    12
   CORRECTED       9205.435    11

RAW R-SQUARED (1-RESIDUAL/TOTAL)  =  1.000
CORRECTED R-SQUARED (1-RESIDUAL/CORRECTED) =    1.000

PARAMETER  ESTIMATE    A.S.E.     LOWER  <95%> UPPER
    U       1.962      0.114      1.705         2.219
    V       4.909      0.170      4.526         5.293
    W       3.136      0.069      2.980         3.291

 ASYMPTOTIC CORRELATION MATRIX OF PARAMETERS

                      U           V           W
          U           1.000
          V           0.724       1.000
          W          -0.937      -0.443       1.000
```

Figure 15.5.2 Data and fitted line for the weed infestation problem.

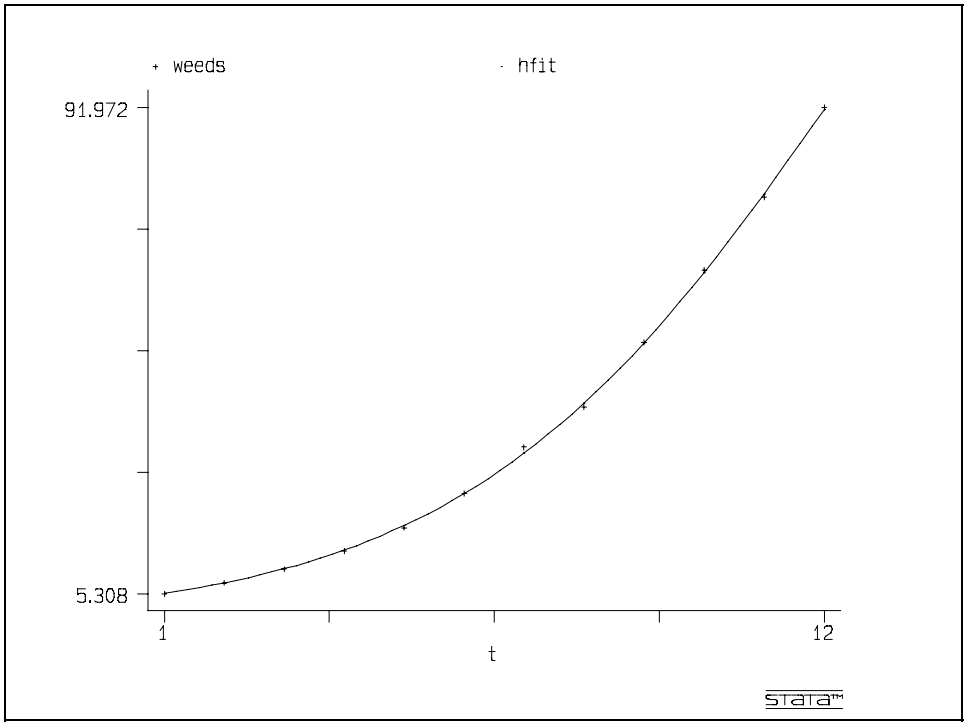


Figure 15.5.3 Solution of the weed infestation problem by the Nash / Marquardt method

```
DRIVER -- GENERAL PARAMETER ESTIMATION DRIVER
       - 851017,851128
       21:52:42      08-16-1992
HOBBSJ.JSD 3-PARAMETER LOGISTIC FUNCTION SETUP
       -  851017
 FUNCTION FORM
   =  100*B(1)/(1+10*B(2)*EXP(-0.1*B(3)*I))
HOBBSJ.JSD 3 parameter logistic fit
bounds on parameters for problem
 0  <=   b( 1 )  <=   100
 0  <=   b( 2 )  <=   100
 0  <=   b( 3 )  <=   30
ENTER INITIAL VALUES FOR PARAMETERS ([cr]=Y)
B( 1 )= 1
B( 2 )= 1
B( 3 )= 1
 are masks or bounds to be set or altered?
   ([cr] = no)
MRT -- MARQUARDT/NASH -- 860412
ITN 0   EVAL'N 1  SS= 10685.29
parameters   1    1    1
LAMDA =  .00004
LAMDA =  .0004
LAMDA =  .004
ITN 1   EVAL'N 4  SS= 1959.699
parameters   .8746042    2.324613    4.944148
LAMDA =  .0016
LAMDA =  .016
ITN 2   EVAL'N 6  SS= 1420.665
parameters   1.003532    2.440965    3.1544
LAMDA =  .0064
...
ITN 9   EVAL'N 13  SS= 2.587254
parameters   1.961861    4.909162    3.135698
LAMDA =  1.048576E-05
LAMDA =  1.048576E-04
LAMDA =  1.048576E-03
LAMDA =  1.048576E-02
  ELAPSED SECS= 4  AFTER 10  GRAD & 16 FN EVAL
CALCULATED FUNCTION MINIMUM =  2.587254
POST-SOLUTION ANALYSIS FOR MARQUARDT-NASH NLLS
SIGMA^2 = LOSS FUNCTION PER DEGREE OF FREEDOM
    = .2874726
PARAMETER CORRELATION ESTIMATES
ROW  1  :   1.00000
ROW  2  :   0.72030  1.00000
ROW  3  :  -0.93651 -0.43731  1.00000

SOLUTION WITH ERROR MEASURES AND GRADIENT OF
SUM OF SQUARES
B(1) = 1.961861 STD ERR = .1130655
    GRAD(1) =  6.923676E-04
B(2) = 4.909162 STD ERR = .1688398
    GRAD(2) = -1.842976E-04
B(3) = 3.135698 STD ERR = 6.863073E-02
    GRAD(3) =  8.602142E-04

radii of curvature for surface along axial
directions
  & tilt angle in degrees
for B( 1 )  R. OF CURV. =  1.580E-04
    tilt =   -0.06543
for B( 2 )  R. OF CURV. =  2.322E-03
    tilt =    2.01501
for B( 3 )  R. OF CURV. =  1.124E-04
    tilt =  -17.24985

RESIDUALS
 .011899 -3.275681E-02  9.203052E-02  .2087812
.3926354  -5.759049E-02  -1.105722    .7157898
-.1076469 -.3483887  .6525879 -.2875595
```

Figure 15.5.5 gives the MINITAB solution of the farm income problem. The results appear satisfactory, though we should check them by plotting residuals against predicted values and against the explanatory variables. From a statistician's perspective, we would want to plot the distribution of residuals and examine some extra information in the output, for instance, the small magnitude of the t-ratio for petroleum products, but we will not continue this discussion here.

For the height difference problem, MINITAB (Figure 15.5.6) unfortunately does not apparently get refined height differences. It gives a warning message The difficulty is that the matrix X is now singular because we have no "absolute zero" of height defined, and MINITAB has acted to resolve the lack of uniqueness in the solution. MATLAB is more revealing, as in Figure 15.5.7. Note that we have carried out the calculations from a file SURVEY.M created with a text editor. MATLAB warns us that the X matrix (called **A** here) is singular (that is, rank deficient). We regularize the MATLAB solution by subtracting b_1 from all the elements of $\boldsymbol{b}$. This is equivalent to making benchmark 1 the "zero" of height. Note that as part of our "solution" we compute residuals from the true heights of both our initial and final estimates, showing a reduction in the sum of squares from 0.0016 to 0.0006. We also compute the errors from the true (but normally unknown) heights used to create this problem. The error sum of squares is reduced from 0.0021 to 0.00065. Generally we will not be able to know how well we have done.

Figure 15.5.4 Hessian of the Hobbs weed growth nonlinear least squares problem for b^T = [200, 50, 0.3]

a) Scaled parameters

```
Initial parameters
 ?      2     5     3
Input scaling
 ?   100.0   10.0   0.1
 Hobbsf problem initiated
WARNING: sumsquares = 158.232   at b       2
  5     3
  H indefinite :   1.0e+004 *
    1.0314   -0.2561    1.2851
   -0.2561    0.0645   -0.3453
    1.2851   -0.3453    1.8578
  eigenvalues   1.0e+004 *
   -0.0017    0.0949    2.8606
End Warning
eigenvalues of analytic Hessian   1.0e+004 *
  -0.00170159022249
   0.09485456572052
   2.86059060485273
```

b) unscaled parameters

```
Initial parameters
 ?   200.0   50.0    0.3
Input scaling
 ?      1     1     1
 Hobbsf problem initiated
WARNING: sumsquares = 158.232   at b  200.0000
50.0000  0.3000
  H indefinite :   1.0e+006 *
    0.0000   -0.0000    0.0013
   -0.0000    0.0000   -0.0035
    0.0013   -0.0035    1.8578
  eigenvalues   1.0e+006 *
   -0.0000    0.0000    1.8578
End Warning
eigenvalues of analytic Hessian   1.0e+006 *
  -0.00000009216630
   0.00000026964909
   1.85779520216555
```

Figure 15.5.5 MINITAB output for the solution of the farm income problem (Table 15.1.1a)

```
 MTB > note REGDATA.XEC: regression of farm income index vs
 MTB > note    index of phosphate and petroleum use
 MTB > read c1-c3
      13 ROWS READ
 MTB > end data
 MTB > regress c3 on 2 c1 c2

 The regression equation is
 income = 299 + 0.557 phosfate - 0.599 petrol

 Predictor       Coef       Stdev    t-ratio        p
 Constant       299.0       179.3       1.67    0.126
 phosfate     0.55724     0.06422       8.68    0.000
 petrol       -0.5989      0.8955      -0.67    0.519

 s = 10.37       R-sq = 96.9%     R-sq(adj) = 96.3%

 Analysis of Variance
 SOURCE       DF          SS          MS         F        p
 Regression    2       34135       17067    158.77    0.000
 Error        10        1075         107
 Total        12       35210

 SOURCE       DF      SEQ SS
 phosfate      1       34087
 petrol        1          48
```

If we assume that the 4th coefficient in the MINITAB solution is zero and regularize, as with MATLAB, so that the first height is zero, we obtain heights at 0, 99.995, 121.015, and 96.02 meters (as we should!). We have simply subtracted -96.02 from each coefficient.

Finally, we may choose or be forced to solve the least squares problem iteratively by a technique specifically designed to minimize the sum of squares function. These techniques are finding growing importance in problems in statistics or geodesy where very large numbers of parameters $\boldsymbol{b}$ (into several thousands) must be estimated. Figure 15.5.8 shows the results of applying Nash J C (1990d), Algorithm 24 to this problem. Adding 79.2575 to all elements of the solution gives benchmark heights of 0, 99.995, 121.015, and 96.02 meters as anticipated.

Figure 15.5.6 Partial MINITAB output for the height difference problem 15.1.1b

```
MTB > exec 'survey.xec'
MTB > note MINITAB attempt to carry out
MTB > note Nash J C CNM2 Surveying example pg 240
MTB > note matrix defines which height differences are involved
MTB > read c1-c4
      5 ROWS READ
MTB > end data
MTB > note the measured height differences
MTB > set c5  (data is entered here)
MTB > end data
MTB > regr c5 on 4 c1-c4;
SUBC> noconstant.
*       C4 is highly correlated with other X variables
*       C4 has been removed from the equation

The regression equation is
C5 = - 96.0 C1 + 3.97 C2 + 25.0 C3

Predictor       Coef       Stdev    t-ratio        p
Noconstant
C1          -96.0200      0.0173   -5543.65    0.000
C2           3.97500     0.01369     290.29    0.000
C3           24.9950      0.0137    1825.35    0.000
s = 0.01732
```

Figure 15.5.7 Edited MATLAB output for the height difference problem. The names of matrices and vectors differ from those used in the text.

```
% Nash CNM2 Surveying example pg 240
% SURVEY.M
% matrix defines which height differences are
        involved
A = [ 1 -1  0  0;
      0  1 -1  0;
      0  0  1 -1;
      1  0 -1  0;
      0  1  0 -1]
% and the measured height differences
y =  [ -99.99; -21.03; 24.98; -121.02; 3.99]
% true values
btrue = [0; 100; 121; 96]
% compute current residuals from true
    differences
w=A*btrue
r=y-w = 0.0100 -0.0300 -0.0200 -0.0200
-0.0100
SS=r'*r = 0.0019
%initial estimates from first 3 data points
AA=A(1:3,1:3)
yy=y(1:3)
xx=AA\yy
xp=[xx;0]
xp=xp-ones(4,1)*xp(1)
xp = 0 99.9900 121.0200 96.0400
%errors
dd=xp-btrue
dd = 0 -0.0100 0.0200 0.0400
%sum of squares
dd'*dd =  0.0021
%residuals from initial estimates
r=y-A*xp = 0 0 -0.0000 0 0.0400
ss=r'*r =  0.0016
% solve, noting singularity
x = A\y
Warning: Rank deficient, rank = 3 tol =
1.9230e-015
x = -96.0200  3.9750 24.9950 0
w=A*x;
% residuals
r=y-w = 0.0050 -0.0100 -0.0150 -0.0050 0.0150
% and sum of squares
SS=r'*r =  6.0000e-004
% regularize solution
[n,k]=size(x);
z=x-x(1)*ones(n,1)=0 99.9950 121.0150  96.0200
w=A*z=-99.995 -21.02 24.995 -121.015 3.975
% residuals
r=y-w = 0.005 -0.01 -0.015 -0.005 0.015
% and sum of squares
SS=r'*r =  6.0000e-004
%errors
dd=z-btrue = 0 -0.0050 0.0150 0.0200
%sum of squares
dd'*dd =  6.5000e-004
```

Figure 15.5.8 Partial output of iterative method for height difference data, part (b) of Table 15.1.1.

```
dr24ls.pas -- linear least squares by conjugate gradients
1992/08/11 18:24:36
Number of rows in coefficient matrix = 5
Number of columns in coefficient matrix = 4
Matrixin.pas -- generate or input a real matrix 5 by 4
Row 1    1.00000   -1.00000    0.00000    0.00000
Row 2    0.00000    1.00000   -1.00000    0.00000
Row 3    0.00000    0.00000    1.00000   -1.00000
Row 4    1.00000    0.00000   -1.00000    0.00000
Row 5    0.00000    1.00000    0.00000   -1.00000
RHS vector
-9.9990E+01 -2.1030E+01  2.4980E+01 -1.2102E+02  3.9900E+00
Initial guess for solution -- all zeros
Normal equations -- coefficient matrix
   2.00000   -1.00000   -1.00000    0.00000
  -1.00000    3.00000   -1.00000   -1.00000
  -1.00000   -1.00000    3.00000   -1.00000
   0.00000   -1.00000   -1.00000    2.00000
Normal equations - RHS
-221.01000   82.95000  167.03000  -28.97000
Step too large -- coefficient matrix indefinite?
Solution after 4 iterations. Est. normal eqn. sumsquares -1.0000000000E+35
 -79.25750   20.73750   41.75750   16.76250
For original least squares problem -- Residuals
-5.000E-03  1.000E-02  1.500E-02  5.000E-03 -1.500E-02
Sum of squared residuals = 6.0000000025E-04
```

15.6 Assessment

For the growth curve problem, the choice among the four general styles of solution tool, that is, statistical package, spreadsheet add-in, special purpose program or package or general mathematical problem-solving environment, will depend on the user's familiarity with the tools, the expected number of times similar problems need to be solved, the additional output required, and the degree of difficulty the problem presents. For the weed data, bad scaling and the singularity of the Hessian means that usually good techniques, such as Newton's method, may fail or will appear inefficient. Supposedly inferior methods can make progress from points where a straightforward Newton method cannot go on. It is possible, of course, to adjust the Newton method to overcome such difficulties. However, the user must now cope with even more detail in the description of the method, without assistance of off-the-shelf software.

Chapter 16

Trajectories of Spacecraft

16.1 Problem statement
16.2 Formulations
16.3 Methods and Algorithms
16.4 Programs or Packages
16.5 Some solutions
16.6 Assessment

This chapter looks at the orbits spacecraft follow near the earth and moon. The problem is a good illustration of differential equation solution.

16.1 Problem Statement

Trajectories of spacecraft are an important class of problems that can be solved by numerical methods. Consider the problem of the Apollo capsule in the U.S. space program of the late 1960s. The system of interest involves the earth, moon, and the spacecraft. We will restrict our attention to trajectories in the plane of rotation of the moon about the earth to simplify our work (Figure 16.1.1).

16.2 Formulations

Forsythe, Malcolm, and Moler (1977, pg. 153-4) and Kahaner, Moler and Nash S G (1989, p. 333) present a version of this problem, but leave out important details of constants and units. The simplified problem is more difficult to relate to the real world, though the equations are simpler. Here we shall sketch a derivation of the appropriate equations based on classical mechanics (Synge and Griffith, 1959) that results in a set of linked ***first order ordinary differential equations***. There are starting values that give the speed and position of the spacecraft whose trajectory we wish to calculate, so this is an ***initial value problem***.

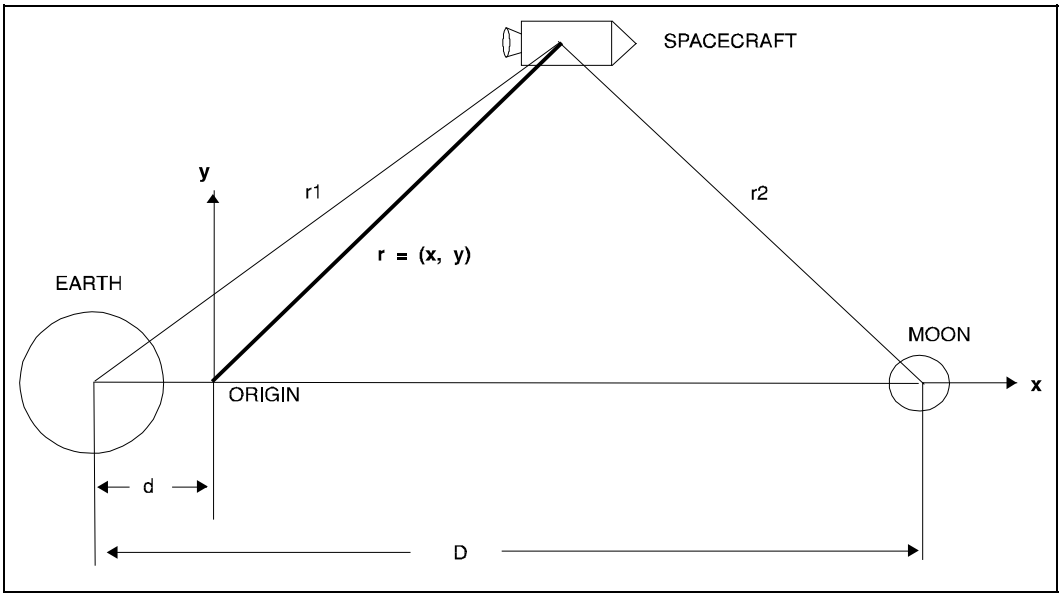
The trajectory is not necessarily a stable orbit (periodic trajectory). If we start with a periodic orbit and perturb them, algebraic eigenproblems are derived from the equations. Such a formulation is appropriate, for example, for earth orbits of artificial satellites influenced by moon gravitation and perturbations of planetary orbits by other planets.

The main equation is Newton's second law of motion

(16.2.1) $$\boldsymbol{F} = w\,\boldsymbol{a} = w\,d^2\boldsymbol{r}_s / dt^2$$

where $\boldsymbol{F}$ is the (vector) force acting on the spacecraft, w its mass (we shall use M and m for the masses of the earth and moon respectively). $\boldsymbol{a}$ is the spacecraft acceleration, and $\boldsymbol{r}_s$ its vector position in a stationary coordinate system. Time is represented by the variable t. We are more likely to be interested in motion of the spacecraft relative to the earth and moon, rather than some abstract but stationary (that is, non-accelerated) coordinate frame. The desired coordinates have these two "large" bodies fixed. In reality the earth-moon coordinate system is rotating, so we introduce corrections to the usual equation of motion 16.2.1. We choose as our coordinate system the rectangular axes in x, y, and z directions defined as follows. The x-axis is taken along the earth-moon line of centers. The y-axis is taken perpendicular to

Figure 16.1.1 Diagram showing the variables of the spacecraft system



the x-axis and lying in the plane of rotation of the earth and moon. The z-axis is taken to be the remaining perpendicular direction the angular velocity is a positive right-handed vector. That is, if the earth and moon are rotating anti-clockwise in the plane of the page, z is pointing up out of the paper).

The corrections to the equation of motion are called the Coriolis force and the centrifugal force. Our corrected equations of motion are

(16.2.2) $$w\, d^2\mathbf{r} / dt^2 = \mathbf{F} - w\,(\mathbf{a}_t + \mathbf{a}_c)$$

where $\mathbf{r}$ is the new position vector relative to the rotating axes, and $\mathbf{a}_t$ and $\mathbf{a}_c$ are the centrifugal and Coriolis accelerations respectively. In general, the vector quantities $\mathbf{a}_t$ and $\mathbf{a}_c$ are given as follows:

(16.2.3) $$\mathbf{a}_t = 2\,\Omega \times (d\mathbf{r}/dt)$$

where Ω (Greek capital omega) is the angular velocity of rotation of the coordinate system. Note the vector cross-product. Further, using a vector dot-product,

(16.2.4) $$\mathbf{a}_c = -\,\Omega^2\,\mathbf{r} + (d\Omega/dt) \times \mathbf{r} + \Omega\,(\Omega \cdot \mathbf{r})$$

By considering only trajectories in the plane of the earth-moon rotation, we greatly simplify these corrections. Consider the coordinates defined in Figure 16.1.1. Note that the earth has its center at $(-d, 0)$, the moon at $(D-d, 0)$, the spacecraft at (x,y). Newton's gravitation law gives the total gravitational force on the capsule as

(16.2.5) $$\mathbf{F} = -\,G\,w\,\{(M / r_1^2)\,\mathbf{i} + (m / r_2^2)\,\mathbf{j}\}$$

where $\mathbf{i}$ and $\mathbf{j}$ are the unit vectors along the earth-spacecraft and spacecraft-moon lines, $M \approx$ 5.977E+24 kg. and $m \approx$ 7.349E+22 kg. are the earth and moon masses, and $G \approx$ 6.6733E-11 $m^3\ kg^{-1}\ s^{-2}$ is the gravitational constant. The distance center-to-center from the earth to the moon is $D \approx$ 3.844E+8 m. The center of mass of the earth-moon system, which we use for our coordinate origin, is therefore at a distance $d \approx$ 4.669E+4 m from the center of the earth, and is actually inside the earth. The angular velocity of the earth-moon rotation $\Omega \approx$ 9.583E-3 hr^{-1} = 2.661E-6 s^{-1}. This gives a period $T = 2\,\pi / \Omega \approx$ 655.66 hrs ≈ 27.32 days (Tennent, 1971).

Combining and simplifying the equations yields the linked second order ordinary differential equations

(16.2.6a) $$d^2x/dt^2 = -GM(x+a)/r_1^3 - Gm(x-(D-a))/r_2^3 + \Omega^2 x + 2\Omega\, dy/dt = g_1(x, x', y, y', t)$$

(16.2.6b) $$d^2y/dt^2 = -GMy/r_1^3 - Gmy/r_2^3 + \Omega^2 y - 2\Omega\, dx/dt = g_2(x, x', y, y', t)$$

where we use the functions g_1 and g_2 as a shorthand for later equations.

16.3 Methods and Algorithms

Solution of equations (16.2.6) from an initial position with a known initial velocity (i.e., x, y, dx/dt, dy/dt known at $t=0$) is not always straightforward because programs and packages such as RKF45 (Forsythe, Malcolm and Moler, 1977) are designed to solve a set of first order differential equations. We can transform our pair of equations into four first-order ordinary differential equations (ODEs) by using new variables u and v

(16.3.1) $$u = x' \text{ and } v = y'$$

(16.3.2a) $$dx/dt = u$$

(16.3.2b) $$du/dt = g_1(x, u, y, v, t)$$

(16.3.2c) $$du/dt = v$$

(16.3.2d) $$du/dt = g_2(x, u, y, v, t)$$

We therefore need methods that handle either linked first or second order differential equations. There is a large literature on such problems (e.g., Kahaner, Moler, and Nash S G, 1989, Chapter 8).

16.4 Programs or Packages

The software tools for the solution of such a problem fall into three categories:

- Existing library subroutines or programs to which we supply our problem by means of custom program code;
- Problem solving environments of a general nature in which our particular problem is expressed in some algebraic language;
- Special-purpose software for the solution of differential equation problems.

The first approach was the only option as recently as 1980. For example, in 1983 we used a BASIC translation (by Kris Stewart) of the FORTRAN program RKF45 given in Forsythe, Malcolm and Moler (1977). The user has to write driver code and write or link to graphical routines.

The last approach, using special-purpose software, is clearly the least work for the user if the software is well-designed. Since spacecraft trajectories are needed by many agencies, such software likely exists, but access to it may be less easy to obtain. For the more general task of solving sets of differential equations we have examples like PLOD (PLotted solutions of Ordinary Differential equations, Kahaner et al., 1989). This package builds and executes FORTRAN programs from a description of the first order differential equations (16.3.2). The equations are entered almost as they appear, though we must also supply

expressions for the distances r_1 and r_2 as well as physical quantities that appear. PLOD lets this information be placed in a file for reuse. Figure 16.4.1 shows the file APOLC.MOD with the starting values

(16.4.1) $x = 461.28; y = 0.0; u = 0.0; v = -3.865412$

Figure 16.4.1 PLOD input file for Apollo spacecraft trajectories

```
APOLC.T
    Me = 5169.26643
    mm = 63.5585
    om = 9.5827E-03
    tmu = 379.73
    r1 = sqrt( (x + mu)**2 + y**2 )
    r2 = sqrt( (x - tmu)**2 + y**2 )
    x'=u
    y'=v
    u' =  2*om*v + x*om**2 - Me*(x+mu)/r1**3 - mm*(x-tmu)/r2**3
    v' = -2*om*u + y*om**2 - Me*y/r1**3 - mm*y/r2**3
```

16.5 Some solutions

Figure 16.5.1 shows a plot of the trajectory computed by PLOD for initial conditions (16.4.1). The PLOD input and output illustrate the "minor" but very annoying difficulties that accompany any real-world scientific problem. First, we must ensure all the constants in the equations are in consistent units. Attaching the units to all quantities and performing careful algebra with these and the conversion factors, we obtained the input in Figure 16.4.1. A second annoyance arose here — PLOD forced us to use distances and velocities expressed in terms of megameters (10^6 meters) because it would not accept the large numbers present when kilometers were used. A third annoyance is that PLOD does not appear to allow us to save high quality image information. Nor can we draw the earth and moon on the output or put labels on. Finally, while it is helpful to plot the position of the spacecraft at regular time intervals (to give us an idea of how fast the spacecraft is moving at different points along its trajectory), PLOD (and most other differential equation integrators) vary the integration time step for efficiency and error control. Thus we have a set of data (t, x, y) with irregular time steps.

Avoiding scale and numerical errors in input quantities is important. A spreadsheet or symbolic algebra package lets us perform unit conversion calculations. By making a program display the data that has been entered we may catch data storage "bugs". This is how we found that PLOD was "truncating" the large numbers for distances in kilometers.

Equispaced time points could be obtained by outputting the (t, x, y) data and using a separate interpolation and graphing package. For each new time point new_t, with two adjacent original time points such that

(16.5.1) $t_{i-1} <= new\_t < t_i$

a linear interpolation gives a corresponding approximate x value

(16.5.2) $new\_x = x_{i-1} + (x_i - x_{i-1}) * (new\_t - t_{i-1})/(t_i - t_{i-1})$

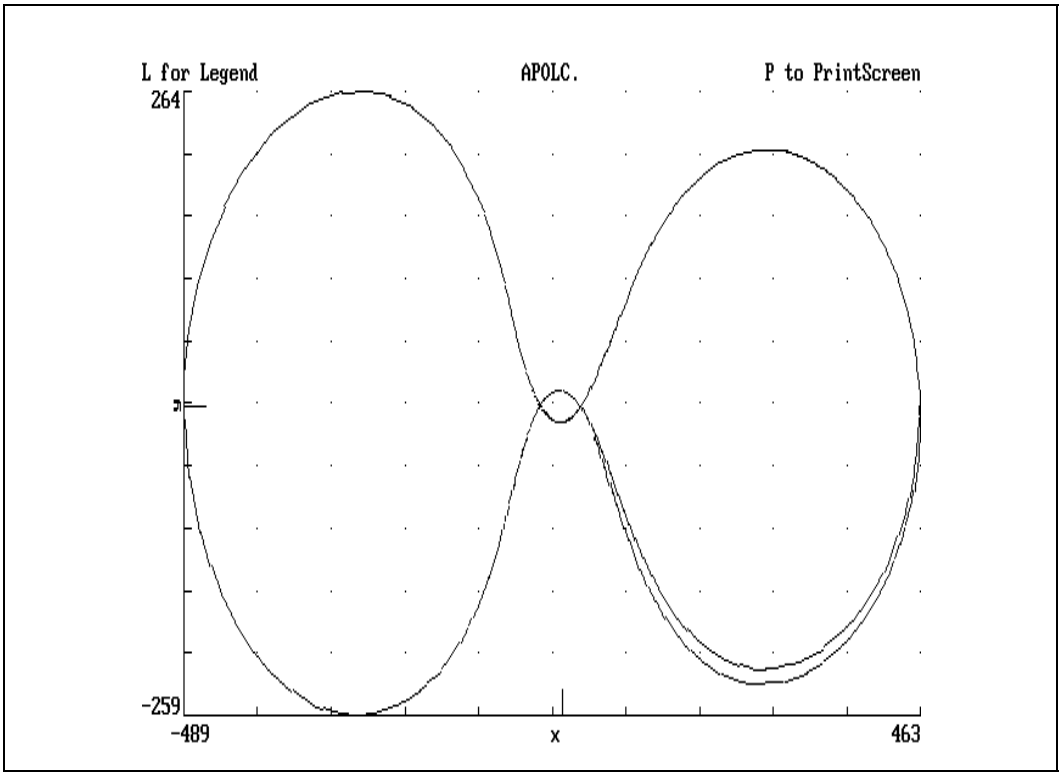
with similar expressions for any other output variables. In a program, check that the inequality 16.5.2 is truly satisfied, and avoid asking for time points outside the available data range. The linear interpolation does result in small but perceptible "jaggies" in the plot, but alternatives require more sophisticated programming. We do not show results here.

A different difficulty is illustrated if we choose to initialize the trajectory at the same place and direction but with a velocity of 5000 kilometers per hour. That is, the initial conditions are

(15.6.4) $x = 461.28; y = 0.0; u = 0.0; v = -5000$

Figure 16.5.2 shows the output from PLOD. Our second software choice, a problem solving environment,

Figure 16.5.1 PLOD screen plot for Apollo spacecraft trajectory from the starting point given as Equation 16.4.1.



lets us lets us understand the situation. Using the Student Edition of MATLAB, the setup and solution of our problem is only slightly more work than with PLOD. The MATLAB integrator (ode23) stopped at about T = 154 hours with the message "SUSPECTED SINGULARITY". Drawing the earth and moon on the MATLAB plot we see why in Figure 16.5.3.

16.6 Assessment

In this case study, we have not used special-purpose programs that directly carry out the trajectory calculation. Clearly, such an approach would be preferred if we had many calculations to perform, as long as the software were known to be reliable. We would not, for instance, want the program to compute a trajectory through the earth as PLOD did. That MATLAB found a singularity was likely accidental. What is more important is that the MATLAB plot of the trajectory includes the earth and moon. We could also have "programmed" MATLAB to perform the equispaced time point interpolation.

The lessons of this case may be summarized as follows.

- To relate the problem and its solutions to the real-world, use units algebra to carry quantities and conversion factors through the equations that make up the formulation.
- Check solutions with graphs that include real-world features.
- Extra features, such as the equispaced time points or high-quality output, may be important. Neither of the two examples here could produce graphs of better than screen-capture quality (the professional version of MATLAB has this capability).

Figure 16.5.2 Another PLOD Apollo spacecraft trajectory

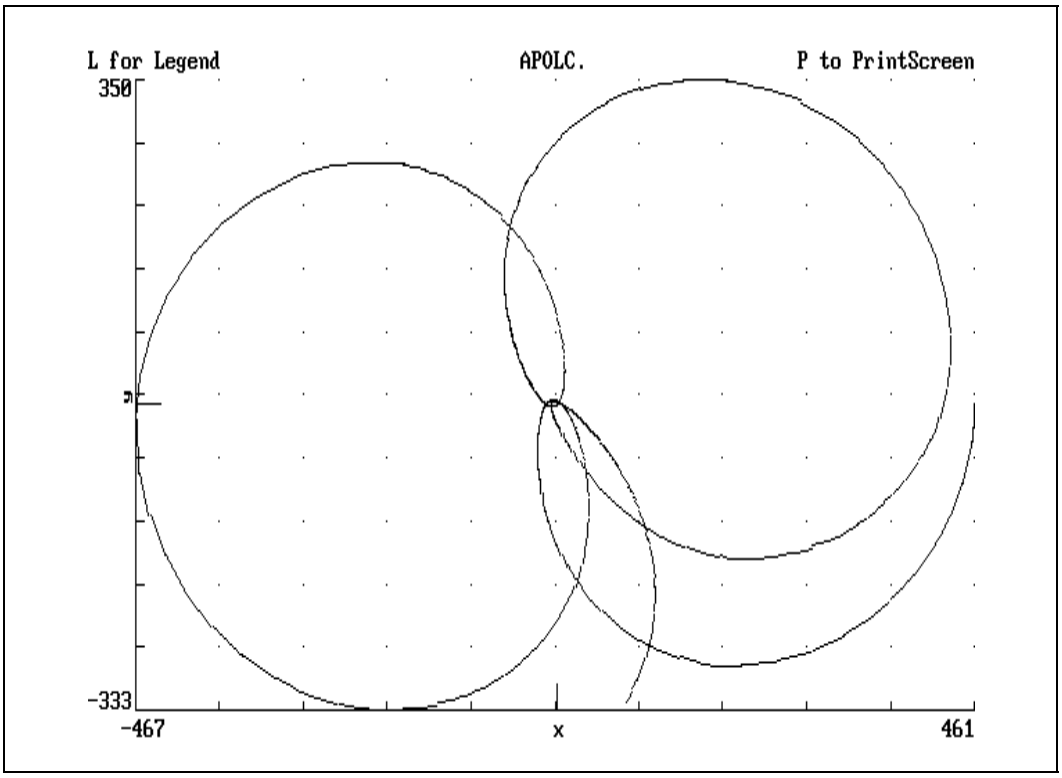
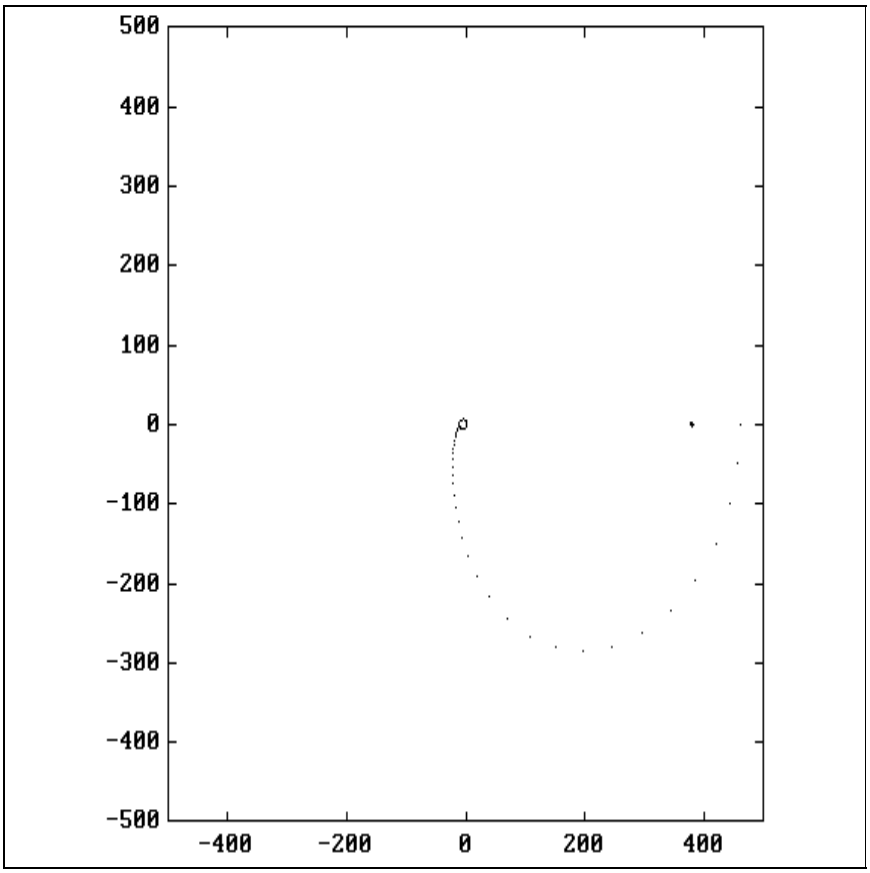


Figure 16.5.3 MATLAB version of the Figure 15.6.3



Chapter 17

Simulating a Hiring Process

17.1 Problem Statement
17.2 Formulations
17.3 Methods and Algorithms
17.4 Programs or Packages
17.5 Some solutions
17.6 Assessment

In this case study, we touch upon the elements that make up a computer simulation or Monte Carlo calculation.

17.1 Problem Statement

Many problems present themselves in ways that do not immediately suggest standard solution methods. Examples arise throughout the physical, biological and social sciences, as well as engineering and management. The "problem" may not be well-specified; indeed, a phenomenon may present itself only partially, so that clear objectives and understandings are impossible. Simulation allows explicit inclusion of knowledge that does not lead to an analytic (i.e., calculus or algebra) solution to the problem. Scenario rules are written down and actually followed through to see what happens. The approach also finds formal expression in ***resampling methods*** in modern statistical estimation.

This "trying out" of ideas relating to problems does not lead to a true solution. Typically we simply want to understand the processes better, but simulations may give a very good picture of what is going. For example, a simulation of the operation of an insurance scheme may allow the premium and regulations to be set using optimization techniques. A simplified example appears in Nash J C (1990d), pp. 165-167.

Our example here considers the hiring of people for several jobs where the employer is thought to discriminate against a specific group of candidates. In our simplified treatment we make only cursory reference to the large literature on this subject. The hiring process is quite difficult to model in detail. Some factors that come into play are the number of jobs available, how the employer discriminates for or against candidates who are members of particular groups, the awareness of candidates of the availability of jobs, perceived policies or conditions of work that may discourage applicants who are members of certain groups, mechanisms used to process applications, and interview / selection procedures.

17.2 Formulations

To simplify our task in simulating the hiring process, we make the following assumptions. First, the population is considered to be made up of only two groups, A and B. Let $P(A)$ be the population proportion of group A, so that $(1-P(A))$ is the proportion of B's. In reality a candidate may belong to several groups (black / white, male / female, anglophone / francophone, college-educated / not college-educated).

Second, the relative odds that an A gets a job compared to a B are

(17.2.1) $d = P(Job \mid A) / P(Job \mid B)$

$P(Job \mid B)$ is the conditional probability a type B candidate gets a job. Fixing d implies a constant policy of "discrimination" by the employer, who does not change his hiring methods or attitudes during the period of our study. Note that d can include factors beyond the employer's control that influence the relative likelihood A's or B's get jobs. The "discrimination" may be unintended.

Third, we assume that the employer fixes his number of jobs available as n and pursues the hiring process until all positions are filled. We ignore the possibility of disappointing candidates or lack of applications.

Fourth, the hiring process will be considered to be a single stochastic trial for the candidate. This ignores the reality that the candidate may withdraw when he is discouraged by a long application form, that he may not get an interview because his application appears weak, or similar occurrences that imply that the process has more than one stage at which selection / rejection can occur.

Finally, in our simulation we fix the chance that an "average" candidate gets a job as $P(Job)$, despite group membership. Using d, we find the probabilities members of each group get jobs as

(17.2.2) $P(Job \mid A) = P(Job)\, d / (1 + (d-1)\, P(A))$

(17.2.3) $P(Job \mid B) = P(Job) / (1 + (d-1)\, P(A))$

We want, given the notation and assumptions above, to derive the probability distribution of the number of candidates $succA$ of type A who get a job. This will vary with n jobs available, $P(A)$ fraction of A's in the population, d relative chances of A getting a job compared to B, and $P(Job)$ average chance of getting hired. That is, there are four dimensions in which we can vary the "world" we simulate. Besides $succA$, the number of A's who get jobs out of the n available, we could look at $succB$, the number of B's who are hired (this is $n - succA$ in each trial, but the distribution may have a different shape), $apply$, the total number of candidates who present themselves before all n jobs are filled, and the partitioning of this into A and B subsets, namely, $applA$ and $applB$.

It may be possible to derive analytic expressions for these distributions. If there are not two groupings, but merely n jobs available with $P(Job)$ chance that an individual applicant gets one, the distribution of the number of applicants follows the Pascal distribution, while the number of rejected candidates follows the Negative Binomial distribution (see Hastings and Peacock, 1975). Under more complicated assumptions, such as those of the previous section, analytic results do not appear obvious and we will use simulation to approximate them.

17.3 Methods and Algorithms

The essentials of simulation are a set of rules by which our system or phenomenon is assumed to operate, a mechanism for translating these rules into mathematical or algorithmic form, tools for generating random numbers corresponding to the uncertainties that influence outcomes, and ways of analyzing the results of operating the simulation several times.

The most technically awkward of these requirements is generating the random numbers. Where real data is available, we can use files of such data. Central statistical agencies have started to offer special files of micro-data drawn from their extensive survey and census information (e.g., Keller and Bethlehem, 1992, and related papers).

Without "real" data files, we must generate the numbers. Though hardware devices do exist, only the most specialized of applications will use them. Software pseudo-random number generators are common, but some have grave deficiencies (Park and Miller, 1988). Most provide sequences of uniformly distributed

pseudo-random numbers on the unit interval, that is between 0 and 1. Sometimes 0 or 1 or both may be left out of the sequence. The generation mechanisms are such that the number sequence will eventually repeat. There may also be patterns, even if difficult to detect, that may be important if we use a single generator to produce values first for one variable, then another, and so on. Successive values for a variable are drawn a fixed number of positions apart in the pseudo-random sequence, and may turn out to be correlated. This difficulty is reduced in linear congruential generators if their period is long, the justification for generators such as that in Nash J C, Sande and Young (1984) and Wichmann and Hill (1987).

If we need numbers distributed from other than a uniform distribution on [0,1), these are usually created by transformation of uniform random numbers (Dagpunar, 1988). We specify the interval to include zero but not one. Users should be cautious of such details in making transformations.

The set of rules by which our hiring process operates can be written down and embedded in a simulation to obtain the distribution of outcomes. We conduct "experiments" that trace applicants through the system. Figure 17.3.1 shows the possible paths. At the nodes of this tree, random numbers will be used to decide the path to be taken. All random numbers are drawn from a uniform distribution on the unit interval [0, 1), so approximate probabilities reasonably well.

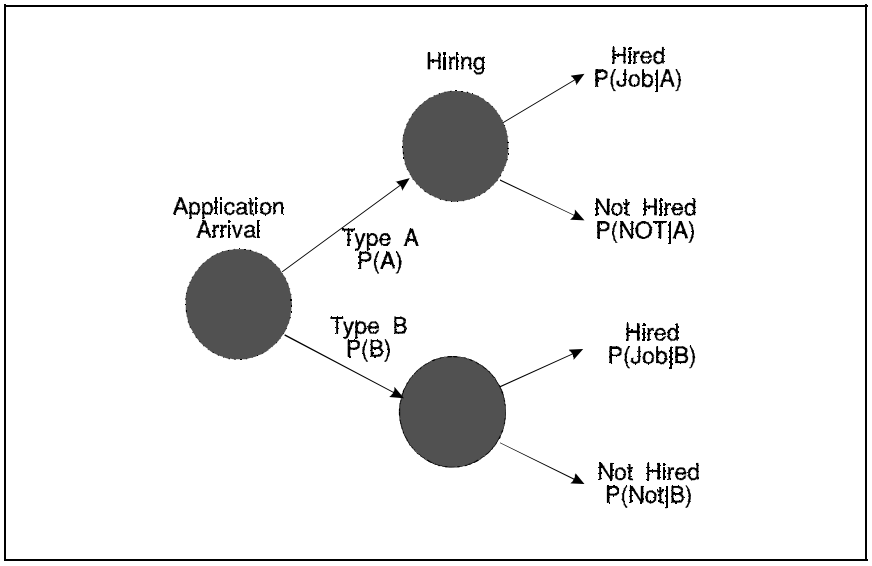
Repeat until all jobs filled:

Step 1: Applicant is presented. A random number $R1$ is drawn.
If $R1>P(A)$, applicant is a B, else an A.

Step 2: A random number $R2$ is drawn.
a. If applicant is an A, and $R2 > P(Job \mid A)$, then reject applicant; otherwise hire applicant.
b. If applicant is a B, and $R2 > P(Job \mid B)$, then reject applicant; otherwise hire applicant.

The distribution of outcomes can only be obtained after conducting a number of trials. For each set of input parameters of interest we will conduct M trials. M should be large enough to draw a sufficiently precise picture of the distribution. Note that we can conduct several experiments, look at the results, then carry out some more simulations and aggregate the results with the first set. Indeed, much of the programming effort in simulation is to keep results in a form that allows its later use, even if the exact manner of use is not known in advance. There are techniques for reducing the size of M in simulations

Figure 17.3.1 Events and their relationship in the hiring process as idealized by our assumptions.



(Hammersley and Handscomb, 1964). Here, however, we will only use direct simulation. More advanced techniques are needed when adequate approximations to desired results cannot be obtained quickly enough.

17.4 Programs or Packages

With the formulation and methods now settled, we can implement our simulation. A decade ago, such computations were performed in an early Microsoft BASIC on an Osborne 1 computer, and even though various simulation packages exist, we believe that ordinary programming languages are still a straightforward choice for performing the simulation calculations. We used Turbo Pascal for the examples below. A technical concern may be the quality of the built-in random number generator. We could use other routines (e.g., that of Wichmann and Hill, 1987). In programming the simulation itself, the program may not do what we intend because there is no natural cross-checking mechanism, so it is easy to code a different set of rules from that intended.

17.5 Some Solutions

Figure 17.5.1 presents the distributions of numbers of successful A and B job-seekers when there are 4 jobs open. A's form 30% of the population, but have a 4 to 1 better "luck" in getting hired. The average probability of being hired is 20%. The figure shows that the "discrimination" in favor of the A's gives them numerical dominance in the people eventually hired. We used $M = 1000$, that is 1000 trials, which gave an execution time of about 10 seconds on our 33 MHz PC. We used the random-number generator internal to Turbo Pascal in our calculations.

Figure 17.5.2 presents the distributions of applicants from each group and in total. Here we see that the bulk of the distribution of the A's is to the left. This implies that there are fewer A's trying for the jobs because they have a greater chance of filling them.

An aspect of the implementation that is important is that our simulation program generates a dataset ready for use by the statistical package **Stata** so that we could easily draw the figures. We have used **Stata**'s capability of drawing spline curves through sets of points in Figure 17.5.2 to bring out the visual aspects of the distribution. We believe that a major difficulty in using simulation is the choice and development of suitable techniques for displaying results in a convenient yet informative way. Such reporting tools are a help in verifying the correctness of the simulation code and in learning about the system under study.

In checking our simulation program, we found it useful to compute the Pascal distribution. That is, we calculated the probability there would be x applicants for n jobs when the probability an individual candidate is successful is $P(J)$. Setting $d=1$ (i.e., A and B candidates have equal chances) allows a check on the simulator to be carried out using a goodness-of-fit test.

17.6 Assessment

Clearly the simulation task is as large as we wish to make it. Here we shall be content with the brief description so far presented as a sample of the type of study that may be carried out with a PC.

Figure 17.5.1 Distributions of successful A and B candidates when 4 jobs are available, A's make up 30% of the population but have a 4:1 better chance of being hired than B's, and the average success rate is 20%.

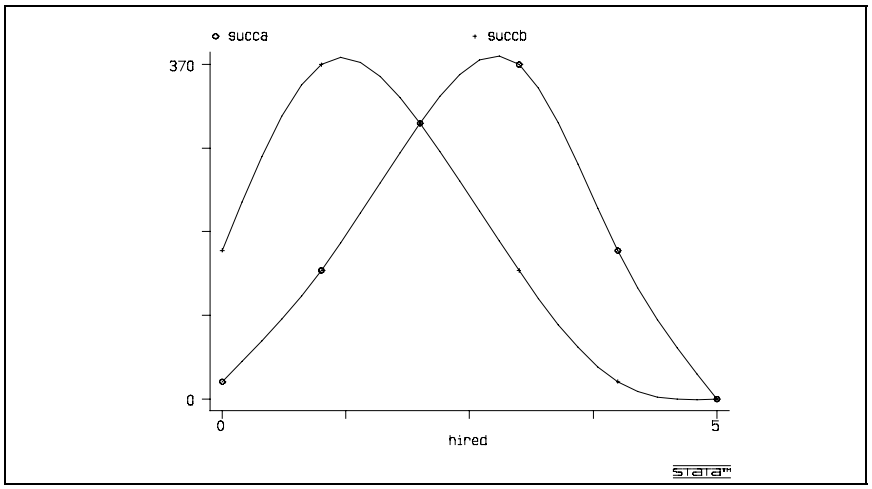
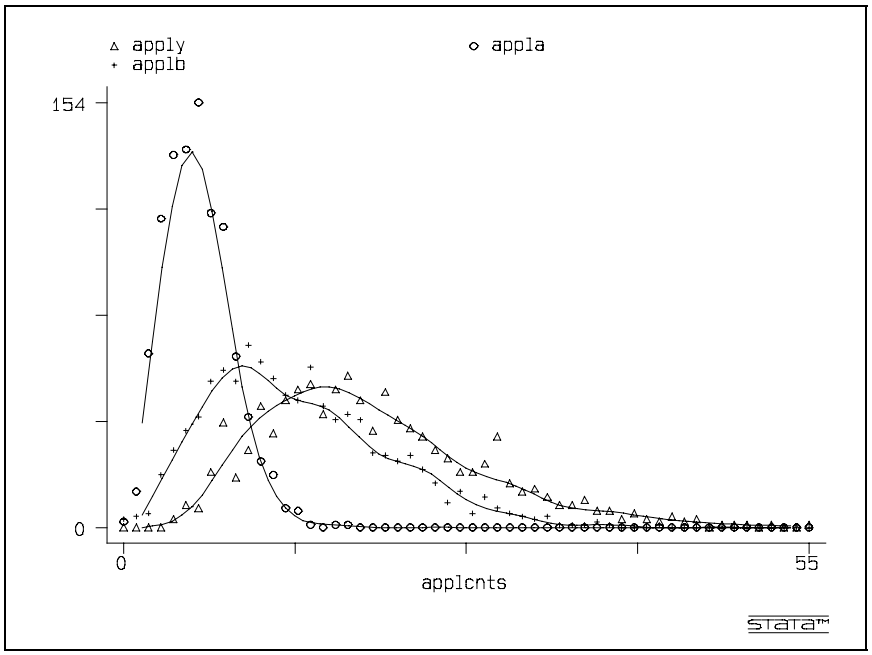


Figure 17.5.2 Distributions of applicants (total, A and B) when 4 jobs are available, A's make up 30% of the population but have a 4:1 better chance of being hired than B's, and the average success rate is 20%.



Chapter 18

A Program Efficiency Study: the Cholesky Decomposition

18.1 Purpose of the study
18.2 The programs and systems compared
18.3 Measuring the differences
18.4 Program sizes and compiler options
18.5 Time differences from program alternatives
18.6 Compiler and arithmetic influences
18.7 Processor and configuration time differences

In this chapter we conduct a study of the performance of three variants of a single algorithm as programmed in several programming languages. A variety of language translators and several computing platforms are used. The variability of computing times and storage requirements to carry out the ***same*** computation is surprising. We will repeat this point for emphasis — the computations are ***equivalent***. Minor organizational changes in the algorithms make demonstrably important differences in the resulting programs and their performance.

18.1 Purpose of the Study

This performance study serves as a warning that claims about the relative efficiency of algorithms should be suspect until proven by tests. We follow recommendations made in earlier chapters that results and performance of programs be verified ***on the target machine***. This is particularly important when a program is to be used heavily or in a situation where erroneous results have an unacceptable cost.

In what follows we will use three slightly different organizations of the ***same*** computational algorithm. The example we use is the Cholesky decomposition, and the three algorithms perform essentially the same computational operations on the matrix elements. The differences in the algorithms are mainly in the way the matrix ***indices*** are developed. Beyond the algorithmic differences we shall look at:

- Differences across programming languages;
- Differences between compilers or interpreters for a single language;
- Differences across arithmetic libraries and compiler options within a single compiler;
- Differences across computing platforms;
- The effects of special hardware, in particular, numeric co-processors
- Timing effects of operational choices, such as the (active) presence of communications facilities or screen blanking programs in the PC.

Along the way, we will note some annoying "glitches" we encountered in carrying out the timings and evaluations.

The main points to be be learned from these Cholesky timings are:

- Programming style has a large effect on execution timing and program size.

- Intuitive ideas of program changes that may speed execution can be incorrect. Experience in one computing environment may not carry over to another.
- Actual timings must be carried out whenever changes are made in the code or computing environment if effects on execution time could be important.

The methods in this study are useful whenever performance becomes critical. For example, the Cholesky decomposition is commonly employed inside many algorithms in optimization and data approximation. If such calculations are required in a real-time or otherwise time-critical application, performance measurement will likely be necessary.

18.2 The Programs and Systems Compared

The Cholesky decomposition of a symmetric positive definite matrix A computes a lower triangular factor L such that

(18.2.1) $$A = L L^T$$

This decomposition can be organized in many ways. Two of the present codes develop the elements of L row by row (row-wise organization), but it is just as simple to develop columnwise variants, and our third code is an example. We will outline the computations briefly to show that they are really quite straightforward, which underlines why the variety of results is so surprising.

First, we note that Equation 18.2.1 can be rewritten in terms of the individual matrix elements, that is,

(18.2.2) $$A_{ij}$$

where we have already taken account of the transposition of L in the product. The key point to note is that the summation, because of the triangular structure of the matrices, only comprises $min(i,j)$ terms. Thus we can immediately find

(18.2.3) $$A_{11} = L_{11}^2$$

The 1,1 element of L is defined as the square root of the corresponding element of A. (The positive definite property of A ensures that this is possible.) Now that L_{11} is known, we can find all the other elements in column 1 of L from

(18.2.4) $$A_{i1} = L_{i1} L_{11}$$

which is a direct result of Equation 18.2.2. If we use Equation 18.2.4 immediately in our program to store the elements L_{i1}, a column-wise organization of the decomposition results. In the row-wise variants of the algorithm, however, we will use Equation 18.2.4 to compute L_{21} only. Once this element is computed, we then use Equation 18.2.2 to get

(18.2.5) $$L_{22}^2 = A_{22} - L_{21}^2$$

Again, because A is positive-definite, this is always possible. To guard against the possibility that rounding errors or inappropriate input render the computed matrix A indefinite, we perform a test that the right hand side of Equation 18.2.5 is positive before taking the square root. If the test fails, then the decomposition has also failed; our codes should report this.

The process of developing L from A proceeds row by row in this organization. Algorithmically, there are some very important considerations that we should note. First, the elements of A are not needed once the corresponding elements of L are computed. Second, because A is symmetric, only a lower triangle of it need be stored. Third, a triangular matrix structure is not provided by any common programming language, so it is more convenient to store A and L in a single ***vector*** of elements. If A and L are of order

n, then the storage vector needed for our program is of length $n*(n+1)/2$. We will call this vector a, and the rule for accessing elements in A and L is that we read our matrix row-wise, that is,

(18.2.6) $$a_{(i*(i-1)/2 + j)} = A_{ij}$$

The indices for $a()$ are thus in the following positions in A or L:

```
1
2  3
4  5  6
7  8  9  10
```

and so on.

Figures 18.2.1, 18.2.2 and 18.2.3 show the FORTRAN code for three different implementations of the Cholesky algorithm. BASIC, PASCAL and C versions of these three codes were prepared by direct translation of programming language structures. Later in the chapter in Table 18.5.2 we summarize execution times, while Table 18.5.1 presents the relative execution rates of the Price and Healy variants to the Nash codes, and various measures of size and performance are presented in graphs.

Figure 18.2.1 Nash J C (1990d) variant of the Cholesky decomposition (FORTRAN)

```
      SUBROUTINE NCHOL(A,N2,N,IFL)
C NASH
      LOGICAL IFL
      DIMENSION A(N2)
      IFL=.FALSE.
      DO 20 J=1,N
      L=J*(J+1)/2
      IF(J.EQ.1) GO TO 11
      J1=J-1
      DO 10 I=J,N
      L2=I*(I-1)/2+J
      S=A(L2)
      DO 5 K=1,J1
      L2K=L2-K
      LK=L-K
      S=S-A(L2K)*A(LK)
5     CONTINUE
      A(L2)=S
10    CONTINUE
11    IF(A(L).LE.0.0) GO TO 21
      S=SQRT(A(L))
      DO 19 I=J,N
      L2=I*(I-1)/2+J
      A(L2)=A(L2)/S
19    CONTINUE
20    CONTINUE
      RETURN
21    IFL=.TRUE.
      RETURN
      END
```

Figure 18.2.2 Price implementation of the Cholesky decomposition

```
      SUBROUTINE PCHOL(A,N2,N,IFL)
C PRICE
      LOGICAL IFL
      DIMENSION A(N2)
      IFL=.FALSE.
      J2=0
      DO 20 J1=1,N
      I2=J2
      DO 10 I1=J1,N
      L=I2+J1
      S=A(L)
      J=1
4     IF(J.EQ.J1) GO TO 5
      K=I2+J
      M=J2+J
      S=S-A(K)*A(M)
      J=J+1
      GOTO 4
5     IF(I1.EQ.J1) GO TO 6
      A(L)=S/T
      GO TO 7
6     IF(S.LE.0.0) GO TO 21
      T=SQRT(S)
      A(L)=T
7     I2=I2+I1
10    CONTINUE
      J2=J2+J1
20    CONTINUE
      RETURN
21    IFL=.TRUE.
      RETURN
      END
```

Figure 18.2.3 Listing of the Healy (1968) variant of the Cholesky decomposition

```
      SUBROUTINE HCHOL(A,N2,N,IFL)
C HEALY
      LOGICAL IFL
      DIMENSION A(N2)
      IFL=.FALSE.
      J=1
      K=0
      DO 10 ICOL=1,N
      L=0
      DO 11 IROW=1,ICOL
      K=K+1
      W=A(K)
      M=J
      DO 12 I=1,IROW
      L=L+1
      IF(I.EQ.IROW) GO TO 13
      W=W-A(L)*A(M)
      M=M+1
12    CONTINUE
13    IF(IROW.EQ.ICOL) GO TO 14
      IF(A(L).LE.0.0) GO TO 21
      A(K)=W/A(L)
11    CONTINUE
14    IF(W.LE.0.0) GO TO 21
      A(K)=SQRT(W)
      J=J+ICOL
10    CONTINUE
      RETURN
21    IFL=.TRUE.
      RETURN
      END
```

The method and algorithm are essentially the same for all three codes. The storage mechanism is a row-wise single vector holding a triangular array. The same equations are used to calculate the elements of L but Nash and Price compute L row by row, while Healy does it column-wise.

The differences between the codes are in their looping controls and in how they get the storage vector index for a particular element of the matrix. The Nash code (Nash J C, 1990d, Algorithm 7) uses the formula

(18.2.7) $$k = i\ (i-1)\ /\ 2 + j$$

to give the storage vector index k corresponding to the i,j element of the matrix A, as we have shown above. The Healy (1968) code and the Price code (personal communication from Kevin Price, a colleague and friend) attempt to avoid the arithmetic involved in Equation 18.2.7 by careful organization of the program. The devices used are discussed partially in Quittner (1977), pages 324.327. In the late 1960s and early 1970s it was common to try to save execution (CPU) time in this way. For the IBM (mainframe) FORTRAN G1 compiler and to some extent for various other computing environments, it is clear such efforts may be useful.

Unfortunately, many PCs and language processors do not behave as anticipated by the Price and Healy codes. The straightforward approach used in the Nash variant then has the advantage of being more directly comprehensible to readers and programmers. Sometimes it turns out to be more efficient, sometimes remarkably so, while in other instances the differences in efficiency may not warrant the attention to detail needed to avoid the index calculation. Our advice, which will be repeated, is that if timing is critical, then measurements must be made for the particular situation in which the computations are important.

Over the years, we have attempted to compare these programs and their variants in other programming languages on a diverse computers. Table 18.2.1 lists some we have looked at.

18.3 Measuring the Differences

Elapsed time for either execution or compilation / linking is the main measure we will be comparing here, with program size a second quantity of interest. Measurement of elapsed time may be non-trivial for several reasons discussed in Section 8.6. Some relevant points follow.

- We want to measure only times for the program code of interest. Other processes active in our PC may interfere, for example, background tasks, disk activity, or time-shared programs. In these Cholesky timings, all PCs had a screen-blanker program to blank the screen after three minutes of no keyboard activity. We sometimes forgot to disable the fax-modem program watching for incoming facsimile messages in one PC (this is noted where it happened).
- Some compilers / interpreters do not allow direct measurement of elapsed time ***within*** a program, for example Microsoft Fortran version 3.2 and Turbo Pascal version 3.01a on MS-DOS computers. Using TIMER (Figure 8.6.1), we timed separate programs for each variant of the Cholesky algorithm and for each matrix order 10, 20, 30, 40 and 50. We also timed the codes ***without*** the decomposition to measure time for program loading, building of the test matrix and reporting of results.
- To minimize human effort, control of timing is carried out using batch command files in the MS-DOS environments. As there may be delays reading and executing such files, we store all the codes to be tested and also the batch files on RAM-disk to minimize input-output times that might create uncertainty in our timings.
- Some timings, performed a long time ago on obsolete machines, are included to illustrate that the issues presented have been a continuing concern in matters of program and algorithm efficiency.
- Near the end of the timing study, we changed versions of the MS-DOS operating system from 3.3 to

5.0 to accommodate the installation of a local area network. There may be subtle effects on the timings due to this change. The network was disabled for timings.

- Occasionally there are results that seem to make no sense at all. For example, the 1980 timing for decomposing an order 35 matrix on the Terak machine was 11.11 seconds, while order 30 took 11.88 seconds. We did not see anything this bizarre in the recent timings.
- The discipline required to record all details for each timing exercise is such that we had to repeat some timings.

For our purposes, we have chosen to find the Cholesky decomposition of the Moler matrix (Nash J C, 1990d, p. 253). This matrix has the elements

(18.3.1) $A_{ij} = i$ for $i = j$
$A_{ij} = min(i,j) - 2$ otherwise

Table 18.2.1 Computers and programming environments used in Cholesky algorithm timing comparisons.

I) timings pre-1984

machine	**programming environment and options**
Control Data Cyber 74	FTN compiler, opt=0,1,2
IBM System 370/168	Fortran HX, OPT=2, single precision
	Fortran G1, single precision
Sperry Univac 1108	FOR
Hewlett-Packard 3000	FORTGO
Terak LSI/11	UCSD PASCAL
Data General Eclipse	Extended BASIC
Imsai Z80	14 digit CBASIC
(courtesy K. Stewart)	14 digit North Star Basic
North Star Horizon	8 digit BASIC
	8 digit FPBASIC, proprietary co-processor
	14 digit FPBASIC, proprietary co-processor

II) 1992 tests

Macintosh SE	*True BASIC*

For the MS-DOS PCs listed, most computing environments were employed across the systems except where noted. As there are many options, not all will be listed here.

machines: 286 = 12 MHz Intel 286/8 MHz Intel 80287 (286)
NBK = Eurocom Notebook (Intel 80386DX 33Mhz, ULSI 80387)
V20 = NEC V20 with Intel 8087 (V20)
386 = 33 MHz Intel 80386DX/80387 with 64K cache (386)

programming environments:

Microsoft Basic 6.0
Borland Turbo BASIC 1.1
True BASIC 3.04 (PC)
Microsoft GW Basic 3.23 interpreter
Microsoft Fortran 3.2
Lahey Fortran F77L 3.01
Microsoft Fortran 4.10
Microsoft Fortran 5.10[++]
Silicon Valley Systems 2.8.1b[++]
Borland Turbo Pascal 3.01a
Borland Turbo Pascal 5.0
Borland Turbo Pascal 5.5
Borland Turbo Pascal for Windows (1991)
Microsoft Quick C 2.5
Turbo C++ 2.0[**]

[**] Note: Turbo C++ and Borland C++ are different products.
[++] compiled by Gordon Sande

Thus the order 5 Moler matrix is

```
 1  -1  -1  -1  -1
-1   2   0   0   0
-1   0   3   1   1
-1   0   1   4   2
-1   0   1   2   5
```

The Cholesky decomposition of this matrix is given by the matrix L having elements that follow the formulas

$$L_{ij} = \begin{cases} 1 & \text{for } j = i \\ 0 & \text{for } j > i \\ -1 & \text{for } j < i \end{cases} \qquad (18.3.2)$$

Thus, for order 5, we have the triangular matrix

```
 1
-1   1
-1  -1   1
-1  -1  -1   1
-1  -1  -1  -1   1
```

18.4 Program Sizes and Compiler Options

Novice users of PCs are frequently surprised at the very large differences between the sizes of programs that ostensibly perform the same tasks. Table 18.3.1 presents a summary of source and execution program sizes for the Cholesky decomposition timing codes in FORTRAN, BASIC, PASCAL and C. We have removed most of the commentary from the source code to avoid hiding the true underlying sizes. We have also removed right hand blanks, but made no effort to minimize program line indentation, as this would render the codes less readable. In any event, readers will see that the programs are relatively "small". The source programs were compiled and linked, and the table shows a summary of the executable program sizes. Occasionally a single compiler allowed several variants of the executable program to be created by various settings of compiler or linker options.

Table 18.4.1 also shows a summary of the size of compressed or DIETed executables (Section 5.5). We have use the compressor DIET (by Teddy Matsumoto) that replaces the executable program with its compressed equivalent. Out of the 20 executables listed here, two compiled with the Silicon Valley Systems compiler could not be compressed by DIET. The Turbo Pascal for Windows program would not run after compression. (The latter program must be run in the Microsoft Windows environment, so anticipates a different program loader.)

Table 18.4.1 Source and executable program sizes for the Cholesky timing tests.

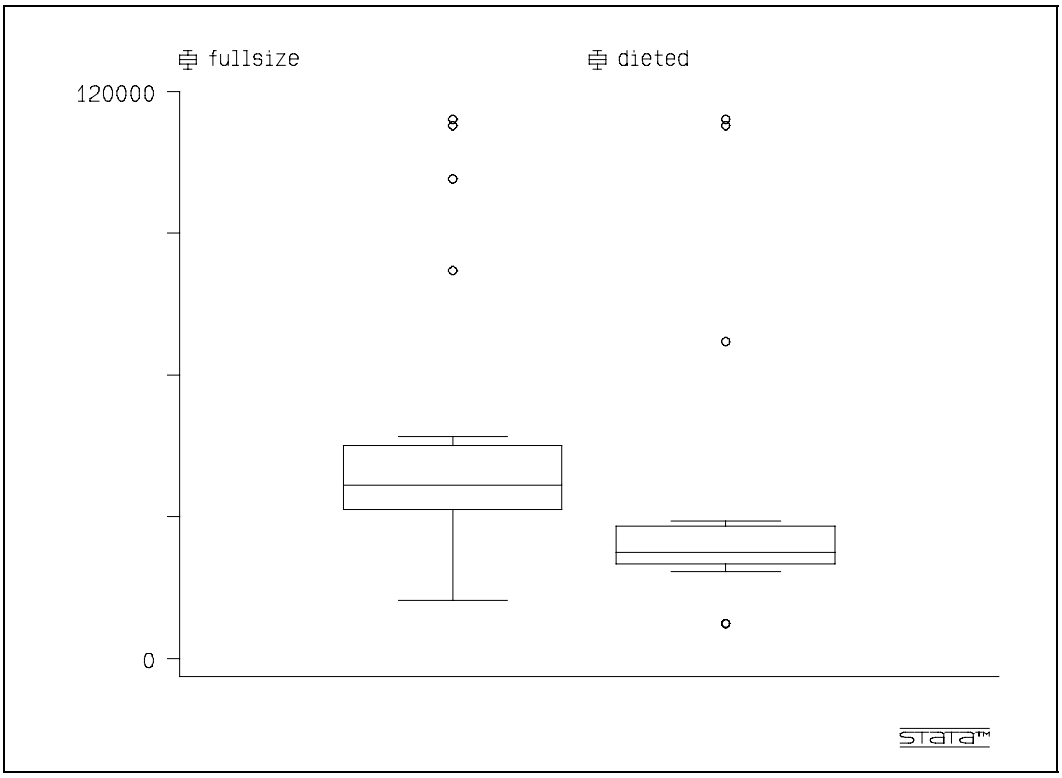
a) Source codes

	bytes	lines
CHOLTEST.BAS	3625	157
CHOLTEST.C	5173	256
CHOLTEST.FOR	4064	182
CHOLTEST.PAS	5694	251

b) Executable codes -- summary statistics

	Mean	StDev.	Min	Max
Size (bytes)	46501.35	30805.2	12240	114072
DIETed	32847.8	29925.29	7349	114072
ratio	.67569	.1658055	.3536	1

Figure 18.4.1 Boxplot showing variability in executable program sizes for the Cholesky tests.



To give a better idea of the program size variability, we can also use boxplots of the full and compressed executable sizes. These are presented in Figure 18.4.1. From the summary table and the graph, we see:

- That executable program sizes vary largely;
- That compression can save space, which is useful if we are trying to pack a set of files onto as few distribution diskettes as possible.

The variability of the executable program sizes is in part due to the manner in which different programming environments store the arrays for the matrices A or L. Note that if we were to store a square matrix of order 50 using 8 bytes per element, we would need 20,000 bytes of storage. Even the lower triangle requires 10,200 bytes. If the executable program includes ***explicit*** space for the array(s), then the file will be correspondingly larger. Since this space is simply a clean blackboard for working on, we could find the memory required at run time. This allows smaller executable files, though at the small risk of a program load failure if there is not enough memory available for the arrays.

Another source of "extra" program size is the mechanism used by different compilers for attaching (linking) the commonly needed pieces of program code to perform arithmetic, input-output, or special functions. This ***run-time support*** can be linked as a lump, or we can select just the needed pieces. Clearly, the "lump" method makes for larger program sizes, but the compiler/linker is easier to prepare. We note that Microsoft BASIC compilers sometimes use a variant of the "lump" method. They allow compiled code to be stored without having the runtime support included. At load time, a special runtime module is loaded along with the compiled code.

A final note concerns the possibility of ***not*** compiling the programs, but interpreting them directly or from some intermediate form. This was the most popular way of executing BASIC programs on early PCs, and we store only the source code that is translated directly. The main drawback is that it is much more difficult to automate the process of finding accelerations of the program execution. For reasons of speed, compiled programs are usually preferred, especially if the task is large or must be carried out often.

18.5 Time Differences from Program Alternatives

The simplest mechanism for comparing the program times is to take ratios, since this avoids issues of underlying machine speed. We shall use the Nash variants of the program as the basis for comparison, and compute the ratios Price / Nash and Healy / Nash. (These have been made into variables ***ponn*** and ***honn*** in our data analysis.) Figures 18.5.1 and 18.5.2 show boxplots (Tukey, 1977) of these variables for recent and older timings respectively, with a line drawn at 1.0 for comparison.

The boxplots seem to indicate that there is some ***average*** advantage for the Price variants in the more recent timings. This is supported by the summary statistics for the ratio variables ***ponn*** and ***honn*** in Table 18.5.1.

Figure 18.5.1 Boxplots comparing relative performance of Cholesky algorithm variants in timings performed in 1992.

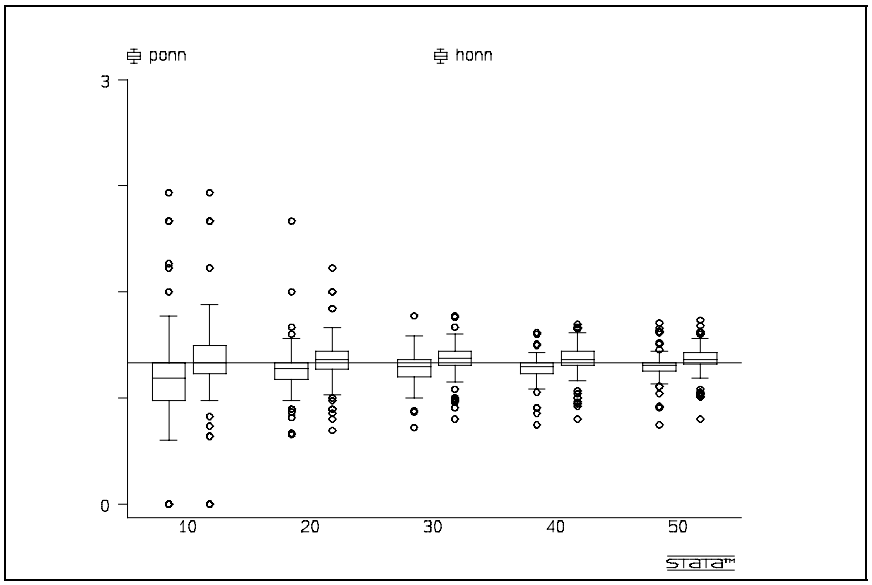


Figure 18.5.2 Boxplots comparing relative performance of Cholesky algorithm variants in timings performed between 1975 and 1983.

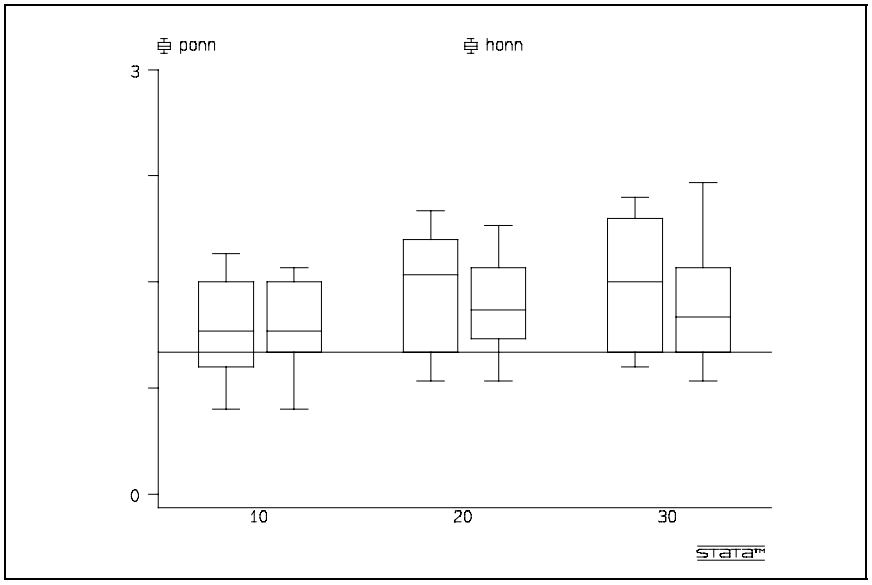


Table 18.5.1 Summary statistics for ratios of Price and Healy Cholesky variant timings on Moler matrices of orders 10, 20, 30, 40, and 50 to the Nash variant.

Var.	Obs	Mean	StDev	Min	Max	Median
ponn	539	.9526	.19798	0	2.2	.97
honn	539	1.0212	.17674	0	2.2	1.02

We can also look at the direct timings on the Nash, Price and Healy variants (Table 18.5.2), but will restrict our attention to PC "386". This table suggests that, for "386" at least, the Nash variant of the Cholesky algorithm enjoys a small advantage for the larger matrices. It also has a lower variability as measured by both the standard deviation and the range (maximum - minimum). However, the existence of a time of zero for matrices of order 10 shows that our "clock" is at the limits of its resolution — it does not "tick" fast enough.

The more recent ratio results indicate that the Price variant, compiler by compiler, generally does a little better than the Nash variant. The Healy variant generally does a little worse than the Nash variant on this basis. However, for some compilers or interpreters, the Nash variant is much better (or the others are much worse), so that the total time taken by the Nash variant, hence its average, is smallest. The lower variability of the Nash variant supports this; it suggests we see fewer really "bad" results.

Table 18.5.2 Summary statistics for Cholesky timings on a 33 MHz 80386DX Tower PC with 80387 co-processor. There were 35 different timings for different compilers or compiler settings. Times are for 10 repetitions of the matrix decomposition of the Moler matrix of order listed.

matrix order		Mean	StDev.	Min	Max
10	nash	.2322857	.435607	0	2.26
	price	.2154286	.4245159	0	2.25
	healy	.2391429	.4773232	0	2.47
20	nash	1.359143	2.551194	.11	12.81
	price	1.34	2.749773	.1	14.67
	healy	1.462	2.919178	.1	15.06
30	nash	4.171143	7.750355	.28	38.67
	price	4.205143	8.664946	.28	46.08
	healy	4.479714	9.014118	.28	46.43
40	nash	9.412286	17.49057	.62	87.22
	price	9.605714	19.82196	.56	105.51
	healy	10.15486	20.4451	.58	105.11
50	nash	17.84857	33.09645	1.14	165.11
	price	18.40486	38.014	1.1	202.12
	healy	19.29686	38.86275	1.16	199.59

Remember, however, that the same PC is decomposing the same five matrices using different methods of running the programs. Yet all the Choleski variants have exceedingly large variations in performance. The Max times are over 100 times bigger than the Min times in Table 18.5.2. We will try to see if we can make any sense of this data.

The relative advantage of the Nash variant in the older timings could be explained by a quirk of some interpreted BASICs. First, execution times were difficult to measure reliably on some of these now-defunct systems. Second, we observed for some BASICs, through simple experiments that added comments to a program code, that GOTO or GOSUB statements in a program were apparently carried out using a forward line-by-line search through the source code to find the target line number. The Price and Healy codes in BASIC used jumps to lines earlier than the current line. Thus the GOTO search must pass through almost the entire program code to find the right line, typically a few lines ahead of the current statement. The Nash code, while using some extra arithmetic, is faster.

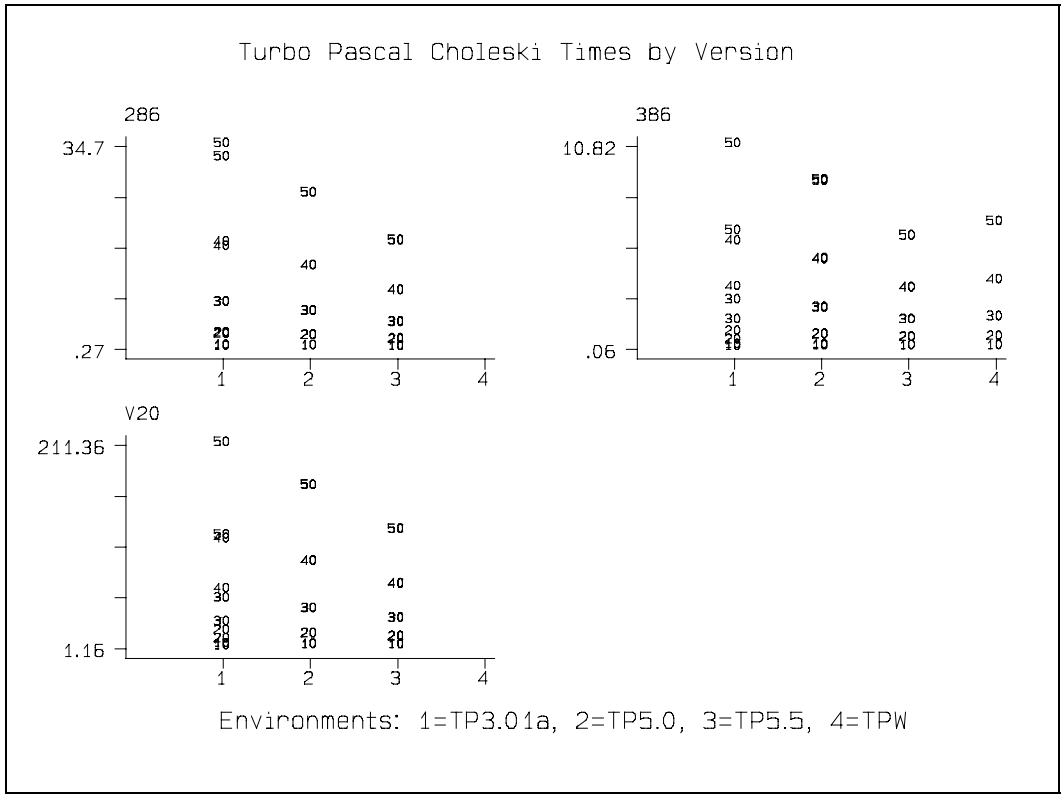
18.6 Compiler and Arithmetic Time Differences

New versions of programming tools are often advertised as "better" and "faster". Let us see if newer versions of the popular Turbo Pascal compilers give better runtime performance. Ignoring some annoyances of obtaining reliable timings, we simply graph the execution times for the Cholesky decomposition against an index for the compiler (Figure 18.6.1). From this graph the improvements in performance from version to version are quite clear, except the slight slowdown with the system overhead in running Turbo Pascal for Windows (TPW).

For other programming languages, we noted some improvement in execution time for Microsoft Fortran between versions 3.2 and 4.1, but no appreciable difference between 4.1 and 5.1. We also noted that the program compiled with version 5.1 failed on the PC with a NEC V20 processor. The fastest execution times were observed with the Silicon Valley Systems compiler. However, this comes at a price: the program code is large and will only run on Intel 80386 and later processors.

We deliberately avoid details in this section, as there are many fine points that would require lengthy discussion. Again, we urge that timings be run for the tasks and systems that will be used regularly.

Figure 18.6.1 Minimum execution time on any of the three Cholesky variants for four versions of the Turbo Pascal compiler.



18.7 Processor and Configuration Time Differences

We conclude this study by considering how processor type and presence of a numeric co-processor affect the speed of our computations.

The first difficulty we encounter is that of timing programs ***without*** the co-processor if it is installed (see Section 8.6). Special system settings to suppress the co-processor did not work as we expected for several of the compilers used. ***Environment variables*** that can be SET to suppress co-processor use have varying

names and control values; they may not be indexed in manuals. To avoid spurious comparisons, we have removed results from consideration if the ratio of timings without and with co-processor was less than 1.1.

The second difficulty is that the arithmetic used with and without the co-processor may not be equivalent. The IEEE 754 (IEEE, 1985) binary floating-point standard has not been followed by all compiler writers, though recent emulations in software seem quite reasonable. Early compilers made no pretence to equivalence, sometimes sacrificing good features of IEEE arithmetic for execution speed. We do not pursue the possibility that co-processors may be incorrectly used.

A third issue is that there are now several manufacturers of co-processors. Some of these (for example Cyrix and ULSI) claim pin for pin compatibility with the Intel 80x87 chips along with higher speed. Others, such as the Weitek co-processor, use a different physical and logical interface to our problems. In either case, timing results and their comparisons may be affected.

Despite these matters, we see from Table 18.7.1 that a co-processor can be highly effective in speeding up execution. Moreover, we gain the added advantage of a documented standard for the arithmetic used. Given the relatively low price of the co-processors, they are very cost-effective if any serious numerical work is required, and we recommend their acquisition and use. On the negative side, we remind readers of a program failure observed on our 80286 PC related to co-processor use (Section 8.3).

Table 18.7.1 Summary results of the average ratio of the times for Cholesky decomposition over the three algorithms and five matrix sizes for different compilers without and with numeric co-processor active.

machine type	number of compilers	mean ratio	StDev ratio	Min ratio	Max ratio
80386	5	8.38	2.93	4.47	11.17
80286	5	3.75	.505	3.14	4.22
NEC V20	7	8.55	3.13	6.11	12.97

Chapter 19

Case study: graphical tools for data analysis

19.1 Purpose of the study
19.2 Example data for analysis
19.3 Display characteristics
19.4 Choices of graphical tools
19.5 Displaying level and variability
19.6 Displaying relative measurements
19.7 Displaying patterns and outliers

In this chapter we present an example of data analysis using graphs. This is typical of the type of exercise that researchers, engineers and statisticians carry out. The particular situation we have chosen is the performance analysis of three program codes for solving nonlinear function minimization problems. This is a task close to the topic of this book, but we do not distinguish our own field from others — the subject may be different, but the tools and methods used are the same.

19.1 Purpose of the Study

The focus of the analysis, which we do not carry to completion here, is the understanding of the differences in the performance of the programs over a set of test problems. We will attempt to address the following issues:

- ***What*** information should we display in any graph or set of graphs?
- ***How*** should we draw graphs — the choice, placement and scale of graphical features for good effect?
- ***Which*** tools should be used for preparing displays easily?

There is rarely a "best" approach or tool for preparing graphical displays, whose effectiveness for data analysis depends on human perception and is colored by personal tastes and preferences. Nevertheless, this case study presents some general ideas we believe are widely applicable.

More detail on the development of statistical graphics can be found in the excellent books by Tufte (1983) and Cleveland (1985). We recommend these to anyone whose job involves the preparation of graphs to be used in data analysis and presentation.

19.2 Example Data for Analysis

The data we wish to analyze consists of a set of performance information for three nonlinear function minimization programs as published by Nash S G and Nocedal (1991). The published paper contains a large amount of numerical data. We shall use only a part of this, namely the data for large test problems their Tables 5 and 11. The programs tested were three nonlinear function minimization codes, written in FORTRAN, and tested on an Encore Multimax computer. The three codes are:

- Truncated Newton method (TN);
- Limited memory Broyden-Fletcher-Goldfarb-Shanno method (LBFGS);

- Polak-Ribière Conjugate Gradient method (CG).

The measures of performance for the codes are:

- The execution time in seconds;
- The number of iterations, that is, major cycles within the codes. These iterations may have vastly different amounts of computational work, and the Nash S G and Nocedal paper addresses this in some detail.
- The number of function and gradient evaluations. This is a major cost in all function minimization methods. For these programs, the function and gradient are evaluated together, which is often efficient since the function and gradient usually have common components. However, some methods may take advantage of situations where the function is very much "cheaper" to evaluate than the gradient or vice-versa, and separate counts for function and gradient evaluations would then be appropriate (Nash J C and Walker-Smith, 1987).

The data we shall study is made up of the following elements:

- The problem size n, that is, the number of parameters in a nonlinear function that are varied to seek a minimum of the function.
- For each program, TN, LBFGS, and CG : the execution time, the number of iterations, and the number of function / gradient evaluations until termination (i.e., convergence to a minimum, a failure, or more function / gradient evaluations than a preset limit).

Very similar sets of data are commonly used in performance evaluations. Another example is found in the paper by J C Nash and S G Nash (1988).

19.3 Display Characteristics

Presenting data graphically is more than simply issuing a command to a computer program to "plot the data". If graphs are to have a useful function in clarifying the information that is partially hidden in a collection of data, then we need to decide what aspects of the data we wish to reveal. This section considers some aspects of drawing graphs.

First, we want to reveal magnitudes to illustrate ***level*** of performance for the computer programs we are trying to understand. In statistics, we would be seeking ***measures of location***. Such graphs are used almost everywhere. They are the substance of most "presentation graphics" or "business graphics" packages. While important, they are not the only form of display needed to help understanding of the information at hand.

Variability is as important as level. In the case of program performance, we would like to know if a program can be expected to take approximately equal times to compute the minima of each of several different functions of the same order (n). Similarly, we want to know if different initial starting points produce widely different executions times for the same test function.

One way to see variability would be to compute a summary statistic such as the standard deviation. (This is one ***measure of dispersion*** to statisticians.) While we could plot the value of the standard deviation for each program using a plot such as a bar graph, this may hide details we want to see. All but one of a set of test functions of order n may have the same execution time, but the remaining problem takes 100 times as long. A set of fairly well spaced timings could have the same value of the standard deviation — clearly a different situation. To display such information about the ***distribution*** of execution times (or other performance measure), we can use:

- Histograms, which are frequency bar charts;
- Box-and-whisker plots, abbreviated as *boxplots*, which summarize distributional information in a way that permits several distributions to be easily compared;

Figure 19.2.1Example data from Nash S G and Nocedal (1991) as entered in a Quattro worksheet

		CG			L-BFGS			TN			
Pnum	N	It	f-g	Time	It	f-g	Time	It	f-g	Time	pname
3	200	3336	6847	2060	7248	7482	2960	76	599	220	C
31	200	3	14	20.3	3	4	5.8	4	20	24.9	I
1	200	4804	9999	3840	9695	9999	5040	38	929	428	A
2	200	1106	2491	657	1734	1785	646	37	456	154	B
53	403	62	144	926	57	63	410	14	100	656	T
29	500	8	98	7.1	48	49	15.4	12	54	8.8	H
6	500	1098	4889	515	1054	1177	389	356	3446	796	D
39	961	161	519	319	165	172	187	27	387	364	K
47	1000	145	302	181	154	157	168	22	160	154	N
49	1000	225	615	104	54	61	35.6	14	68	31.8	P
51	1000	41	91	93.7	46	57	80.1	35	370	467	R
50	1000	294	591	116	457	476	328	30	210	118	Q
43	1000	16	56	23.3	16	20	15.4	15	75	59.1	M
28	1000	167	456	72.1	54	61	35.8	15	75	34.6	G
10	1000				103	114	89.4	30	200	142	F
8	1000	13	36	7.3	30	34	21	12	58	23.9	E
38	1000	285	573	138	405	423	302	33	208	121	J
42	10000	11	33	68.9	14	17	102	24	111	696	L
52	10000	5	13	21	6	8	32.5	5	19	90.9	S
48	10000	18	76	103	37	50	261	29	118	639	O

- Dotplots (MINITAB) or one way scatter plots (**Stata**) that display each observation as a dot or vertical bar along a single line. These give a quick visual view of the density of occurrence of observations;
- Stem-and-leaf diagrams (Tukey, 1977) that serve simultaneously as a summary of the data (with or without loss of information depending on the manner of their development) and as a form of histogram.

We note that such graphs will be important not only for measuring the variability exhibited ***within*** a single program code but also for comparing variability ***between*** programs.

A third class of graphs will show ***relative*** performance. We want to know which situations reflect ***winners*** and which ***losers***. We want to make ***comparisons*** between different situations, problems, and program codes.

Finally, we want to detect both ***patterns*** and deviations from patterns, or ***outliers***. Graphs are helpful for this as the human eye is very good at seeing patterns and deviations from pattern, especially if information is presented clearly. Unfortunately, humans are so good at this that they may see patterns where none really exist. The use of plots to detect both patterns and outliers is an exploratory exercise where we are looking for suggestions for further investigation. The graphs do not "prove" anything, but they may guide us toward such proof.

In this case study, patterns help us to discover the overall performance of each program relative to problem size and other factors. We call these algorithm characteristics: behavior on small versus large problems or nearly linear versus very nonlinear problems. Outliers help us to detect special cases, program errors, or notable successes in solving problems.

In considering ***how*** a display should be drawn we suggest:

- The utility of graphs is enhanced if they contain as much information as possible. For example, a graph comparing the performance of several program codes simultaneously is likely to be more useful than several graphs for individual programs.
- Good visual appearance enhances understanding of the information in the plot.
- The presentation should be easily understood. Obscure diagrams or jargon labelling confuses readers.

- Points on XY plots should be labelled by the "case" or problem or program. Without some care in choice of labels, we cannot locate particular special cases or isolate problems.
- Appropriate use of color or other graphical features helps the viewer. In this book we will ***not*** use color — color plates are expensive — but will try to illustrate different display features.
- Graphical analysis tools are more likely to be used if we do not have to work too hard to produce them. Appropriate software should be acquired. If necessary, command scripts for this software to simplify the creation of selected types of graphs should be prepared.

19.4 Choices of Graphical Tools

We present only a sample of the many choices of graphical display software here. We use this sample to illustrate the range of features in such software. Desirable features of such software include:

- Ease of data manipulation. We will commonly want to manipulate data to improve displays. Frequently data must be sorted to have graph points presented in the correct order. Labels may need to be added because the original identifiers are simply too cumbersome to display without cluttering the graph. Transformations of data, e.g., taking logarithms, are often needed to render information visible.
- Good automatic settings for drawing displays save the user effort. Effective scaling of axes should ensure that the graph points fill the display area yet the axis ticks are at reasonable numbers. For example, an X-axis from -2.345 to +123.3 with 4 ticks between is less easy to understand than a graph with an X-axis from -25 to 125 with tick marks (possibly labelled) at 0, 25, 50, 75, and 100. Labels and titles should be easily legible without forcing the graph itself to postage stamp size. Automatic selection of reasonable and clear graphing symbols, fonts, line types, colors or shadings saves much effort, though automatic selections that the user cannot change make for a worthless program.
- Ease of annotation. It should be easy to add extra notes or to identify special cases by adding text in appropriate places on a graph. Positioning — or moving — such notes should be easy and natural.
- Identification of observations (cases). We may have a label for each case. It should be possible to use this label as the plotting symbol if needed. Even better is a facility to use a pointing device (mouse, light pen, etc.) to move a cursor to a point and have it identified. This lets us pinpoint situations that are special or abnormal in some way.
- Ease of file export. Once a graph is displayed, it should be easy to save the image so that it can be printed or imported into other software for inclusion in documents, reports, presentations or displays. The purpose of graphical displays is the communication of ideas, first to ourselves, then to others, so data transfer capabilities are extremely important.
- Generally, the ease of use of a graphics package encourages the use of graphical data analysis.

We now present some examples of graphical software. We limit our discussion here to packages on MS-DOS machines. In our opinion Macintosh software has had better graphical tools, in part because of the more consistent screen control design of the Macintosh.

LOTUS 1-2-3: This well-known, easy to use, spreadsheet package allows users to plot up to six data series at once, but lacks tools to display variability (e.g., boxplots). To get good quality displays and printouts it has been necessary to use add-ins such as **ALWAYS**.

QUATTRO: This spreadsheet package has display-quality graphics; graph manipulation and annotation tools are built-in. Since Quattro can be used in "Lotus" mode, 1-2-3 users avoid learning new commands. Of interest to us in preparing this book has been the availability of PostScript output, though we can also import graphs into WordPerfect 5.1 in the Lotus PIC format. Spreadsheet packages have very convenient features for data entry, edit, transformation, sorting and manipulation. We have used a spreadsheet as the primary data entry mechanism for this study.

Stata: Though designed as a general statistics package, **Stata** has excellent two-dimensional graphical tools based on an easy-to-learn command language. It has good facilities for exporting graphs to other software and facilities. (We generally use the PIC file options.)

SYSTAT: This is a full-featured statistical package. Graphics include three-dimensional point cloud spinning. This feature essentially takes a graph such as that in Figure 19.7.1 below (minus grid lines) and allows the user to rotate the plot about different axes in order to try to discover patterns. SYSTAT programs are very large; we have experienced some "insufficient memory" problems depending on PC configuration and operating system.

EXECUSTAT: The Student Edition of this commercial statistical package has interesting three-dimensional (3D) graphics both in the form of Figure 19.7.1 and point cloud spinning. It includes interactive data-analysis tools such as point brushing: points are colored differently if a fourth variable is greater than or less than a user-set control value. This control value may be changed by mouse or arrow commands, with the graph points dynamically changing color ("brushed") accordingly. Unfortunately import and export may be awkward. Section 19.7 tells how we managed to export displays for use in this book.

MATLAB: (Student Edition) allows for easy manipulation of matrix data. Graphical tools for displaying variability are missing, except for histograms. 3D plots are possible. The Student Edition has limited capabilities for export of graphical data, for example to documents such as this book. However, the regular versions offer full capability in export.

For those who must include graphic capability in a user-written program, there are libraries of graphical functions or sub-programs to ease the task (Nash J C, 1994). Three of these are ***GraphiC***, ***VG*** and ***GraphPak Professional***. They are designed for programmers who write in C, FORTRAN and BASIC, respectively. None appears to provide graphical displays for variability measures (not even histograms). ***GraphiC*** and ***GraphPak Professional*** provide some facilities for three-dimensional graphics. ***VG*** allows multiple displays on the same "screen" or page. More remarkably, ***VG*** is available at no charge from the National Institute for Standards and Technology (NIST) using the FTP protocol on academic computer networks. Versions exist for several FORTRAN compilers.

Of the above packages, ***VG*** is the only one we have used to prepare a graph. We have received and run demonstrations of the other two, but have not used them in a practical situation. Frankly, we regard the programming of graphical displays as a very heavy task. If there are tools available (such as **Stata** or QUATTRO) that allow us to develop the displays we need, then we will choose these easier-to-use tools. If something special is needed, one could consider *True BASIC*, which offers add-on packages such as a Statistics Graphics Toolkit (which includes boxplots) and a 3D Graphics Toolkit. Programs are easy to write, but the language is nonstandard, though it does exist on multiple platforms, in particular MS-DOS, Macintosh and some UNIX workstations.

19.5 Displaying Level and Variability

In Figure 19.5.1 we have used **Stata** to display both variability and level via boxplots and one-way plots of execution time. Note that in this display we have stacked the displays to enable some comparison of the execution times of the three programs. We note a wide variation in scale. There are a very few points at the right hand side of each one-way scatter plot; most points are scrunched together at the left-hand side. Taking logarithms of the data (Figure 19.5.2) brings out more detail.

Figure 19.5.1 Level and variability — natural scale

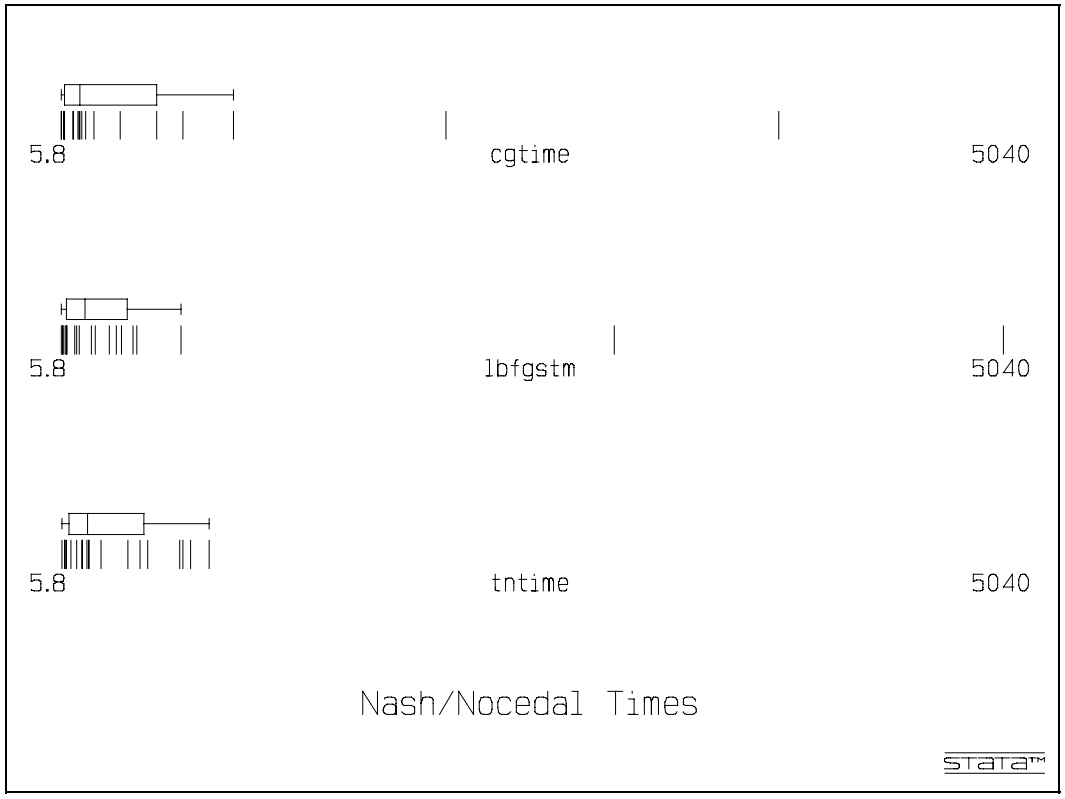


Figure 19.5.2 Level and variability — logarithmic scale

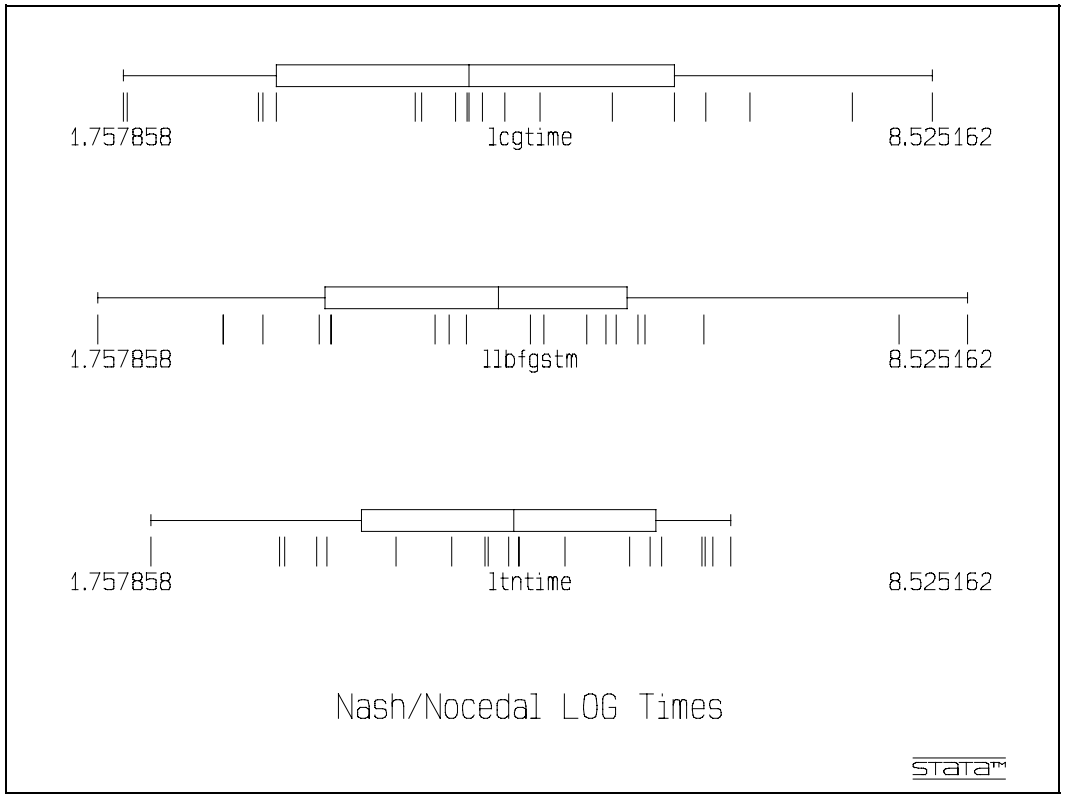
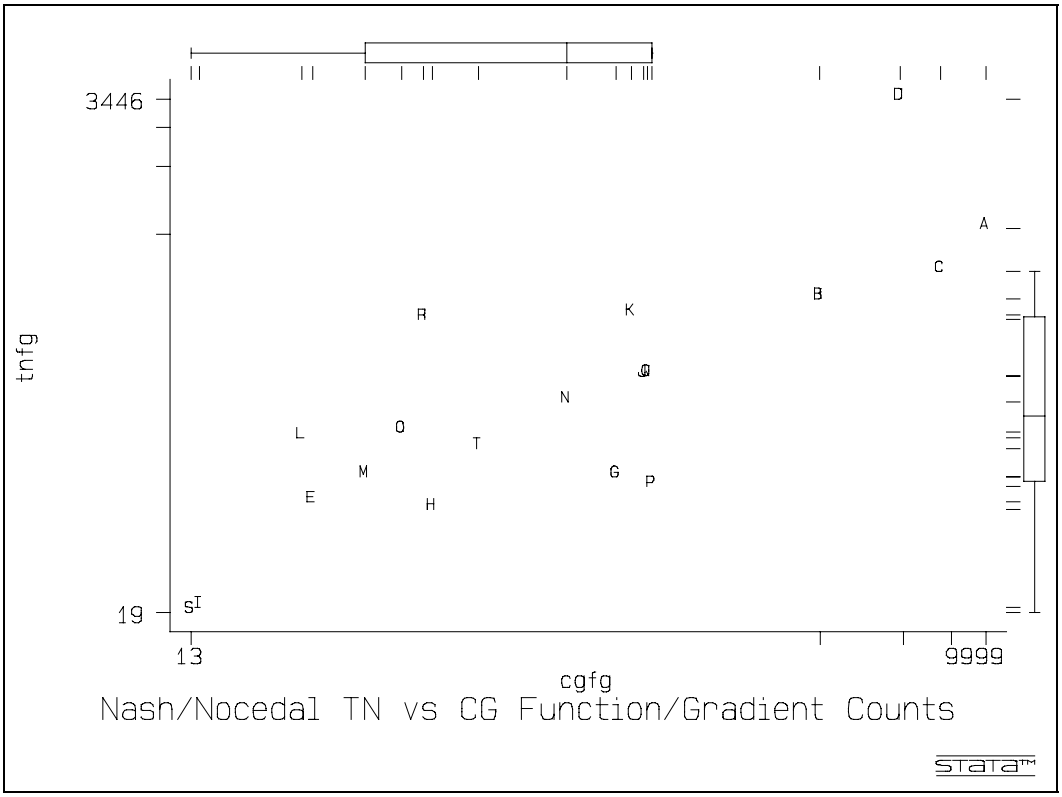


Figure 19.5.2 has a reasonable scale for comparing the relative levels and variabilities of the execution

times of the programs. However, a direct comparison of the times for given problems is ***not*** possible because we cannot label the points. To overcome this we plot the times for one program versus those for another and use the problem name — the letters of the alphabet A through T that we added into the QUATTRO worksheet during data entry — as the point label. **Stata** offers the possibility of adding boxplots and one-way scatterplots along the axes of the graph, so we get more direct visualization of the variability by selecting this option. Interestingly, we need not transform to logarithmic data before plotting this display since **Stata** offers a "log scale" option for XY plots, though not for the simpler one dimensional plots. Figure 19.5.3 shows the output. We note in passing that similar plots can be prepared for iteration count and function/gradient count data.

Figure 19.5.3 Level and variability — enhanced XY plot in log scale



19.6 Displaying Relative Measurements

The purpose of the Nash S G and Nocedal study was to try to understand which algorithms (using Fortran program implementations as proxies) were better in dealing with different types of problems. We are trying to find the winners and losers in a set of computer program races. This calls for some form of ***relative measurement*** rather than the plotting of the actual numbers as above.

One useful tool (used in Nash J C and Nash S G, 1988) has been a graph of ***ratio-to-best*** information. That is, we find the best outcome for a given case (problem) over all the competing methods (programs). We then compute the ratio of the performance of each method to the best performance. For timings, the ratio of the "winner" to the "best" will naturally be 1, while all other methods will have larger ratios. With measures of performance that increase with "better" performance, we may want to use reciprocals or otherwise alter our approach. However, the general idea stays the same. Watch out for zero divides caused by missing values!

A spreadsheet can easily develop the "best" and "ratio-to-best" information. This can be plotted using

simple bar graphs. Figure 19.6.1 is an example. We would like for each case (problem) to flag the "winner" more clearly. In an attempt to bring out the best case, we reverse the sign of the ratio that was 1.0, and use -2 as the quantity to plot so that the "winner" stands out. Unfortunately, We found it quite easy to make an error in this process. We recommend checking several random graph points to see that they are in the correct position.

The prevalence of any one program as "winner" is highlighted by the different shadings, but could be made more prominent by use of color. We have manually colored printouts from conventional printers. Color printing would, of course, be useful, but at the time of writing is still relatively expensive to reproduce. Figure 19.6.1 was produced with Lotus 1-2-3 v.2.2. Similar displays can clearly be used to show "losers" by obvious changes in the computation of the ratios and "flag" values.

An alternative graph that displays the relative performance of the method is called an "area plot" by QUATTRO (DOS version). We present an example as Figure 19.6.2, where again we use the ratio-to-best figures for timings. Note that a narrow band is "better" here. It is more difficult to flag the "winner" or "loser" in each case — an unsatisfactory aspect of this type of plot. Still, the use of shaded areas allows the human eye to "integrate" the overall performance, with a larger area being poorer. An alternative would adjust the ratios to make larger imply "better". Different choices of shadings could alter our perceptions of the relative performance of the programs.

We note that while QUATTRO makes this plot easy to generate, it is not, to our knowledge, a common feature of many graphics packages. A common difficulty that arises when selecting graphics software is that we really want to use two different types of graphs that are each only available in ***separate*** packages. As in this case study, we must then move data around and spend time and effort learning more than one package.

Figure 19.6.1 Relative performance — ratio-to-best bar chart

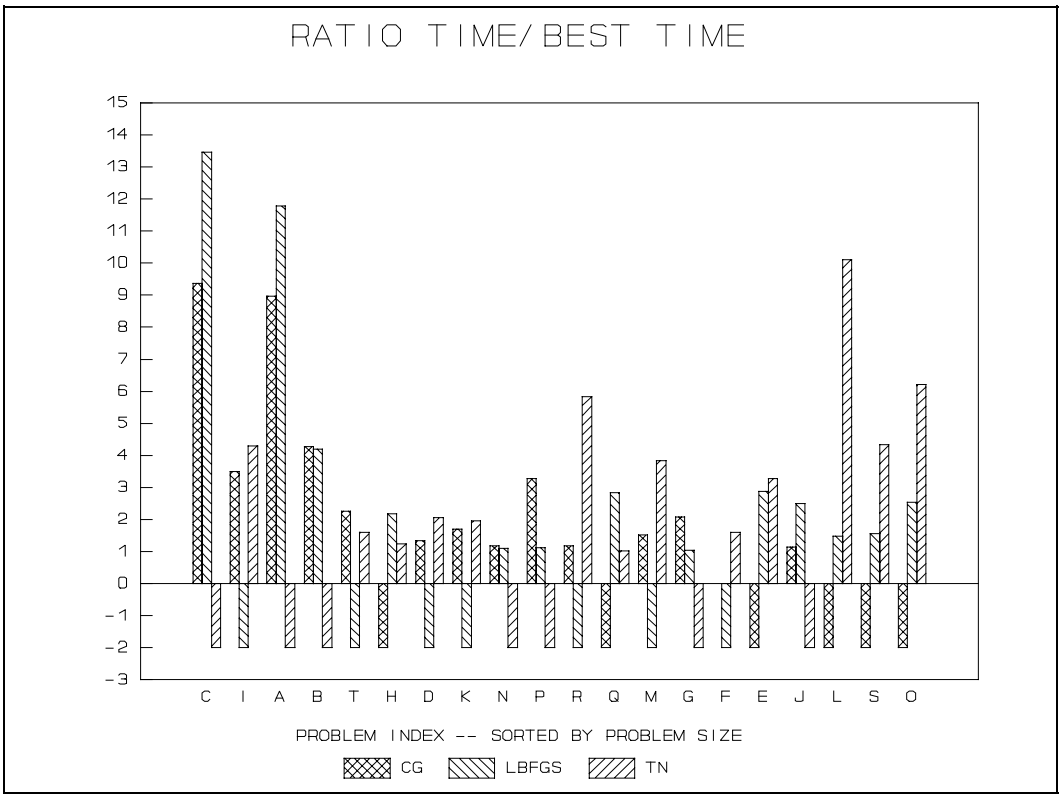
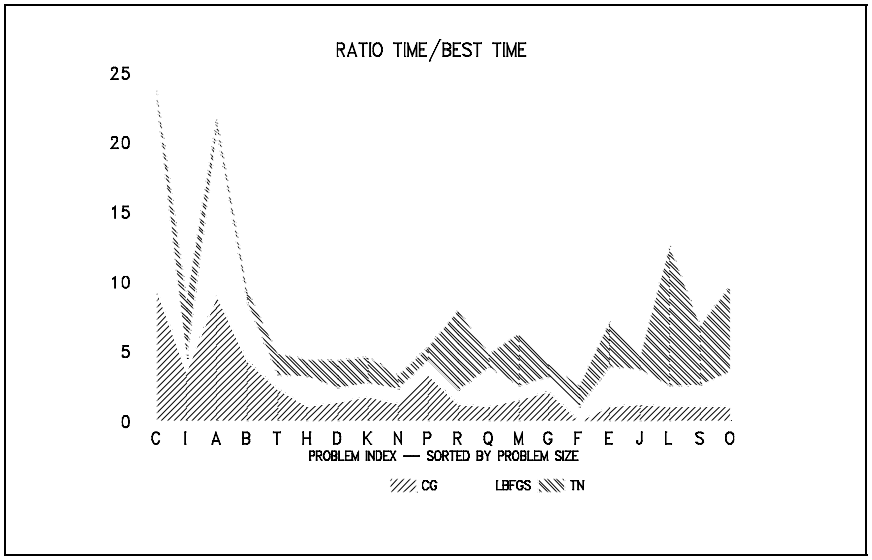


Figure 19.6.2 Relative performance — ratio-to-best area plot



19.7 Displaying Patterns and Outliers

Much of the work of researchers is devoted to understanding patterns that lead to principles explaining phenomena. Therefore tools that help us to discover or "see" such patterns are important in aiding the process of developing an understanding of phenomena.

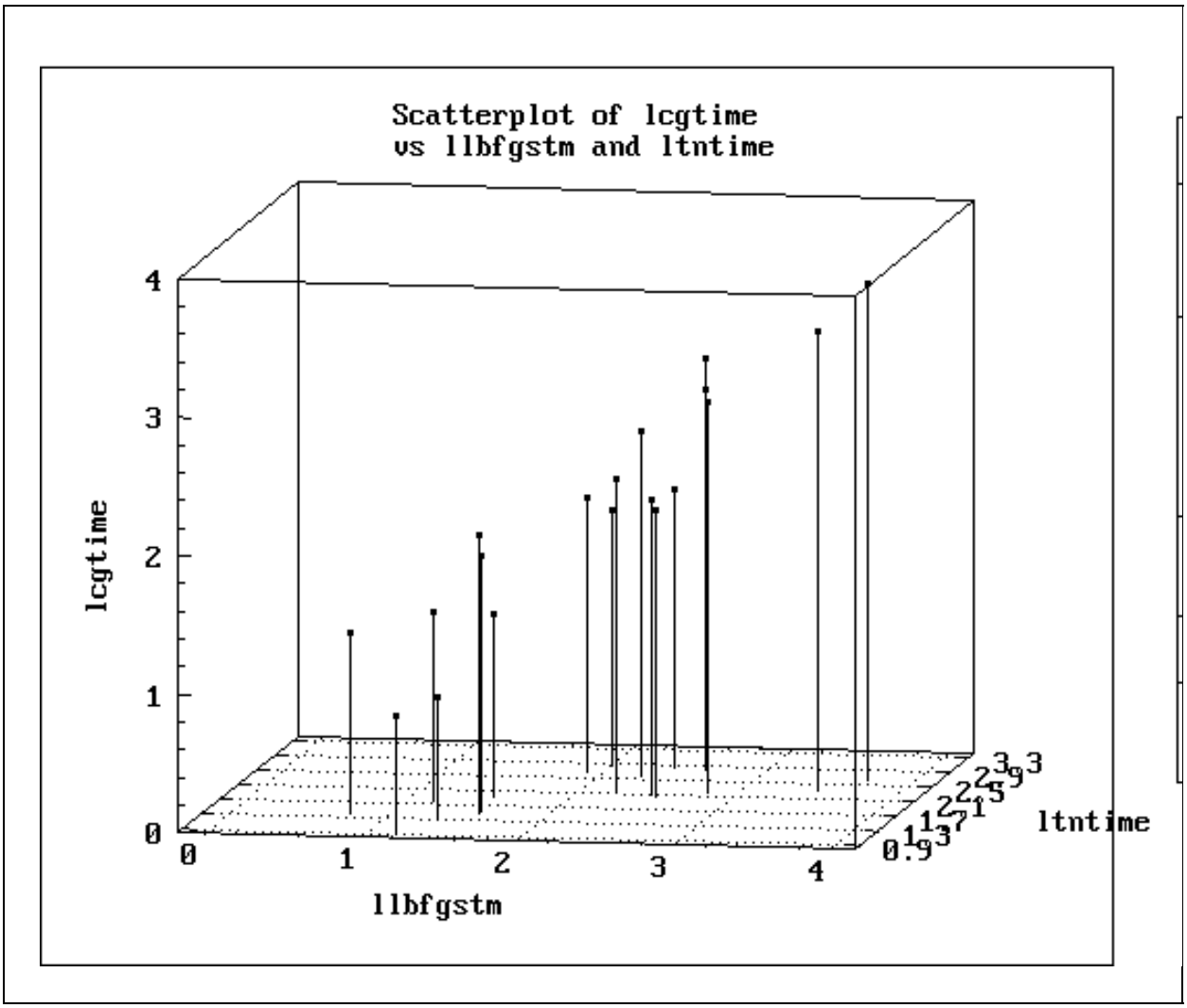
One such tool is the three-dimensional plot, abbreviated ***3D plot***. Figure 19.7.1 displays simultaneously the execution times using all three of the program codes for all the test problems except the one labelled *F* (which has no timing for the CG program code).

Readers will note that Figure 19.7.1 is ***not*** clear, with a vertical line on the right-hand side of the plot and "jaggy" diagonal lines. The Student Edition of EXECUSTAT we used to prepare this graph does not include facilities for exporting graphics into our word processing software (WordPerfect 5.1). Figure 19.7.1 was created as follows:

1. A screen capture program (we used SNAP) was run. This intercepts "Print Screen" commands.
2. EXECUSTAT is started and the desired plot displayed on the screen. Adjustments are made to the horizontal and vertical display "angles".
3. The Print Screen command is issued. SNAP intervenes and presents a dialog box that allows us to name a file to hold the graphic image and to set the file format. (We chose monochrome PCX format.)
4. After leaving EXECUSTAT, we load our word processor and import the graph. EXECUSTAT leaves some control information on the screen and this is captured along with the graph. Some of this extraneous material may be moved out of sight by adjusting the graph size in the "window" for our figure.

Screen capture is inferior to facilities to transfer clear, scalable graphic images to other software. Nevertheless, it is the type of mechanism we must sometimes use to save useful graphs or other screen displays.

Figure 19.7.1 Three-dimensional point plot (EXECUSTAT)



As a tool for interactively finding patterns, the rotation of 3D plots around both horizontal and vertical axes is useful. An excellent implementation is the statistical package **Data Desk** for the Macintosh, written by Paul Velleman of Cornell University. While other packages — e.g., EXECUSTAT and SYSTAT — use keyboard or mouse commands to rotate the cloud point image about the horizontal or vertical axes, **Data Desk** uses the idea that the cloud point is like a globe or ball floating in a dish. With an icon that looks like a human hand and is manipulated by the Macintosh mouse, one can "click" anywhere on the image and "roll" it around in any direction. One can even "click", roll and let go, leaving the image to rotate around whatever axis the motion implied. This is masterful human factors engineering.

Even with the less elegant horizontal / vertical rotations, cloud point spinning can bring to life patterns in data. We will illustrate this with an example outside the present study and consider a plot of some data for automobiles, namely number of cylinders, displacement and price. These are plotted in Figure 19.7.2, the images of which were captured as above. Nevertheless, the idea comes through clearly.

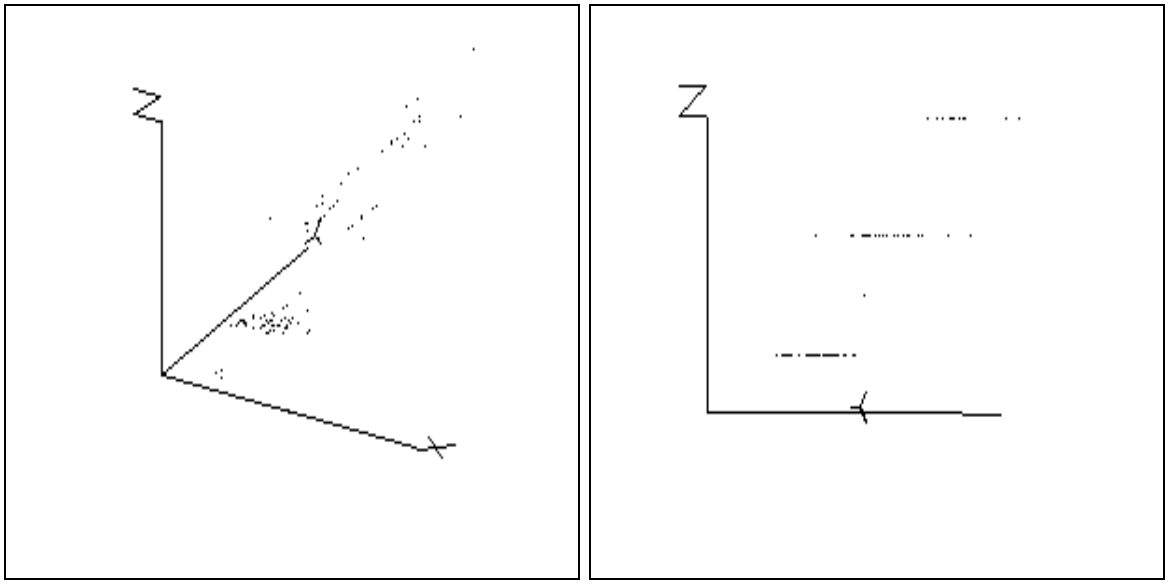
While 3D plots are useful for seeing patterns, some details influence their effectiveness in revealing data features:

- If the points displayed are too small we cannot see them; if too large, they clutter the display and hide other points.

- For best effect, near/far perspective needs to be shown by making "closer" points larger or a different shape, a non-trivial programming task for developers, especially given the comment above.
- Grid lines are helpful to the viewer in assessing the level represented by a point for one or more of the three variables plotted, ***but*** such lines clutter the graph. Users should have control of rotations and which (if any) grid lines to include.
- So users can discern which points are "special", the graph points need to be identified by using a labelling letter or symbol as we have done in Figure 19.5.3. Unfortunately, the identifiers may make the points so large on the display that other features are hidden. Again we have to balance between including wanted information in the graph and maintaining a clear and uncluttered image. An alternative to labelled points is the possibility of pointing an arrow cursor at a given point to have it identified. Developing such attractive capabilities requires a lot of programming effort.
- Color can be very useful in adding extra information to a display. We have also already mentioned in Section 19.4 (in describing EXECUSTAT) how point ***brushing*** and ***spinning*** are useful in interactive data analysis.
- It may be helpful if data are pre-processed before display to focus on certain features present in the data that we want to emphasize. Our use of the ratio-to-best transformations, or even the logarithmic transformation of the data, may be regarded in this light. Other possibilities include ***clustering*** (with cluster membership indicated) or ***robust regression*** to select and label points that may be outliers.

A different type of pattern — that of similarity of cases — requires us to attempt to graph many variables at once for a number of different cases. Several tools have been developed that try to squeeze many more dimensions out of a flat, two-dimensional page than are immediately available. In the present example we could, for example, consider each row of the table that makes up Figure 19.2.1 as an observation vector.

Figure 19.7.2 Point cloud spinning: Left hand graph — unrotated
Right hand graph — rotated



(We would probably leave out the observation labelled *F* because it lacks information on the three variables ***time***, ***function/gradient count***, and ***iteration count*** for the program *CG*.) We now wish to plot some display for each problem that uses the information for all variables. Note that we nearly always need to scale the data so that actual plotted line lengths are similar for different variables. Thus ratios-to-best or ratios-to-maxima are commonly used, and logarithmic scaling may be necessary. Some possibilities include:

- ***Star plots*** — for each case, we plot each variable as a radial distance "spoke" from a center. We join the ends of the centers for effect. If we do not join the ends of the spokes, the plot is sometimes referred to as a ***glyph plot*** (Gnanadesikan, 1977, p.63)
- ***Castles*** — each observation yields a small bar graph representing the values of all the variables. These "castles" are arrayed as in the star or glyph plot so we have every case displayed.
- ***Chernoff's faces*** — the values of each variable for a given case are represented by human facial features such as roundness of face, form of smile, size of ears, roundness and slant of eyes, etc. It is possible to represent over a dozen variables at once in this way. Because it is important for us to recognize facial features of our own species, we can quickly spot similarities and differences, though assignment of variables to features can alter perceptions. (Tufte, 1983, p.142)

It is relatively easy to develop the bar charts for castles, and some packages, for example **Stata**, have star charts. Software for Chernoff's faces is rarer; in our personal library we have only experimental code in BASIC to draw crude faces using regular text symbols as characters.

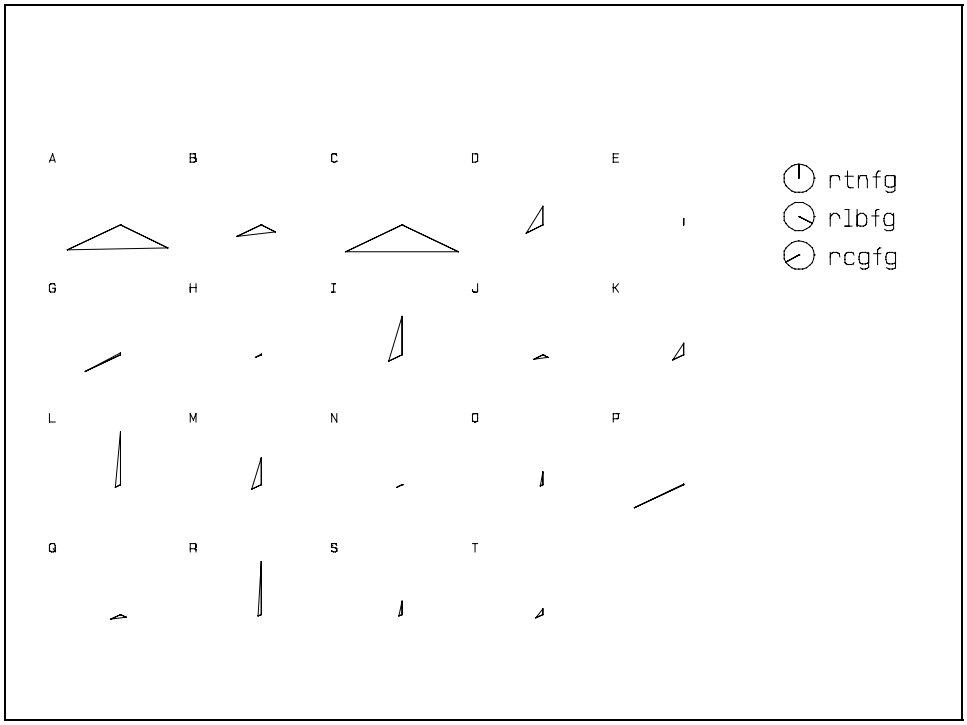
We illustrate the use of star charts in Figure 19.7.3, which displays the execution times for the three program codes simultaneously on all problems. Note the similarity of the following sets of problems:

problems A, B, C, J, and Q
problems D, E, I, K, L, M, O, R, S, and T
problems G, H, N, and P

Note that this does not "prove" the problems are similar. It simply allows us to pick out similarities and differences for further study.

Outliers are rendered more detectable if we have a model for the phenomena that underlie the data we are analyzing. For the present data we could, for example, compute approximate models of execution times for the three optimization codes using, say, a cubic polynomial. Then the residuals — the deviations from the model — could be computed and plotted for each method, possibly as a star chart.

Figure 19.7.3 Star plots to compare optimization test problems
Nash S G / Nocedal ratio-to-best execution times.



Chapter 20

Your Own Strategy for Scientific Computing on PCs

20.1 Identifying needs and wants
20.2 Acquiring the right computing environments
20.3 Tools and methods
20.4 Add-ons, extras and flexibility
20.5 Personal choice and satisfaction

This last chapter is a restatement of our basic theme that PCs should suit the individual who uses them. As far as possible, it is the PC that must adapt to the user, not the user to the PC. We review the elements of developing the hardware and software mix that will allow you to fulfil your scientific computing needs.

In doing this, we consider your problems and the strategy that will be used to solve them. By ***strategy*** we mean the overall approach, including the methods and type of software to attempt a solution. If there is a choice of computing environment, we will also want to select the most appropriate one for the particular need. We will, of course, continue to look at the suitability of PCs for the job.

Tactics to overcome the detailed obstacles that arise during the evolution of a solution to a problem will only be mentioned in passing. Developing and improving such tactics requires experimentation of the type used in the Cholesky timing study in Chapter 16, where the importance of details in computational solutions is made abundantly clear. While tactical ideas for use in improving the features or efficiency of a solution may be suggested by many sources — books, magazines, conversations with colleagues — we believe such ideas ***must*** be tested before being accepted as applicable to a specific problem, solution method, or computing system.

20.1 Identifying Needs and Wants

Since becoming known as "PC experts" by virtue of our writings on personal computing, we have often been asked questions such as:

> What type of computer (or software) should I buy?

or

> Is ***(name of brand)*** any good?

We do not answer these questions directly because the person asking has not generally given us any information ***why*** they want a computer or a piece of software. Computers and software are expensive junk unless there are well-defined reasons for their acquisition. Usually — and this is a delight of PCs and their software — one later discovers several very interesting uses not envisaged at the time of purchase. Nevertheless, acquisitions should be justified by well-specified needs and wants.

We discussed the capabilities of PCs in research applications in Chapters 2 and 3. A list of headings from these chapters could serve as a preliminary checklist for the types of applications for which one may want a PC. We suggest that this list be augmented with some detail to reflect the size and complexity of

problems anticipated, the special graphical or text processing features required, and any unusual interfacing needs. Without these details, one may purchase good equipment that nevertheless is unsuitable for solving our problems.

If you require software of a certain type to do your scientific work, then you must ensure that the equipment you purchase is can run this software along with any operating system or utility software to support it, such as memory managers or graphics drivers.

Our first piece of closing advice is then:

Identify what you want to do and how you want to do it before acquiring hardware and software.

We also would point out that while this book concerns the management of scientific computing when one has to do it oneself, we do not recommend this option if there are staff to carry out all the annoying work of backing up files, managing installations of software, maintaining and cleaning equipment etc. Our message is mainly for those without the helpers.

Choose the easiest means to get the job done — if there are competent helpers, let them help!

Assuming we are forced to be self-sufficient, we should be aware of the computing and data-processing tasks that our job entails. Listing these and selecting those that place the greatest demands on our computing resources, we can establish some guidelines for the computer we will need, be it PC or otherwise.

For some tasks, the methods will be well-known to us. For others, we must work through formulations to potential reasonable methods as in Chapters 13 to 17. The word "reasonable" is important here. We may solve a linear least squares problem as a general unconstrained function minimization as mentioned in Section 14.2. However, this is only useful in the rare instance that a function minimization algorithm is available while a method for least squares solutions is not. Clearly, if we do not know many possible formulations, our choice of methods is correspondingly limited. In the situation where the problem has a large computational or memory requirement, being able to choose a method that can be used at all within the computing resources available may depend on our knowledge of the possible formulations of our problem.

We want to recognize quickly whether a particular PC or type of PC can be used to attempt a solution. In making this decision we need to know:

- The total amount of input data required by the problem;
- The minimum set of data that must be held in the main memory during solution to define the problem;
- The precision of each of these data elements, so that the total memory requirement for the problem data can be determined;
- The likely amount of working storage needed, along with a rough estimate of the size of the program needed;
- Amount of memory needed, that is, the sum of program storage, operating system and language processor storage, and working storage;
- The amount of output generated by a solution to the problem;
- Typical solution times on other PCs, leading to a rough estimate of run time on the target PC;
- Computational precision required, as opposed to storage precision.

With the above information we can make an intelligent guess at the possibility of tackling the problem on our machine. We should choose not to proceed in the following situations:

- The total amount of data required is too large to be stored on our mass storage devices in any reasonable way. For example, attempts to solve problems requiring all the data in a national census with a PC having only floppy disks would generally be regarded as foolish. However, the Senegal census was conducted in the mid-1980s with a few such machines, aided by one or two with fixed disks, in a well-designed data entry and tabulation effort.
- The amount of data in the problem is considerably larger than memory available on the target PC system. (Note that we do not even consider working storage or program space yet, as these are determined by the algorithm.)
- Conversion of data from its external form to computational form, e.g., from small integers in a data file to floating-point numbers, will overload memory. Careful programming may overcome such difficulties.
- The anticipated amount of output is such that peripherals cannot cope in a reasonable time, e.g., the printer will take all weekend to print the results.
- A "fast" PC (in comparison with the target PC) has required a considerable time to compute solutions to problems similar to the one at hand. We must be honest and scrupulous in estimating the time requirements for the proposed solution.
- We need reliable, high precision answers, for example in a navigation or spacecraft tracking problem, yet our programming languages and hardware cannot guarantee this precision. Fortunately, good tools do exist on PCs, but they may not be available to us.

In all the above, the aim is to avoid ***impossible*** tasks. In the past, we have been accused of just this offense. However, there is a distinction to be made between ***testing*** the limits of computational systems — where they are rarely used effectively — and trying to solve problems that strain PC limits in a ***production*** mode. The "try-it-and-see" exercise is valuable in providing data upon which the decision discussed in this section can be based. If our goal is to solve problems effectively, we do not want to be constantly risking memory overflow or similar disasters in mid-solution, after much human and PC work has been performed.

20.2 Acquiring the Right Computing Environments

Most workers performing scientific computations now have a choice of several computing environments for their work. Our recommendation:

> ***Choose the computing environment that will do the whole job with the least amount of bother for the users — us!***

If computing resources that can do the job already exist, we must decide which to use. The questions in Section 20.1 are relevant in eliminating candidate machines that cannot do the job. We now wish to select the best PC available to us. If an already available system has software suited to our problems, this will be the preferred candidate if it has adequate features, speed and storage resources. Whereas in Section 20.1 we considered ***if*** a particular PC would be adequate, we now wish to put a scale on the answers to the questions and decide ***how well*** it will work for us.

An important consideration concerns the burdens the operation of a particular machine places on the user? For example, will it require tedious or difficult responses or commands, many disk exchanges, or having to remember complicated sequences of events that must occur in a definite and precise order.

Issues of special interfacing of equipment or devices are best left to the specialists, not the salespersons. Being the first person to try a particular interface nearly always implies expenditure of time and money. We consider some cases that deserve caution by examples.

Any interface where there are time constraints on signals or movement of data can be troublesome, since

minor changes in the way in which our system works may result in annoying failures. This can be illustrated by the (non-scientific) example of our fax-modem. This inexpensive but important part of one of our PCs functioned without problems until we connected its host PC (an aging XT-class MS-DOS PC) to our other PCs in a small local area network. We noticed our incoming fax messages were of poor quality, and modem communications seemed to suffer from "line noise". Finally, some experiments involving the sending and receiving of faxes with a friend showed that timing delays imposed on disk storage were apparently the source of the problem. That is, the PC was not fast enough to save all the "dots" in the incoming fax message, so we lost some information. We ran this PC off-line from the network. It was eventually replaced with a faster unit that can handle both the LAN and fax messages simultaneously.

It may not be possible to operate all installed devices that require interrupt allocation to work. The IBM PC is particularly notorious for having too few interrupt request lines (IRQs). Thus vendors are happy to sell equipment "guaranteed to work with your PC". However, they may neglect to mention that to use your CD ROM drive you must disconnect your printer! We have observed a situation in a government office where two secretaries were to have their PCs connected to a single laser printer via a printer sharing box. The installer arrived, duly hooked up the box with appropriate cables, and departed with the words "Oh, your mouse might not work." (It did not.)

If PCs must be obtained, then we want to minimize the acquisition effort. While cash can be saved by careful shopping for PC system components from multiple suppliers, our feeling is that this activity demands much time from the user. In case of trouble, we can insist that a single supplier find and repair it, usually under warranty. We can also arrange a fully configured system before delivery, saving our time for research work. While we prefer to deal with the same supplier over time, this is proving more difficult as PCs become commodity merchandise and specialty shops give way to merchandising chains. Of course, even specialty PC suppliers are rarely knowledgeable in scientific computing.

Our policy is to overbuy in some respects. In particular, we recommend that one ensures the maximum in fixed storage ("hard disk") capacity, main memory (RAM) capacity and processing speed given the money available for the purchase. Generally we have found ourselves best served in terms of performance / price ratios by machines that have just been superseded as the most powerful in their class. By buying late in the product cycle, we feel we get reliable, well-tested technology at a reasonable price. Our own MS-DOS PCs were all bought in this way. We bought a XT-class (Intel 8088 / NEC V20) machine as the AT class (Intel 80286) was introduced, a "fast" AT-clone as 80386 PCs were appearing, a high-end 80386 / 80387 machine as 80486s were delivered, and a similar notebook configuration when 80486 notebooks were first widely offered.

We recommend against the use of multiple computing platforms. Our own experiences of trying to mix PCs or operating systems have been uniformly unsatisfactory. We managed to get the job done, but were not happy in so doing (see Sections 1-5, 2-6, and 11-8).

20.3 Tools and Methods

As with choosing a PC on which to compute solutions to a problem, selecting software or programming language(s) is often Hobson’s choice.
The machine we must use is on our desk. If we want to use equipment belonging to others, then we must generally put up with the facilities provided. Many PCs are not used for technical or research work, so lack the software most suitable to such tasks.

If the method chosen to solve the problem is not already developed within available software, then we must program it. This may mean:

- Writing of a program "from scratch" in a traditional programming language such as FORTRAN, C, BASIC or PASCAL;

- Working within a system such as MATLAB or *True BASIC* where a range of typical scientific computations is already available, so that our "program" becomes a sequence of calls to macro commands or functions. Symbolic manipulation packages such as ***DERIVE***, **Maple** or *Mathematica* offer considerable computational power along with the capability to manipulate mathematical expressions.
- If our problem is statistical in nature, linking commands for a statistical package into scripts that can be executed automatically may be a reasonable approach. We have used such ideas extensively to present examples to students in university statistics courses, where the calculation can be made to evolve on the screen as the student watches and interacts. The tools with which we have worked — and this a very restricted list — are MINITAB, **Stata** and SYSTAT (or its educational version MYSTAT).
- Developing macros or worksheet templates for a spreadsheet processor such as Lotus 1-2-3, QUATTRO or **Excel**. We may also be able to take advantage of special Add-In software to enhance the capabilities of the spreadsheet package to carry out scientific computations. We have reviewed such Add-Ins for optimization computations (Nash J C 1991b). Our experience is such that we caution ***against*** the development of any but the simplest of macros. They are, in our opinion, too difficult to develop and revise and much too easy to prepare incorrectly.
- Where problems involve extensive data manipulation we may wish to write command scripts for a database language such as that for dBase III/IV or PARADOX.

If we decide to write a conventional program, then we need a compiler or interpreter for the language in which we choose to write the program. Fortunately powerful yet inexpensive language translators are available for the principal programming languages. Since many PCs are never used as program development environments, we may not find programming tools installed on the PC we are going to use to solve our problem. While Microsoft supplies an interpreter for BASIC with MS-DOS version 5 (called QBASIC), no manual is supplied for this in versions we have seen. Previous versions of MS-DOS (e.g., version 4.01) were accompanied by the GWBASIC interpreter plus a manual for this version of the Microsoft BASIC programming language. The interpreter, as we have seen in the timed Chapter 16, gives slow run times when compared to equivalent compilers.

For those users with the luxury of a choice of solution tools, the following set of questions are pertinent to the selection:

- What computational features of a programming language does the problem at hand require?
  - Floating-point or integer variables;
  - Precision of computation and range of exponents;
  - Maximum array size and maximum dimensionality (number of subscripts allowed);
  - Speed of computation.
- Do we have subroutines, functions, macros or command scripts already available to us that can save effort if they are usable? If so, from what computing environments can we use these tools? For example, we may be able to call subroutines written in one language from other programming languages that provide better file management of input/output features.
- Can we efficiently make use of the candidate solution software? That is, if we have chosen to use a spreadsheet package and need to write macros, can we do this without difficulty and delay? If we have decided to program our method in Pascal, do we know how to effectively use the compiler at hand, for example, in controlling options such as floating-point arithmetic and memory models?

Clearly it is wise, where possible, to choose a method for which an algorithm is available. That is, we have a recipe for using a particular method in our possession. If we are lucky, this has already been programmed and exists in machine readable form. It may even have been implemented and tested, a considerable saving of time and effort to us. We usually find programs that take at least several hours to implement unless unusual care has been taken to ease this task for the user.

When an algorithm is already available, we enjoy many advantages compared to the situation where only a reference is known.

First, the properties of the algorithm are presumably better known, if not by the user himself, at least by other users. Thus, some knowledge of the features, advantages or pitfalls of an algorithm, or at least an implementation of an algorithm, can be determined from experience, available documentation or other users.

If the algorithm has been implemented by the user on his or her own PC, then there is a reasonable chance that the method is quite well understood. Many methods require a good comprehension of their workings to use them successfully. To attempt, for example, the blind use of a quadrature program for integrating a function with singularities is foolhardy unless it is specifically designed to handle such difficulties. Equally, for smooth functions, it is overkill to use a highly sophisticated adaptive quadrature method; a simple method is sufficient. One may also want to check tables of integrals to see if analytic solutions have been devised, in which case quadrature may be unnecessary.

If a method is "available" we also need to ensure that it fits the task. The Hooke and Jeeves function minimization uses very little working storage and has an extremely low requirement for memory to store program code. Nevertheless, it is very poorly suited to problems with large numbers of parameters due to the number of function evaluations occasioned by each axial search step. Thus, even if the Hooke and Jeeves method fits the memory size requirements for minimizing a function of many parameters, it cannot be said to "fit" the task overall, which must always presume a modicum of efficiency.

The method chosen must fit the PC on which computations will be done. This goes beyond the question of program and working storage. We must also consider the precision and speed of calculation, as well as the capacity of peripherals to store or transmit data at the required rate or to present it in a suitable format.

Finally, we should be comfortable in using the method. This may seem incongruous, since users are primarily interested in a solution rather than the route by which it is obtained. However, many problems are sufficiently difficult that there is a real chance that methods may fail to find a solution. Therefore, it can be important to understand the method sufficiently well to recognize, and if possible recover from, such failures. For example, in nonlinear least squares or function minimization calculations there may be a premature convergence to a false solution. By noting certain features of a tentative solution, the user may restart the search for a solution and obtain a correct result. Such questions are quite separate from matters of personal taste, that may also influence the choice of method.

20.4 Add-ons, Extras and Flexibility

In the best of all worlds, we could easily choose between computing platforms to select the most appropriate system in which to perform our computations. Furthermore, we could easily switch platforms without a huge effort in porting data and software.

The unkindness of the real world is such that few of us are prepared to switch machines frequently (see Sections 1-5, 2-6, and 11-8). Nevertheless, we may be prepared to change software within a given platform if this is easy to do. In this respect we urge users:

- To get hardware with sufficient power or capability to accommodate alternative uses. This implies sufficient memory and disk space, good hard-copy output devices such as printers, and floppy disk drives that can read several formats for diskettes. We also advise that there be several input/output ports for data transfer and pointing devices.
- To acquire software that is common or popular for our day-to-day work. This increases the likelihood that there is a colleague or associate using the software so that we can compare notes on "bugs" or fixes. For specialty work, one may be willing to try out esoterica. If it works, fine; if it does not, at

least our bread-and-butter tasks can carry on as usual.

Some users make the mistake of getting a portable machine when one is not appropriate. The possibility "I might like to take it home to do some work" overpowers the flexibility of a system with slots for add-in circuit boards, a larger and more colorful display and a full size keyboard. There are good applications for portable machines, but the flexibility of a desktop or tower unit is generally greater even if its mobility is restricted. For scientific users, we note that numeric co-processors are generally power-hungry and have been only rarely provided on portable machines, even as an option.

We think it is wise to avoid unnecessary extras such as games, utility programs we will not use, graphical curiosities, or noise makers.
Games distract from technical computing, they clutter the fixed disk and are common vectors of computer virus infections. We believe games should usually be kept off PCs used for technical computing except for those games used or being developed in the pursuit of educational goals. Games traded informally may be a vehicle for computer viruses.

PCs are often supplied with some interesting but inexpensive utility software. It is probably worth trying it out, but we recommend deletion or archiving of such software unless it is used regularly, as it will tend to get in the way of useful programs. We have noted that some programs have similar or identical names — a definite source of trouble.

The capability of laser printers and other high-resolution raster graphic devices to produce interesting print or display fonts and icons has led to a growing tendency for people to play with such capabilities. Rarely is this productive of research. Worse, graphics chew disk space and memory much faster than programs or scientific data. Moreover, when one really wants to prepare a display for a publication or presentation, it is necessary to wade through much unwanted material to find the useful fonts or designs.

Programs that make interesting sounds or "talk" using the standard loudspeaker of most PCs are pleasant toys. For the handicapped, there are proper versions of such tools, For the rest of us, leave them alone. On the Macintosh, we have observed some users changing the "attention" sound (usually beeps on MS-DOS machines) to duck quacks, breaking glass, or thunder noises.

The choice of method and algorithm for a given problem may be highly sensitive to goals ancillary or subsidiary to the solution itself. There may be concerns about the time required to obtain a solution, the availability of diagnostic checks of the method, the tests we can apply to the solution, additional information about the problem revealed by the method, or approximations or refinements of the solution.

Some examples may help to highlight these ideas. In tasks where the solution must be obtained within a specified time, such as control of industrial processes, it makes sense to disregard methods that are quite slow in computing answers, even if they offer other significant benefits. Where speed is not essential, we are better off to choose reliability. In linear least squares approximation, for example, we have preferred to use the singular value decomposition so we can know the extent of multicollinearity in our predicting data, although the svd is "slow" compared to other methods. Some methods provide information about the quality of solution as we proceed. Many quadrature methods and differential equation integrators provide an estimate of errors made in the approximations used. If such estimates are smaller than the accuracy required in our particular calculation there is no need for us to refine the results further.

We think the most useful extras for computational methods test the solution for correctness. (The numerical integration methods generally only provide error estimates, not error bounds.) Knowing that an answer is right gives great peace of mind, even if the answer is only for a subproblem.

Unfortunately, the specific data produced by a method and the format of its presentation are features that may outweigh all other considerations. If a particular layout of data is not generated, users or clients may reject a program based on a method of proven reliability in favor of less trustworthy software with a more familiar layout. For example, the Gauss-Jordan reduction for the solution of linear least squares regression calculations may suffer from severe (and usually undetectable) numerical instability. Yet this approach

lends itself extremely well to the determination of linear regression models in a stepwise fashion, with convenient statistical tests for the variables that should enter or leave the regression. The same Gauss-Jordan steps (or ***sweeps***) are similarly useful for linear programming calculations. The use of numerically more reliable approaches such as the QR decomposition achieved by Householder or Givens transformations or by the modified Gram-Schmidt method (Dahlquist and Bjorck, 1974) may leave the numerical analyst happy that the code is secure from computational disaster. However, the users or clients may still use the "old" programs, even if some efforts are made to discourage them.

Providing the intermediate output that users want while still using stable methods in their computation usually requires a good deal of extra program code. This may be an unwelcome addition to a computer program. The extra code is an annoyance not only because it requires effort to develop, but also because it increases the chance of errors and enlarges the chore of maintenance and documentation. If memory is scarce, then the extra code length and temporary variable and array storage may also create difficulties.

The weaning of users from unstable codes may require some compromise for both programmer and user. Sometimes, of course, these are the same person trying to reconcile conflicting objectives. When the method we would like to implement does not offer precisely the same output as wanted, there are often alternative possibilities that may ultimately prove more satisfactory. In linear regression, stepwise operation may be replaced, for instance, by a user selection of variables to appear in the model.

Where programs are provided as a service to others, the preservation of desired output formats can be helpful in the avoidance of objections based solely on unfamiliarity. If the benefits of the "new" method can be convincingly shown, then adoption of this method will generally follow. In linear regression, failures of the existing programs are a tremendous encouragement to change, but only if such failures occur on the user's own problems. Test cases, unless extremely realistic and relevant to the user's experience, may be written off as contrived. In our own experience however, users have often unwittingly brought us problems that provided far more challenges to software and methods than conventional tests found in the literature.

The ability to use a program with existing software and data is an important consideration for users, particularly if they have made a considerable investment of time, effort and money in existing collections.

20.5 Personal Choice and Satisfaction

The ultimate reason we use PCs is because they are under our own control. We can choose to follow or ignore fashions in computing. We can use our favorite program long after others have condemned it to the museum, or we can be the first on the block to break the seal on the diskette envelope of some new and untried software product. The main point is that we find we can do our job and find satisfaction in so doing.

We find the pressure to upgrade annoying, and the cost to our stretched budgets painful, especially as many "upgrades" seem only to repair errors or deficiencies in the versions for which we have already paid good money. Unfortunately, we may eventually be forced to adopt the new software as colleagues want to exchange data with us in new formats, or want us to carry out operations on this data using features only found in more recent versions of software.

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Some items are not cited in the body of the book but were used for background information. Section number references are given in square brackets.

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