

CONTENTS

Preface to the Second Edition	ix
Preface to the First Edition	xi
1. A STARTING POINT	1
1.1. Purpose and scope	1
1.2. Machine characteristics	3
1.3. Sources of programs	9
1.4. Programming languages used and structured programming	11
1.5. Choice of algorithms	13
1.6. A method for expressing algorithms	15
1.7. General notation	17
1.8. Software engineering issues	17
2. FORMAL PROBLEMS IN LINEAR ALGEBRA	19
2.1. Introduction	19
2.2. Simultaneous linear equations	19
2.3. The linear least-squares problem	21
2.4. The inverse and generalised inverse of a matrix	24
2.5. Decompositions of a matrix	26
2.6. The matrix eigenvalue problem	28
3. THE SINGULAR-VALUE DECOMPOSITION AND ITS USE TO SOLVE LEAST-SQUARES PROBLEMS	30
3.1. Introduction	30
3.2. A singular-value decomposition algorithm	31
3.3. Orthogonalisation by plane rotations	32
3.4. A fine point	35
3.5. An alternative implementation of the singular-value decomposi- tion	38
3.6. Using the singular-value decomposition to solve least-squares problems	40
4. HANDLING LARGER PROBLEMS	49
4.1. Introduction	49
4.2. The Givens' reduction	49
4.3. Extension to a singular-value decomposition	54
4.4. Some labour-saving devices	54
4.5. Related calculations	63
5. SOME COMMENTS ON THE FORMATION OF THE CROSS- PRODUCTS MATRIX $\mathbf{A}^T \mathbf{A}$	66

6. LINEAR EQUATIONS-A DIRECT APPROACH	72
6.1. Introduction	72
6.2. Gauss elimination	72
6.3. Variations on the theme of Gauss elimination	80
6.4. Complex systems of equations	82
6.5. Methods for special matrices	83
7. THE CHOLESKI DECOMPOSITION	84
7.1. The Choleski decomposition	84
7.2. Extension of the Choleski decomposition to non-negative definite matrices	86
7.3. Some organisational details	90
8. THE SYMMETRIC POSITIVE DEFINITE MATRIX AGAIN	94
8.1. The Gauss-Jordan reduction	94
8.2. The Gauss-Jordan algorithm for the inverse of a symmetric positive definite matrix	97
9. THE ALGEBRAIC EIGENVALUE PROBLEM	102
9.1. Introduction	102
9.2. The power method and inverse iteration	102
9.3. Some notes on the behaviour of inverse iteration	108
9.4. Eigensolutions of non-symmetric and complex matrices	110
10. REAL SYMMETRIC MATRICES	119
10.1. The eigensolutions of a real symmetric matrix	119
10.2. Extension to matrices which are not positive definite	121
10.3. The Jacobi algorithm for the eigensolutions of a real symmetric matrix	126
10.4. Organisation of the Jacobi algorithm	128
10.5. A brief comparison of methods for the eigenproblem of a real symmetric matrix	133
11. THE GENERALISED SYMMETRIC MATRIX EIGENVALUE PROBLEM	135
12. OPTIMISATION AND NONLINEAR EQUATIONS	142
12.1. Formal problems in unconstrained optimisation and nonlinear equations	142
12.2. Difficulties encountered in the solution of optimisation and nonlinear-equation problems	146
13. ONE-DIMENSIONAL PROBLEMS	148
13.1. Introduction	148
13.2. The linear search problem	148
13.3. Real roots of functions of one variable	160

14. DIRECT SEARCH METHODS	168
14.1. The Nelder-Mead simplex search for the minimum of a function of several parameters	168
14.2. Possible modifications of the Nelder-Mead algorithm	172
14.3. An axial search procedure	178
14.4. Other direct search methods	182
15. DESCENT TO A MINIMUM I: VARIABLE METRIC ALGORITHMS	186
15.1. Descent methods for minimisation	186
15.2. Variable metric algorithms	187
15.3. A choice of strategies	190
16. DESCENT TO A MINIMUM II: CONJUGATE GRADIENTS	197
16.1. Conjugate gradients methods	197
16.2. A particular conjugate gradients algorithm	198
17. MINIMISING A NONLINEAR SUM OF SQUARES	207
17.1. Introduction	207
17.2. Two methods	208
17.3. Hartley's modification	210
17.4. Marquardt's method	211
17.5. Critique and evaluation	212
17.6. Related methods	215
18. LEFT-OVERS	218
18.1. Introduction	218
18.2. Numerical approximation of derivatives	218
18.3. Constrained optimisation	221
18.4. A comparison of function minimisation and nonlinear least-squares methods	226
19. THE CONJUGATE GRADIENTS METHOD APPLIED TO PROBLEMS IN LINEAR ALGEBRA	234
19.1. Introduction	234
19.2. Solution of linear equations and least-squares problems by conjugate gradients	235
19.3. Inverse iteration by algorithm 24	241
19.4. Eigensolutions by minimising the Rayleigh quotient	243
APPENDICES	253
1. Nine test matrices	253
2. List of algorithms	255
3. List of examples	256
4. Files on the software diskette	258
BIBLIOGRAPHY	263
INDEX	271