



# SCIENTIFIC COMPUTING

## AN INTRODUCTORY SURVEY

SECOND EDITION

MICHAEL T. HEATH

INTERNATIONAL EDITION

# Contents

<b>Preface</b>	<b>vii</b>
<b>Notation</b>	<b>xi</b>
<b>1 Scientific Computing</b>	<b>1</b>
1.1 Introduction	1
1.2 Approximations in Scientific Computation	4
1.3 Computer Arithmetic	16
1.4 Mathematical Software	33
1.5 Historical Notes and Further Reading	38
<b>2 Systems of Linear Equations</b>	<b>49</b>
2.1 Linear Systems	49
2.2 Existence and Uniqueness	51
2.3 Sensitivity and Conditioning	52
2.4 Solving Linear Systems	63
2.5 Special Types of Linear Systems	84
2.6 Iterative Methods for Linear Systems	89
2.7 Software for Linear Systems	89
2.8 Historical Notes and Further Reading	92
<b>3 Linear Least Squares</b>	<b>105</b>
3.1 Linear Least Squares Problems	105
3.2 Existence and Uniqueness	109
3.3 Sensitivity and Conditioning	113
3.4 Problem Transformations	117
3.5 Orthogonalization Methods	121
3.6 Singular Value Decomposition	137
3.7 Comparison of Methods	143
3.8 Software for Linear Least Squares	144
3.9 Historical Notes and Further Reading	145
<b>4 Eigenvalue Problems</b>	<b>157</b>
4.1 Eigenvalues and Eigenvectors	157
4.2 Existence and Uniqueness	160
4.3 Sensitivity and Conditioning	166

4.4	Problem Transformations	169
4.5	Computing Eigenvalues and Eigenvectors	173
4.6	Generalized Eigenvalue Problems	201
4.7	Computing the Singular Value Decomposition	202
4.8	Software for Eigenvalue Problems	202
4.9	Historical Notes and Further Reading	204
<b>5</b>	<b>Nonlinear Equations</b>	<b>216</b>
5.1	Nonlinear Equations	216
5.2	Existence and Uniqueness	217
5.3	Sensitivity and Conditioning	221
5.4	Convergence Rates and Stopping Criteria	222
5.5	Nonlinear Equations in One Dimension	224
5.6	Systems of Nonlinear Equations	237
5.7	Software for Nonlinear Equations	243
5.8	Historical Notes and Further Reading	244
<b>6</b>	<b>Optimization</b>	<b>256</b>
6.1	Optimization Problems	256
6.2	Existence and Uniqueness	259
6.3	Sensitivity and Conditioning	269
6.4	Optimization in One Dimension	270
6.5	Unconstrained Optimization	276
6.6	Nonlinear Least Squares	285
6.7	Constrained Optimization	288
6.8	Software for Optimization	295
6.9	Historical Notes and Further Reading	296
<b>7</b>	<b>Interpolation</b>	<b>309</b>
7.1	Interpolation	309
7.2	Existence, Uniqueness, and Conditioning	312
7.3	Polynomial Interpolation	313
7.4	Piecewise Polynomial Interpolation	326
7.5	Software for Interpolation	331
7.6	Historical Notes and Further Reading	333
<b>8</b>	<b>Numerical Integration and Differentiation</b>	<b>339</b>
8.1	Integration	339
8.2	Existence, Uniqueness, and Conditioning	341
8.3	Numerical Quadrature	342
8.4	Other Integration Problems	359
8.5	Integral Equations	362
8.6	Numerical Differentiation	365
8.7	Richardson Extrapolation	369
8.8	Software for Integration and Differentiation	371
8.9	Historical Notes and Further Reading	373

<b>9</b>	<b>Initial Value Problems for ODEs</b>	<b>382</b>
9.1	Ordinary Differential Equations	382
9.2	Existence, Uniqueness, and Conditioning	387
9.3	Numerical Solution of ODEs	390
9.4	Software for ODE Initial Value Problems	413
9.5	Historical Notes and Further Reading	414
<b>10</b>	<b>Boundary Value Problems for ODEs</b>	<b>422</b>
10.1	Boundary Value Problems	422
10.2	Existence, Uniqueness, and Conditioning	424
10.3	Shooting Method	427
10.4	Finite Difference Method	430
10.5	Collocation Method	432
10.6	Galerkin Method	436
10.7	Eigenvalue Problems	440
10.8	Software for ODE Boundary Value Problems	441
10.9	Historical Notes and Further Reading	442
<b>11</b>	<b>Partial Differential Equations</b>	<b>447</b>
11.1	Partial Differential Equations	447
11.2	Time-Dependent Problems	453
11.3	Time-Independent Problems	461
11.4	Direct Methods for Sparse Linear Systems	464
11.5	Iterative Methods for Linear Systems	467
11.6	Comparison of Methods	480
11.7	Software for Partial Differential Equations	483
11.8	Historical Notes and Further Reading	485
<b>12</b>	<b>Fast Fourier Transform</b>	<b>495</b>
12.1	Trigonometric Interpolation	495
12.2	FFT Algorithm	498
12.3	Applications of DFT	502
12.4	Wavelets	504
12.5	Software for FFT	505
12.6	Historical Notes and Further Reading	506
<b>13</b>	<b>Random Numbers and Simulation</b>	<b>511</b>
13.1	Stochastic Simulation	511
13.2	Randomness and Random Numbers	512
13.3	Random Number Generators	513
13.4	Quasi-Random Sequences	515
13.5	Software for Generating Random Numbers	516
13.6	Historical Notes and Further Reading	517
	<b>Bibliography</b>	<b>523</b>
	<b>Index</b>	<b>549</b>