Contents

Preface v

Chapter 1 A summary of FORTRAN 77 1

1.1 Program body 2
1.1.1 Subprograms 2
1.1.2 Continuation lines 2
1.1.3 Statement labels 3
1.1.4 Comments 3
1.2 Constants 3
1.3 Variables 4
1.3.1 Type specifications 4
1.4 Arrays 5
1.5 Assignment statements 6
1.5.1 Mixed-mode expressions 7
1.5.2 Order of priority 8
1.5.3 Intrinsic functions 9
1.6 The PARAMETER statement 10
1.7 The GO TO statement 11
1.8 IF statements 11
1.8.1 The logical IF 11
1.8.2 The block IF structure 13
1.9 Loops 15
1.9.1 DO loop 15
1.9.2 Repeat-until loop 16
1.10 Input 17
1.10.1 Inputting arrays 18
1.10.2 Inputting from a file 20
1.11 Output 20
1.11.1 Outputting arrays 22
1.11.2 Outputting to a file 23
1.12 Functions and subroutines 24
1.12.1 Function subprograms 24
1.12.2 Subroutines 25
1.12.3 Dynamic bounds 26

1.12.4 INTRINSIC statement 27
1.12.5 EXTERNAL statement 28

Chapter 2 Program construction 29

2.1 Example 1 30
2.1.1 Defining the algorithm 30
2.1.2 Bounding the number of iterations 31
2.1.3 Planning the program 32
2.1.4 Writing the subroutine 34
2.1.5 Multi-exit loops 38
2.1.6 Testing the program 42
2.2 Example 2 45
2.2.1 The main subprogram 45
2.2.2 The subroutines 46
2.2.3 Use of files 47

Chapter 3 Rounding errors, conditioning and stability 51

3.1 Round-off errors 52
3.1.1 Computer arithmetic 55
3.1.2 Relative error test 61
3.2 Conditioning and stability 62

Chapter 4 Non-linear algebraic equations 65

4.1 Methods without derivatives 66
4.1.1 Bisection method 66
4.1.2 Regula falsi method 75
4.1.3 Secant method 77
4.1.4 Successive substitution 83
4.1.5 Successive substitution with bisection 92
4.1.6 Aitken's Δ^2 process 93
4.2 Methods with derivatives 97
4.2.1 Newton's method 97
4.2.2 The order of an iterative method 103
4.3 Polynomial equations 105
4.3.1 Real zeros and Newton's method 106
4.3.2 Complex zeros and Bairstow's method 111
Exercises 119

Chapter 5 Linear algebraic equations 123

5.1 Direct methods 124
5.1.1 Gaussian elimination 126
5.1.2 Pivoting strategy 133
5.1.3 Scaling 139
5.1.4 *LU* decomposition 141

	5.1.5 The inverse matrix	156
	5.1.6 Tri-diagonal systems	157
	5.1.7 Iterative refinement	161
	5.1.8 Ill-conditioning	166
5.2	Iterative methods	169
	5.2.1 Jacobi's method	169
	5.2.2 The Gauss–Seidel method	174
	5.2.3 Successive over-relaxation	176
	5.2.4 Convergence	176
	Exercises	181
Chapter 6	**Eigenvalues and eigenvectors**	**187**
6.1	Basic theory	188
6.2	Methods for a single eigenvalue	192
	6.2.1 The power method	192
	6.2.2 Acceleration techniques	197
	6.2.3 Deflation	203
	6.2.4 The inverse power method	204
6.3	Methods for a complete eigensystem	210
	6.3.1 Jacobi's method	210
	Exercises	220
Chapter 7	**Discrete function approximation**	**223**
7.1	Polynomial interpolation	224
	7.1.1 Lagrangian interpolation	225
	7.1.2 Cubic spline interpolation	232
7.2	Data fitting	242
	7.2.1 Least squares approximation	244
	7.2.2 Piecewise polynomial approximation	248
	7.2.3 Alternative approximating functions	255
	Exercises	258
Chapter 8	**Differentiation and integration**	**261**
8.1	Differentiation	262
	8.1.1 Differentiating a tabulated function	262
	8.1.2 Differentiating an analytic function	265
	8.1.3 Rounding error versus truncation error	266
	8.1.4 Richardson extrapolation	267
8.2	Integration	269
	8.2.1 Newton–Cotes formulae	270
	8.2.2 Composite rules	273
	8.2.3 Romberg integration	276
	8.2.4 Gaussian quadrature	282
	8.2.5 Adaptive quadrature	287
	Exercises	296

Chapter 9 Ordinary differential equations 299

9.1 First-order initial-value problems 300
9.1.1 Series method 301
9.1.2 Single-step methods 303
9.1.3 Multistep methods 328
9.1.4 Comparison of Runge–Kutta and predictor–corrector methods 342
9.2 Systems and higher order initial-value problems 343
9.2.1 Systems of first-order equations 344
9.2.2 Higher order initial-value problems 350
9.3 Boundary value problems 351
9.3.1 The shooting method 352
9.3.2 Finite-difference methods 358
Exercises 366

Appendix A Useful mathematical results 371

Appendix B FORTRAN operators and intrinsic functions 375

Appendix C Programs, subroutines and functions 379

Answers to exercises 381

Bibliography 385

Index 387