Notes on Applied Science

No. 16

MODERN COMPUTING METHODS

NATIONAL PHYSICAL LABORATORY

Notes on Applied Science
No. 16

MODERN COMPUTING METHODS

LONDON
HER MAJESTY'S STATIONERY OFFICE
1957

PREFACE

The series of *Notes on Applied Science* is published by the National Physical Laboratory to provide industrialists and technicians with information on various scientific and technical subjects which is not readily available elsewhere. The experience of the Laboratory has indicated a number of subjects on which short monographs would be of value, and a list of those already written is given below:

No. 1.	Gauging and Measuring Screw Threads	Price 5*s*. 0*d*. (5*s*. 4*d*.)
No. 2.	The Industrial Application of Aerodynamic Techniques . .	Price 3*s*. 6*d*. (3*s*. 10*d*.)
No. 3.	Electrical Insulating Materials and Methods of Test . . .	Price 1*s*. 3*d*. (1*s*. 5*d*.)
No. 4.	Measurement of Humidity . .	Price 1*s*. 0*d*. (1*s*. 2*d*.)
No. 5.	Gauge Making and Measuring . .	Price 3*s*. 6*d*. (3*s*. 9*d*.)
No. 6.	Volumetric Glassware—Scientific Aspects of Design and Accuracy .	Price 1*s*. 6*d*. (1*s*. 8*d*.)
No. 7.	Balances, Weights, and Precise Laboratory Weighing . . .	Price 2*s*. 0*d*. (2*s*. 2*d*.)
No. 8.	Audio Frequency Power Measurements	Price 1*s*. 0*d*. (1*s*. 2*d*.)
No. 9.	Measurement of Pressure with the Mercury Barometer . . .	Price 1*s*. 0*d*. (1*s*. 2*d*.)
No. 10.	Noise Measurement Techniques .	Price 2*s*. 0*d*. (2*s*. 2*d*.)
No. 11.	Wind Effects on Bridges and other Flexible Structures . . .	Price 1*s*. 9*d*. (1*s*. 11*d*.)
No. 12.	Calibration of Temperature Measuring Instruments . . .	Price 2*s*. 6*d*. (2*s*. 8*d*.)
No. 13.	Standard Capacitors and their Accuracy in Practice . . .	Price 1*s*. 3*d*. (1*s*. 5*d*.)
No. 14.	Photometry of Telescopes and Binoculars	Price 2*s*. 0*d*. (2*s*. 2*d*.)
No. 15.	Application of Spring Strips to Instrument Design . . .	Price 2*s*. 0*d*. (2*s*. 2*d*.)
No. 17.	High Voltage Impulse Testing .	Price 1*s*. 6*d*. (1*s*. 8*d*.)
No. 18.	High Voltage Bridge Measurements at Power Frequencies . . .	In the press

Further information, or advice on specific questions, can be obtained by writing to the Director of the Laboratory.

The scientific work of the Laboratory is made generally known through the contributions which are made to learned societies, etc., and which appear in their journals. Details of these papers are contained in the Quarterly List of Papers Published. Application to be placed on the mailing list to receive, free, the Quarterly List and the List of N.P.L. Publications should be made to the Laboratory.

NATIONAL PHYSICAL LABORATORY
TEDDINGTON, MIDDLESEX
1957

INTRODUCTION

These notes on computation are based on lectures delivered by various members of the staff of Mathematics Division, N.P.L., as part of a vacation course on "Computers for Electrical Engineering Problems", organized by the Electrical Engineering Department of the Imperial College of Science and Technology, and attended by representatives of industrial firms. The course was designed to teach the basic principles of the use of analogue machines, high-speed digital computers, and the techniques of numerical mathematics involved in the solution of problems in electrical engineering.

Numerical methods are required in all branches of science, and the techniques are generally independent of the source of the problem. For example, the same type of differential equation may represent a problem in physiology as well as a problem in electrical engineering. The opportunity has therefore been taken to present, as one of the N.P.L. series of *Notes on Applied Science*, suitably edited versions of those lectures contributed to the course by members of Mathematics Division.

The first four chapters discuss "algebraic" problems. Chapter 3 considers the determination of the real and complex roots of polynomial equations, while Chapters 1, 2 and 4 are concerned with the basic problems of "linear algebra", the solution of simultaneous linear algebraic equations, the inversion of matrices, and the determination of their latent roots and vectors. Methods are included for use with desk machines and also with high-speed digital equipment.

The "analytical" part is contained in Chapters 5–9. Chapter 5 introduces the theory of finite differences, used in Chapters 6 and 7 to solve ordinary differential equations respectively of boundary-value and initial-value types. Chapter 8 considers the solution of hyperbolic partial differential equations by the method of "characteristics", and Chapter 9 discusses various methods of solving parabolic and elliptic partial differential equations.

Many problems in linear algebra, and the simultaneous finite-difference equations, linear or non-linear, used to represent the solution of differential equations, ordinary or partial, are often conveniently solved by methods of successive approximation, and the use of relaxation methods is described in Chapter 10.

Chapter 11 discusses the problems arising in the construction of mathematical tables, and Chapter 12 demonstrates the necessity of using a variety of techniques in the various stages of solving a given problem.

It is not possible, in twelve short chapters, to cover in detail all branches of the subject. Appendix 1, however, contains a fairly comprehensive bibliography of the most useful books and papers covering the various topics of numerical analysis, including some not considered in earlier chapters.

Appendix 2 gives a brief description of the DEUCE, the high-speed digital machine in operation in Mathematics Division, and illustrates its application to a given problem. The Division also operates a mechanical differential analyser, and Appendix 3 describes the basic features of such a machine and indicates the types of problem for which it might profitably be used.

It is not possible, and would certainly be misleading, to attempt an enumeration of the physical problems which can be solved by computation. Suffice it to say that almost any problem which can be represented by one or more mathematical formulae or equations is amenable to computing methods.

NATIONAL PHYSICAL LABORATORY

NOTES ON APPLIED SCIENCE No. 16

Modern Computing Methods

ERRATA

Page 49. Delete Table 2 and substitute the following:

x	η		δ^2		δ^4
+0·0	−0·00000				
		−11			
0·2	0·00011		+ 2		
		− 9		+5	
0·4	0·00020		+ 7		−4
		− 2		+1	
0·6	0·00022		+ 8		+1
		+ 6		+2	
0·8	0·00016		+10		
		+16			
+1·0	−0·00000				

National Physical Laboratory
June 1957

(70143) Wt. 4408/772 K20 6/57 Hw.

CONTENTS

APPENDICES

1

LINEAR EQUATIONS AND MATRICES (1)

DEFINITIONS AND PROPERTIES

1. A general set of linear simultaneous algebraic equations can be written in the form

$$\left.\begin{aligned} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n &= b_1, \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n &= b_2, \\ &\dots\dots\dots\dots \\ a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n &= b_n. \end{aligned}\right\} \quad (1)$$

The coefficients a_{rs} form a *square matrix*,

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}, \quad (2)$$

and the column of constants b_r forms a *column matrix* or *vector* $\mathbf{b}$. The unknowns x_r form a vector $\mathbf{x}$. Equations (1) can then be written in the shortened form

$$\mathbf{Ax} = \mathbf{b}, \quad (3)$$

and the left of (1) gives the rule for premultiplication of a vector by a matrix.

2. The solution of (1) can be written in general terms as

$$\left.\begin{aligned} x_1 &= \alpha_{11}b_1 + \alpha_{12}b_2 + \dots + \alpha_{1n}b_n, \\ x_2 &= \alpha_{21}b_1 + \alpha_{22}b_2 + \dots + \alpha_{2n}b_n, \\ &\dots\dots\dots\dots \\ x_n &= \alpha_{n1}b_1 + \alpha_{n2}b_2 + \dots + \alpha_{nn}b_n, \end{aligned}\right\} \quad (4)$$

or in matrix notation as

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}, \quad (5)$$

where $\mathbf{A}^{-1}$ has the same form as (2) with a replaced by α. The matrix $\mathbf{A}^{-1}$ is called the *inverse* or *reciprocal* of the matrix $\mathbf{A}$.

The elements α_{rs} of $\mathbf{A}^{-1}$ depend only on the elements a_{rs} of $\mathbf{A}$ and, in equations (4) for the solution of the given equations (1), it is clear that a knowledge of α_{rs} enables the answers to be obtained with relative ease: in particular if many sets of equations require solution for which only the right-hand sides b_r change, the evaluation of the elements α_{rs} of $\mathbf{A}^{-1}$, followed by insertion in (4) of the various b_r, may give the quickest method of solution. On the other hand, the determination of the α_{rs} is not trivial.

Equations (4) indicate one method of doing this: if in these equations we write $b_1 = 1, b_2 = b_3 = \ldots = b_n = 0$, we obtain the elements of the first column of the inverse. It follows that the various columns of $\mathbf{A}^{-1}$ can be found by solving in succession equations (1), in which the right-hand sides are replaced by successive columns of the matrix

$$\mathbf{I}_n = \begin{bmatrix} 1 & 0 & 0 & \ldots & . & 0 \\ 0 & 1 & 0 & \ldots & . & 0 \\ 0 & 0 & 1 & \ldots & . & 0 \\ . & . & . & \ldots & . & . \\ . & . & . & \ldots & . & . \\ 0 & 0 & 0 & \ldots & 0 & 1 \end{bmatrix}. \tag{6}$$

This is the *unit matrix* of order n or *identity matrix*, so called in virtue of the relation

$$\mathbf{I}_n \mathbf{x} = \mathbf{x}. \tag{7}$$

Another important property of $\mathbf{I}_n$ (or just $\mathbf{I}$ when the order is obvious) is derived from (5) by premultiplication with $\mathbf{A}$, giving

$$\mathbf{A}\mathbf{x} = \mathbf{A}\mathbf{A}^{-1}\mathbf{b} = \mathbf{b}$$

in virtue of (3), so that

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}. \tag{8}$$

3. The main properties of matrices required in practice are those of addition, multiplication, and transposition.

Matrices can be added only when of the same order, and if $\mathbf{B}$ is the matrix (2) in which a is replaced by b, then

$$\mathbf{A}+\mathbf{B} = \begin{bmatrix} a_{11}+b_{11}, & a_{12}+b_{12}, \ldots, a_{1n}+b_{1n} \\ a_{21}+b_{21}, & a_{22}+b_{22}, \ldots, a_{2n}+b_{2n} \\ \ldots\ldots & \ldots\ldots \\ a_{n1}+b_{n1}, & a_{n2}+b_{n2}, \ldots, a_{nn}+b_{nn} \end{bmatrix}. \tag{9}$$

If a matrix $\mathbf{A}$ is multiplied by a number k, the resulting matrix has elements ka_{rs}, that is every element is multiplied by k.

Square matrices of the same order can be multiplied, to give

$$\mathbf{AB} = \begin{bmatrix} a_{11}b_{11}+a_{12}b_{21}+a_{13}b_{31}+\ldots, & a_{11}b_{12}+a_{12}b_{22}+a_{13}b_{32}+\ldots, \ldots \\ a_{21}b_{11}+a_{22}b_{21}+a_{23}b_{31}+\ldots, & a_{21}b_{12}+a_{22}b_{22}+a_{23}b_{32}+\ldots, \ldots \\ \ldots\ldots & \ldots\ldots \end{bmatrix}. \tag{10}$$

If we use the notation $r_r(\mathbf{A}), c_r(\mathbf{A})$ to denote respectively the rth row and rth column of matrix $\mathbf{A}$, and $r_r c_s$ to denote the result of multiplying corresponding elements of r_r and c_s and adding the results (*scalar product*), we can write (10) in the simpler form

$$\mathbf{AB} = \begin{bmatrix} r_1(\mathbf{A})c_1(\mathbf{B}) & r_1(\mathbf{A})c_2(\mathbf{B}) & \ldots & r_1(\mathbf{A})c_n(\mathbf{B}) \\ r_2(\mathbf{A})c_1(\mathbf{B}) & r_2(\mathbf{A})c_2(\mathbf{B}) & \ldots & r_2(\mathbf{A})c_n(\mathbf{B}) \\ \ldots & \ldots & & \ldots \\ r_n(\mathbf{A})c_1(\mathbf{B}) & r_n(\mathbf{A})c_2(\mathbf{B}) & \ldots & r_n(\mathbf{A})c_n(\mathbf{B}) \end{bmatrix}. \tag{11}$$

From (11) it is obvious that in general $\mathbf{AB} \neq \mathbf{BA}$, so that the order of multiplication is important. In (11) we refer to $\mathbf{AB}$ as $\mathbf{B}$ premultiplied by $\mathbf{A}$, or multiplied on the left by $\mathbf{A}$, or as $\mathbf{A}$ postmultiplied by $\mathbf{B}$, or multiplied on the right by $\mathbf{B}$.

The transposed matrix of $\mathbf{A}$, called $\mathbf{A}'$, is derived from $\mathbf{A}$ by interchanging rows and columns. If a matrix is symmetric, so that $a_{rs} = a_{sr}$, then $\mathbf{A}' = \mathbf{A}$, and it follows from (11) that in this case

$$\mathbf{A}'\mathbf{A} = \mathbf{A}\mathbf{A}'. \tag{12}$$

The only other important cases in which the order of multiplication is immaterial are contained in the equations

$$\mathbf{AI} = \mathbf{IA}, \tag{13}$$

$$\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}. \tag{14}$$

The transpose of a product is given by

$$(\mathbf{AB})' = \mathbf{B}'\mathbf{A}'. \tag{15}$$

The final important rule is that for inversion of a product, and is given by

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}, \tag{16}$$

the order of multiplication being reversed as in (15).

4. Associated with a matrix $\mathbf{A}$ is its *determinant* det. A or $|A|$. Whereas the matrix is an array of numbers and can be regarded in many ways as an operator, the determinant is a pure number. For example

$$\begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix} = a_1 \begin{vmatrix} b_2 & b_3 \\ c_2 & c_3 \end{vmatrix} - a_2 \begin{vmatrix} b_1 & b_3 \\ c_1 & c_3 \end{vmatrix} + a_3 \begin{vmatrix} b_1 & b_2 \\ c_1 & c_2 \end{vmatrix}$$
$$= a_1(b_2c_3 - b_3c_2) - a_2(b_1c_3 - b_3c_1) + a_3(b_1c_2 - b_2c_1), \tag{17}$$

and the general rule for evaluation should be obvious. The determinant

$$A_1 = \begin{vmatrix} b_2 & b_3 \\ c_2 & c_3 \end{vmatrix}$$

is called the *first minor* of a_1, and is the determinant obtained by omitting from the original determinant the row and column containing a_1.

It can be shown that the inverse $\mathbf{A}^{-1}$ of $\mathbf{A}$ is given by

$$\frac{1}{|A|}\begin{bmatrix} A_{11} & -A_{21} & A_{31} & -A_{41} & \cdots \\ -A_{12} & A_{22} & -A_{32} & A_{42} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}. \tag{18}$$

Note that in (18) the minors A_{rs}, obtained by omitting from the original determinant the row and column containing a_{rs}, occur with alternate signs and are transposed in comparison with the corresponding elements a_{rs} of $\mathbf{A}$.

5. When $|A| = 0$, it is clear from (18) that the matrix **A** has no inverse. Such a matrix is called *singular*, and the corresponding linear equations have in general no solution. If $|A| = 0$ it means that the rows of **A** are not linearly independent, at least one being obtained by linear combinations of the others. For example in the equations

$$\left.\begin{aligned} x_1 + x_2 + x_3 &= b_1, \\ x_1 - x_2 + 2x_3 &= b_2, \\ 3x_1 + x_2 + 4x_3 &= b_3, \end{aligned}\right\} \tag{19}$$

it can be verified that the determinant

$$\begin{vmatrix} 1 & 1 & 1 \\ 1 & -1 & 2 \\ 3 & 1 & 4 \end{vmatrix} = 0,$$

and the third of (19) is obtained by adding twice the first to the second. In this case the equations are incompatible unless $2b_1 + b_2 = b_3$, and if this holds we have effectively only two equations in three unknowns, and there is an infinity of solutions.

If the equations are homogeneous, so that the constants b are all zero, the equations have no solution other than $x_1 = x_2 = \ldots = x_n = 0$ unless the determinant vanishes, in which case we can omit one equation and solve the rest to find the ratios of the x_r. For example, in (19), we can omit the last equation and solve

$$\left.\begin{aligned} x_1/x_3 + x_2/x_3 + 1 &= 0, \\ x_1/x_3 - x_2/x_3 + 2 &= 0, \end{aligned}\right\} \tag{20}$$

finding $x_1/x_3 = -1{\cdot}5$, $x_2/x_3 = 0{\cdot}5$, which also satisfy $3x_1/x_3 + x_2/x_3 + 4 = 0$, the last of (19).

In solving equations or inverting matrices in which the elements of the inverse matrix are large, often associated with a determinant small compared with the original coefficients, it is difficult to get accurate solutions: such equations are often called *ill-conditioned*.

SOLUTION OF EQUATIONS BY ELIMINATION OR PIVOTAL CONDENSATION

6. It is convenient, particularly if the coefficients in the equations differ widely, to multiply the rows by constants, making no change in the equations, and the columns by constants, involving a trivial change in the unknowns, so that the maximum coefficient in each row and column, including the constants column, lies between 0·1 and 1·0.

The simple elimination method taught at school is in practice carried out systematically and with the inclusion of frequent checks. If in equations (1), already treated as suggested in the last paragraph, we select the largest element of the coefficients of x_1, say a_{k1}, and add suitable multiples of the corresponding equation to all the other equations, so that in each resulting equation the coefficient of x_1 is zero, we shall be left with $(n-1)$ equations in the $(n-1)$ unknowns $x_2, x_3, \ldots, x_n$. The multipliers are clearly $-a_{11}/a_{k1}$, $-a_{21}/a_{k1}$, etc., and are all less than unity. The row containing

a_{h1}, the *pivot*, is called the *pivotal row*, and this equation is of course left unchanged and temporarily put aside. We now select as pivot the largest coefficient of x_2 in the new set of $(n-1)$ equations and repeat the process. Continuing in this way we have finally a single equation in the unknown x_n. The various pivotal rows are then assembled, and have the form

$$\left.\begin{aligned} c_{11}x_1+c_{12}x_2+\ldots \qquad\qquad +c_{1n}x_n &= d_1,\\ c_{22}x_2+c_{23}x_3+\ldots+c_{2n}x_n &= d_2,\\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots &\\ c_{n-1,n-1}x_{n-1}+c_{n-1,n}x_n &= d_{n-1},\\ c_{n,n}x_n &= d_n, \end{aligned}\right\} \tag{21}$$

and the production of this set of equations has been carried out by a process of *elimination* or *pivotal condensation*.

We can now calculate x_n directly from the last of (21), and inserting its calculated value in the previous equation we can obtain x_{n-1}, and so on. This process is called *back-substitution*.

Several sets of equations, for the same **A** and varying **b**, can be solved almost simultaneously as far as the elimination goes by keeping several columns **b**, and in particular these may be the columns of the unit matrix if $\mathbf{A}^{-1}$ is required. Each back-substitution process is of course performed separately.

The basic check on the elimination consists in carrying an extra column, whose rth element is formed of the sum of all the elements of **A** and **b** in the rth row. These elements are treated in the elimination exactly like the columns of constants, and after each elimination the "sum" element should be equal, apart from small end-figure discrepancies through accumulation of rounding errors, to the sum of the other elements in its row.

The final results are checked by direct insertion in the original equations or, usually sufficiently, into an equation given by the sum of the original equations, a check corresponding to the sum check in the elimination.

It is important to choose as pivot the largest element in a column; the multipliers are all then less than unity, and we can work with a constant number of decimals.

If the matrix of coefficients is symmetric, however, symmetry is maintained if pivots are chosen on the diagonal, and the work of elimination is reduced by a factor somewhat less than two.

Example

7. The solution of the equations

$$\left.\begin{aligned} 0{\cdot}4096x_1+0{\cdot}1234x_2+0{\cdot}3678x_3+0{\cdot}2943x_4 &= 0{\cdot}3597,\\ 0{\cdot}2246x_1+0{\cdot}3872x_2+0{\cdot}4015x_3+0{\cdot}1129x_4 &= 0{\cdot}1260,\\ 0{\cdot}3645x_1+0{\cdot}1920x_2+0{\cdot}3728x_3+0{\cdot}0643x_4 &= 0{\cdot}4810,\\ 0{\cdot}1784x_1+0{\cdot}4002x_2+0{\cdot}2786x_3+0{\cdot}3927x_4 &= -0{\cdot}3359, \end{aligned}\right\}$$

is carried out as follows. The pivots are in italics, and the sum column is labelled Σ. The multipliers are called m.

Elimination

m	x_1	x_2	x_3	x_4	**b**	**Σ**
	0·4096	0·1234	0·3678	0·2943	0·3597	1·5548
−0·5483	0·2246	0·3872	0·4015	0·1129	0·1260	1·2522
−0·8899	0·3645	0·1920	0·3728	0·0643	0·4810	1·4746
−0·4355	0·1784	0·4002	0·2786	0·3927	−0·3359	0·9140
−0·9221		0·3195	0·1998	−0·0485	−0·0712	0·3996(7)
−0·2372		0·0822	0·0455	−0·1976	0·1609	0·0910 ✓
		0·3465	0·1184	0·2645	−0·4925	0·2369 ✓
			0·0906	−0·2924	0·3829	0·1811(2)
−0·1921			0·0174	−0·2603	0·2777	0·0348 ✓
				−0·2041	+0·2041	0·0000 ✓

Back-substitution

x_1	x_2	x_3	x_4
1·0008	−0·9993	0·9989	−1·0000

Check in sum of original equations:

$$1{\cdot}1771x_1 + 1{\cdot}1028x_2 + 1{\cdot}4207x_3 + 0{\cdot}8642x_4 = 0{\cdot}6308\ (0{\cdot}6310).$$

The equations are somewhat ill-conditioned, seen by the loss of a significant figure in the third pivot, and the results cannot be guaranteed to more than three significant figures, even though the last check is good. If the constant terms are uncertain to the extent of half a unit in the last figure the solutions have greater tolerances.

If the pivots are selected at each stage from the largest coefficient in the complete relevant matrix, rather than from the columns in order, the tendency is for the pivots to lose significant figures gradually, and the last pivot is usually the smallest. It is unlikely that this choice leads to significantly greater accuracy in the final results.

There are several variations of this straightforward elimination process, described in detail in the first reference.

COMPACT ELIMINATION METHODS

8. For desk machines the disadvantage of the simple elimination method is the large amount of recording: there is a corresponding loss of accuracy, since at each recording a number is rounded and a small error introduced. This is avoided in the "compact" elimination methods, of which we describe the method of Doolittle applied to the set of four equations

$$\text{(i)}\quad a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 = b_1,$$
$$\text{(ii)}\quad a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + a_{24}x_4 = b_2,$$
$$\text{(iii)}\quad a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + a_{34}x_4 = b_3,$$
$$\text{(iv)}\quad a_{41}x_1 + a_{42}x_2 + a_{43}x_3 + a_{44}x_4 = b_4.$$

The procedure is as follows:

(*a*) Add a multiple of (i) to (ii) to eliminate x_1 from (ii), thus forming a new equation (ii).

(*b*) Add multiples of (i) and the new (ii) to (iii) to eliminate x_1 and x_2 from (iii), thus forming a new equation (iii).

(*c*) Add multiples of (i), the new (ii) and the new (iii) to (iv) to eliminate x_1, x_2 and x_3 from (iv), thus forming a new (iv).

The resulting equations (i), the new (ii), the new (iii) and the new (iv) have the form of (21), and can be solved as before by back-substitution. As before, a sum column is used as a check.

The computing sheet has the following appearance:

$$\begin{array}{ccccccccc} m_{12} & m_{13} & m_{14} & a_{11} & a_{12} & a_{13} & a_{14} & b_1 & \Sigma_1 \\ & m_{23} & m_{24} & & \alpha_{22} & \alpha_{23} & \alpha_{24} & \beta_2 & \Sigma_2 \\ & & m_{34} & & & \alpha_{33} & \alpha_{34} & \beta_3 & \Sigma_3 \\ & & & & & & \alpha_{44} & \beta_4 & \Sigma_4 \end{array}$$

The first multiplier m_{12} is obtained from the equation

$$m_{12}a_{11}+a_{21}=0,$$

and the coefficients of the new (ii) are obtained from equations typified by

$$\alpha_{24}=m_{12}a_{14}+a_{24}.$$

The second column of multipliers is obtained from the equations

$$m_{13}a_{11}+a_{31}=0,$$
$$m_{13}a_{12}+m_{23}\alpha_{22}+a_{32}=0,$$

and the coefficients of the new (iii) from equations typified by

$$\beta_3=m_{13}b_1+m_{23}\beta_2+b_3.$$

Finally, the last column of multipliers is obtained from the equations

$$\begin{aligned} m_{14}a_{11}+a_{41} &= 0, \\ m_{14}a_{12}+m_{24}\alpha_{22}+a_{42} &= 0, \\ m_{14}a_{13}+m_{24}\alpha_{23}+m_{34}\alpha_{33}+a_{43} &= 0, \end{aligned}$$

and the coefficients of the new (iv) from equations typified by

$$\alpha_{44}=m_{14}a_{14}+m_{24}\alpha_{24}+m_{34}\alpha_{34}+a_{44}.$$

The final equations from which back-substitution is performed are closely allied to the pivotal rows of the previous method. If in the latter the chosen pivot was at each stage the first element of successive columns the two sets of final equations would be identical.

The saving in recording time and space is clear. The arrangement is also satisfactory in that quantities to be multiplied together lie in the same row of the computing sheet. The method of Crout, described in the first reference, has an apparently still more compact lay-out but is less proof against error, since numbers to be multiplied together do not have this favourable combination of position.

In the case of symmetric matrices there is a saving of labour, since the m are computed trivially from the α by the relation $m_{tj} = -\alpha_{tj}/\alpha_{tt}$.

METHODS DEPENDING ON MATRIX PROPERTIES

9. The matrix of coefficients c_{rs} in (21) is denoted by **U** and called upper triangular, since all its elements are zero below the main diagonal. A matrix with zero elements above this diagonal is labelled **L** and called lower triangular. Triangular matrices are obviously more convenient than complete matrices for solving linear equations: the determinant of such a matrix, moreover, is just the product of the diagonal terms.

With the Gauss elimination method, the original equations (1), for which the matrix is complete, were transformed into equations (21), for which the matrix is upper triangular. It can be shown that the elimination was effectively equivalent to multiplying the original **A** by a lower triangle **L**, producing an upper triangle **U**, so that

$$\mathbf{LA} = \mathbf{U}, \tag{22}$$

and

$$\mathbf{LAx} = \mathbf{Ux} = \mathbf{Lb}, \tag{23}$$

were the equations from which the answers were obtained by back-substitution. The matrix **L** has units in its diagonal so that, since **LA** = **U**, it follows that the determinant of **A** is the same as that of **U** and equal to the product of the diagonal terms of **U**. (If the pivots do not all lie on the diagonal, the sign of the determinant may be changed.) The Doolittle method can be regarded similarly as the result of matrix operations.

Another class of method, the best for desk machines, uses the fact that a square matrix with non-singular principal minors can be expressed as the product of two triangles, in the form

$$\mathbf{A} = \mathbf{LU}. \tag{24}$$

The diagonal terms of either **L** or **U** can be chosen arbitrarily, the rest being then determined uniquely. If the matrix is symmetric the diagonals of **U** are best taken to be the same as those of **L**, and then **U** is the transpose of **L**, so that only one triangle has to be determined from the equation

$$\mathbf{A} = \mathbf{LL}', \tag{25}$$

though some elements may be imaginary if **A** is not positive definite.

10. When multiplying two matrices with desk machines, it is best to record the transpose of the right-hand matrix, vertically beneath the left-hand matrix, so that the rule (11) for multiplication can be written as

$$\mathbf{AB} = \begin{bmatrix} r_1(\mathbf{A})r_1(\mathbf{B}') & r_1(\mathbf{A})r_2(\mathbf{B}') & \dots \\ r_2(\mathbf{A})r_1(\mathbf{B}') & r_2(\mathbf{A})r_2(\mathbf{B}') & \dots \\ \dots & \dots & \dots \end{bmatrix},$$

and elements of rows are multiplied together, corresponding elements lying in the same column. In particular, if **B** is **A**′, we have

$$\mathbf{AA}' = \begin{bmatrix} \{r_1(\mathbf{A})\}^2 & r_1(\mathbf{A})r_2(\mathbf{A}) & \dots \\ r_1(\mathbf{A})r_2(\mathbf{A}) & \{r_2(\mathbf{A})\}^2 & \dots \\ \dots & \dots & \dots \end{bmatrix}. \tag{26}$$

The determination of **L** and **U** in general is sufficiently illustrated by consideration of a matrix of order three. The notation and arrangement are as follows, the triangle **L** being taken as unit triangle, and the transpose of the upper triangle **U** being the lower triangle **U**′.

	A			**b**	**Σ**
	a_{11}	a_{12}	a_{13}	b_1	Σ_1
	a_{21}	a_{22}	a_{23}	b_2	Σ_2
	a_{31}	a_{32}	a_{33}	b_3	Σ_3
	L				
	1				
	l_{21}	1			
	l_{31}	l_{32}	1		
	U′			**s**	**x**
	u_{11}			s_1	x_1
	u_{12}	u_{22}		s_2	x_2
	u_{13}	u_{23}	u_{33}	s_3	x_3
y′	y_1	y_2	y_3		
S	S_1	S_2	S_3		

The method and order of calculation are as follows. The multiplication rule gives

$a_{11} = r_1(\mathbf{L})r_1(\mathbf{U}') = u_{11}$, $a_{12} = r_1(\mathbf{L})r_2(\mathbf{U}') = u_{12}$, $a_{13} = r_1(\mathbf{L})r_3(\mathbf{U}') = u_{13}$, giving the first column of **U**′;

$a_{21} = r_2(\mathbf{L})r_1(\mathbf{U}') = l_{21}u_{11}$, giving the second row of **L**;

$a_{22} = r_2(\mathbf{L})r_2(\mathbf{U}') = l_{21}u_{12}+u_{22}$, $a_{23} = r_2(\mathbf{L})r_3(\mathbf{U}') = l_{21}u_{13}+u_{23}$, giving the second column of **U**′;

$a_{31} = r_3(\mathbf{L})r_1(\mathbf{U}') = l_{31}u_{11}$, $a_{32} = r_3(\mathbf{L})r_2(\mathbf{U}') = l_{31}u_{12}+l_{32}u_{22}$, giving the third row of **L**; and finally

$a_{33} = r_3(\mathbf{L})r_3(\mathbf{U}') = l_{31}u_{13}+l_{32}u_{23}+u_{33}$, giving the last element in **U**′.

In the symmetric case **U**′ is **L** and need not be recorded, the diagonal terms of **L** are denoted by l_{11}, l_{22} and l_{33}, and we have the equations

$$
\begin{aligned}
a_{11} &= l_{11}^2, \quad a_{12} = l_{11}l_{21}, \quad a_{13} = l_{11}l_{31},\\
a_{22} &= l_{21}^2 + l_{22}^2, \quad a_{23} = l_{21}l_{31} + l_{22}l_{32},\\
a_{33} &= l_{31}^2 + l_{32}^2 + l_{33}^2,
\end{aligned}
$$

for the successive determination of the l_{rs}.

11. When this triangular resolution is finished, we can solve the linear equations (3) by two processes of back-substitution. Introducing the auxiliary vector **y**, defined by

$$\mathbf{Ux} = \mathbf{y}, \tag{27}$$

we can write
$$\mathbf{Ax} = \mathbf{LUx} = \mathbf{Ly} = \mathbf{b}, \tag{28}$$
solving for **y** from the last of (28), and for **x** from (27).

The elements of **y** are obtained in the same way as those of **U′**. If these are written in transposed form as a row vector with components y_1, y_2, y_3, shown in position in the arrangement of § 10, then the equation $\mathbf{Ly} = \mathbf{b}$ gives
$$y_1 = b_1, \quad l_{21}y_1 + y_2 = b_2, \quad l_{31}y_1 + l_{32}y_2 + y_3 = b_3,$$
from which the y_r are obtained in succession.

As a check on all this work we form the sum column Σ, composed of the row sums of **A** and **b**, and a sum row **S**, composed of the column sums of **U′** and **y′**. As each of the latter becomes available we use the successive relations
$$r_1(\mathbf{L})\,\mathbf{S} = \Sigma_1, \quad r_2(\mathbf{L})\,\mathbf{S} = \Sigma_2, \quad r_3(\mathbf{L})\,\mathbf{S} = \Sigma_3,$$
or
$$S_1 = \Sigma_1, \quad l_{21}S_1 + S_2 = \Sigma_2, \quad l_{31}S_1 + l_{32}S_2 + S_3 = \Sigma_3.$$

We finally calculate **x** from (27) from equations typified by
$$c_r(\mathbf{U}')\,\mathbf{x} = y_r. \tag{29}$$
The elements of **x** are recorded as shown, and calculated from the successive equations obtained by taking $r = 3, 2, 1$ in (29), and given by $u_{33}x_3 = y_3$, $u_{23}x_3 + u_{22}x_2 = y_2$, $u_{13}x_3 + u_{12}x_2 + u_{11}x_1 = y_1$. If **s** is the column formed of the row sums of **U′**, a suitable check on this back-substitution is given by
$$s_1x_1 + s_2x_2 + s_3x_3 = y_1 + y_2 + y_3.$$

If the matrix is symmetric, equations (27) and (28) are replaced by
$$\left.\begin{aligned} \mathbf{L}'\mathbf{x} &= \mathbf{y}, \\ \mathbf{Ax} = \mathbf{LL}'\mathbf{x} &= \mathbf{Ly} = \mathbf{b}, \end{aligned}\right\} \tag{30}$$
so that $\mathbf{U}' = \mathbf{L}$ and the only change in arrangement is the complete omission of **U′**, the sums **S** and **s** being attached to **L**.

12. The solution by this method of the previous example is given below. The fact that the answers are exactly correct to four decimals is rather fortuitous, though the accuracy might be expected to be slightly better than that of the previous method.

	A			**b**	**Σ**
0·4096	0·1234	0·3678	0·2943	0·3597	1·5548
0·2246	0·3872	0·4015	0·1129	0·1260	1·2522(1)
0·3645	0·1920	0·3728	0·0643	0·4810	1·4746
0·1784	0·4002	0·2786	0·3927	−0·3359	0·9140

	L		
1			
0·5483	1		
0·8899	0·2572	1	
0·4355	1·0844	16·6509	1

	U′				s	x
	0·4096				0·4096	+1·0000
	0·1234	0·3195			0·4429	−1·0000
	0·3678	0·1998	−0·0059		0·5617	+1·0000
	0·2943	−0·0485	−0·1851	3·3992	3·4599	−1·0000
y′	0·3597	−0·0712	0·1792	−3·3992	(−2·9315√)	
S	1·5548√	0·3996√	−0·0118√	0·0000√		

13. For matrix inversion there are various possibilities following the triangular resolution. We can invert both **L** and **U**, then finding $\mathbf{A}^{-1}$ from

$$\left.\begin{aligned} \mathbf{A}^{-1} &= \mathbf{U}^{-1}\mathbf{L}^{-1} \text{ (unsymmetric case)},\\ \mathbf{A}^{-1} &= (\mathbf{L}')^{-1}\mathbf{L}^{-1} \text{ (symmetric case)}. \end{aligned}\right\} \quad (31)$$

In the second of (31), of course, $\mathbf{L}^{-1} = \{(\mathbf{L}')^{-1}\}'$, so that only one triangle has to be inverted.

The arrangement for inversion of triangles and the final multiplication, together with other still more compact methods in which the triangles are not inverted, are described fully in the references. These compact methods are important for the economical use of desk machines.

14. The application of methods of iteration or successive approximation are described in Chapter 10.

REFERENCES

Fox, L. 1954 Practical solution of linear equations and inversion of matrices. *Appl. Math. Ser. U.S. Bur. Stand.*, 39, 1–54. Washington: Government Printing Office.

Compact methods of inversion are also described in

Fox, L. and Hayes, J. G. 1951 More practical methods for the inversion of matrices. *J. R. Statist. Soc.* B, 13, 83–91.