

# **Contents**

<i>Preface</i>	1
<b>INTRODUCTION</b>	7
<b>1. FUNDAMENTALS OF UNCONSTRAINED OPTIMIZATION</b>	
1.1 Introduction	7
1.1.1 Vectors, functions and derivatives	7
1.1.2 Types of unconstrained minimum	9
1.2 Necessary and Sufficient Conditions for an Unconstrained Minimum	14
1.2.1 The first-order condition	14
1.2.2 Second-order conditions	15
1.3 Quadratic Functions	16
1.3.1 Derivatives of quadratic functions	16
1.3.2 Types of quadratic function	17
1.3.3 The eigensystem of the Hessian matrix	19
1.4 The Convergence of Minimization Algorithms	23
1.4.1 Stability	23
1.4.2 Rate of convergence	24
1.5 Summary	25
<b>2. UNIVARIATE MINIMIZATION</b>	26
2.1 Introduction	26
2.1.1 Linear search and univariate minimization	26
2.2 Function Comparison Methods	27
2.2.1 Basic principles	28
2.2.2 Fibonacci search	30
2.2.3 Golden Section search	31
2.2.4 Bisection	34
2.3 Polynomial Interpolation Methods	35
2.3.1 Quadratic interpolation	36
2.3.2 Cubic interpolation	38
2.4 Interval Location	41
2.4.1 Function comparison methods	41
2.4.2 Polynomial extrapolation methods	41
2.5 Hybrid Methods	46
2.5.1 Combined quadratic approximation and Golden Section	46
2.5.2 Combined cubic approximation and bisection	50

2.6 Aspects of Univariate Minimization Specific to Linear Search	51
2.6.1 Use of derivatives in linear search	51
2.6.2 Termination criteria for inaccurate linear search	53
2.7 Summary	55
<b>3. MULTIVARIATE MINIMIZATION</b>	<b>56</b>
3.1 Introduction	56
3.1.1 Gradient methods	56
3.1.2 Descent directions and directions of negative curvature	57
3.1.3 Exact linear search	58
3.1.4 Finite difference techniques	58
3.2 The Method of Steepest Descent	59
3.2.1 Convergence	60
3.3 Modified Newton Methods	61
3.3.1 Newton's method	62
3.3.2 Convergence of Newton's method	63
3.3.3 Using the eigensystem of the Hessian matrix	64
3.3.4 Using the Cholesky factorization of the Hessian matrix	65
3.3.5 Saddle points	66
3.3.6 Sparsity in the Hessian matrix	68
3.3.7 The performance of modified Newton methods	69
3.4 Conjugate Gradient Methods	73
3.4.1 Conjugacy and linear independence	74
3.4.2 Quadratic termination	75
3.4.3 The construction of conjugate search vectors	76
3.4.4 Conjugate gradient methods for non-quadratic functions	79
3.4.5 Convergence	80
3.4.6 Projection matrices	81
3.4.7 The derivation of particular conjugate gradient methods	81
3.4.8 Partial conjugate gradient methods	82
3.4.9 The performance of conjugate gradient methods	83
3.5 Quasi-Newton Methods	84
3.5.1 The David–Fletcher–Powell formula	85
3.5.2 The heredity condition	86
3.5.3 Huang's family of updating formulae	87
3.5.4 Broyden's family of updating formulae	88
3.5.5 B-matrix formulation of quasi-Newton methods	90
3.5.6 Positive definiteness in Broyden's family	92
3.5.7 Conjugacy and the heredity property in Broyden's family	94
3.5.8 The choice of parameter in Broyden's family	95
3.5.9 The convergence of rank-one methods	96
3.5.10 The convergence of rank-two methods	97
3.5.11 The implementation of numerically stable quasi-Newton methods	98

3.5.12 Updating Cholesky factors	99
3.5.13 Methods using finite difference techniques	100
3.5.14 Optimal conditioning, self-scaling, sparsity and other topics	101
3.5.15 The performance of quasi-Newton methods	103
3.6 Summary	106
<b>4. NON-LINEAR LEAST SQUARES</b>	<b>110</b>
4.1 Introduction	110
4.1.1 Non-linear regression	110
4.1.2 Simultaneous non-linear equations	111
4.1.3 Derivatives of sum-of-squares functions	112
4.1.4 Newton's method	113
4.2 Small Residual Algorithms	113
4.2.1 The Gauss–Newton method	114
4.2.2 The Levenberg–Marquardt method	115
4.2.3 Powell's hybrid method	118
4.2.4 Solution of the normal equations	121
4.2.5 Finite difference techniques	124
4.2.6 Quasi-Newton methods	125
4.2.7 Simultaneous non-linear equations	127
4.3 Large Residual Algorithms	130
4.3.1 Quasi-Newton methods	130
4.3.2 The Gill–Murray method	132
4.3.3 Hybrid and general minimization methods	136
4.4 Summary	136
<b>5. FUNDAMENTALS OF CONSTRAINED OPTIMIZATION</b>	<b>139</b>
5.1 Introduction	139
5.1.1 Some notation and basic concepts	139
5.2 Necessary and Sufficient Conditions for a Linearly Constrained Minimum	142
5.2.1 Definition of a linearly constrained minimum	142
5.2.2 First-order necessary condition for equality constraints	142
5.2.3 Second-order conditions for equality constraints	144
5.2.4 First-order necessary condition for inequality constraints	146
5.2.5 Second-order conditions for inequality constraints	146
5.3 Necessary and Sufficient Conditions for a Non-linearly Constrained Minimum	147
5.3.1 Definition of a non-linearly constrained minimum	147
5.3.2 First-order necessary conditions for equality and inequality constraints	148
5.3.3 Second-order conditions for equality and inequality constraints	150
5.4 Summary	150

<b>6. LINEARLY CONSTRAINED MINIMIZATION</b>	152
6.1 Introduction	152
6.1.1 Active set strategy	152
6.1.2 Lagrange multiplier estimates	154
6.1.3 Updating after a change of basis	156
6.2 Modified Newton Methods	159
6.2.1 Newton's method	159
6.2.2 The Gill-Murray modified Newton method	160
6.3 Quasi-Newton Methods	165
6.3.1 H-matrix formulation	165
6.3.2 B-matrix formulation	169
6.4 Determination of a Feasible Initial Point	174
6.4.1 Equality constraints	174
6.4.2 Inequality constraints	175
6.5 Summary	177
<b>7. NON-LINEARLY CONSTRAINED MINIMIZATION</b>	179
7.1 Introduction	179
7.2 Penalty and Barrier Function Methods	180
7.2.1 Barrier function methods	180
7.2.2 Simple penalty function methods	184
7.2.3 Powell's penalty function	189
7.3 Augmented Lagrangian Methods	194
7.3.1 Exact augmented Lagrangian methods for equality constraints	195
7.3.2 Exact augmented Lagrangian methods for inequality constraints	203
7.3.3 Sequential augmented Lagrangian methods for equality constraints	205
7.3.4 Sequential augmented Lagrangian methods for inequality constraints	213
7.4 Direct Projection Methods	215
7.4.1 Direct projection methods for equality constraints	215
7.4.2 Direct projection methods for inequality constraints	218
7.5 Projected Lagrangian Methods	222
7.5.1 Projected Lagrangian methods for equality constraints	222
7.5.2 Projected Lagrangian methods for inequality constraints	228
7.6 Summary	228
<b>References</b>	232
<b>Index</b>	240