

Contents

Preface

xiii

1	Introduction to Process Optimization	1
1.1	Scope of Optimization Problems	1
1.2	Classification of Optimization Problems	3
1.3	Optimization Applications in Chemical Engineering	5
1.4	Nonlinear Programming Examples in Chemical Engineering	6
1.4.1	Design of a Small Heat Exchanger Network	7
1.4.2	Real-Time Optimization of a Distillation Column	9
1.4.3	Model Predictive Control	11
1.5	A Motivating Application	13
1.6	Summary and Notes for Further Reading	15
1.7	Exercises	15
2	Concepts of Unconstrained Optimization	17
2.1	Introduction	17
2.2	Basic Concepts	19
2.2.1	Vectors and Matrices	19
2.2.2	Quadratic Forms	22
2.2.3	Classification of Functions	25
2.3	Optimality Conditions	27
2.4	Algorithms	30
2.4.1	Direct Search Methods	30
2.4.2	Methods That Require Derivatives	33
2.5	Summary and Notes for Further Reading	37
2.6	Exercises	37
3	Newton-Type Methods for Unconstrained Optimization	39
3.1	Introduction	39
3.2	Modification of the Hessian Matrix	40
3.3	Quasi-Newton Methods	42
3.4	Line Search Methods	46
3.5	Trust Region Methods	52
3.5.1	Convex Model Problems	53
3.5.2	Nonconvex Model Problems	56

3.6	Summary and Notes for Further Reading	60
3.7	Exercises	60
4	Concepts of Constrained Optimization	63
4.1	Introduction	63
4.1.1	Constrained Convex Problems	64
4.2	Local Optimality Conditions—A Kinematic Interpretation	68
4.3	Analysis of KKT Conditions	72
4.3.1	Linearly Constrained Problems	75
4.3.2	Nonlinearly Constrained Problems	76
4.3.3	Second Order Conditions	79
4.4	Special Cases: Linear and Quadratic Programs	84
4.4.1	Description of Linear Programming	84
4.4.2	Description of Quadratic Programming	85
4.4.3	Portfolio Planning Case Study	86
4.5	Summary and Notes for Further Reading	89
4.6	Exercises	90
5	Newton Methods for Equality Constrained Optimization	91
5.1	Introduction to Equality Constrained Optimization	91
5.2	Newton's Method with the KKT Matrix	92
5.2.1	Nonsingularity of KKT Matrix	94
5.2.2	Inertia of KKT Matrix	95
5.3	Taking Newton Steps	96
5.3.1	Full-Space Newton Steps	96
5.3.2	Reduced-Space Newton Steps	99
5.4	Quasi-Newton Methods	102
5.4.1	A Quasi-Newton Full-Space Method	103
5.4.2	A Quasi-Newton Reduced-Space Method	105
5.5	Globalization for Constrained Optimization	109
5.5.1	Concepts of Merit Functions	109
5.5.2	Filter Method Concepts	112
5.5.3	Filter versus Merit Function Strategies	113
5.6	Line Search Methods	114
5.6.1	Line Search with Merit Functions	115
5.6.2	Line Search Filter Method	119
5.7	Trust Region Methods	122
5.7.1	Trust Regions with Merit Functions	123
5.7.2	Filter Trust Region Methods	126
5.8	Combining Local and Global Properties	128
5.8.1	The Maratos Effect	128
5.9	Summary and Conclusions	130
5.10	Notes for Further Reading	131
5.11	Exercises	131
6	Numerical Algorithms for Constrained Optimization	133
6.1	Constrained NLP Formulations	133

6.2	SQP Methods	135
6.2.1	The Basic, Full-Space SQP Algorithm	137
6.2.2	Large-Scale SQP	144
6.2.3	Extensions of SQP Methods	148
6.3	Interior Point Methods	151
6.3.1	Solution of the Primal-Dual Equations	154
6.3.2	A Line Search Filter Method	155
6.3.3	Globalization with Trust Region Methods	158
6.4	Nested Strategies	160
6.4.1	Gradient Projection Methods for Bound Constrained Problems	164
6.4.2	Linearly Constrained Augmented Lagrangian	167
6.5	Nonlinear Programming Codes	168
6.5.1	SQP Codes	169
6.5.2	Interior Point NLP Codes	170
6.5.3	Nested and Gradient Projection NLP Codes	171
6.5.4	Performance Trends for NLP Codes	171
6.6	Summary and Conclusions	175
6.7	Notes for Further Reading	176
6.8	Exercises	178
7	Steady State Process Optimization	181
7.1	Introduction	181
7.2	Optimization of Process Flowsheets	183
7.2.1	Importance of Accurate Derivatives	188
7.2.2	Ammonia Process Optimization	191
7.3	Equation-Oriented Formulation of Optimization Models	193
7.3.1	Reformulation of the Williams–Otto Optimization Problem	196
7.4	Real-Time Optimization	200
7.4.1	Equation-Oriented RTO Models	201
7.4.2	Case Study of Hydrocracker Fractionation Plant	203
7.5	Equation-Oriented Models with Many Degrees of Freedom	206
7.6	Summary and Notes for Further Reading	209
7.7	Exercises	209
8	Introduction to Dynamic Process Optimization	213
8.1	Introduction	213
8.2	Dynamic Systems and Optimization Problems	214
8.3	Optimality Conditions for Optimal Control Problems	220
8.3.1	Optimal Control without Inequalities	223
8.3.2	Optimal Control with Inequality Constraints	225
8.4	Handling Path Constraints	232
8.4.1	Treatment of Equality Path Constraints	232
8.4.2	Treatment of State Path Inequalities	237
8.5	Singular Control Problems	239
8.6	Numerical Methods Based on NLP Solvers	243

8.7	Summary and Conclusions	246
8.8	Notes for Further Reading	247
8.9	Exercises	248
9	Dynamic Optimization Methods with Embedded DAE Solvers	251
9.1	Introduction	251
9.2	DAE Solvers for Initial Value Problems	253
9.2.1	Runge–Kutta Methods	255
9.2.2	Linear Multistep Methods	256
9.2.3	Extension of Methods to DAEs	259
9.3	Sensitivity Strategies for Dynamic Optimization	260
9.3.1	Direct Sensitivity Calculations	261
9.3.2	Adjoint Sensitivity Calculations	262
9.3.3	Evolution to Optimal Control Problems	265
9.4	Multiple Shooting	271
9.4.1	Dichotomy of Boundary Value Problems	273
9.5	Dynamic Optimization Case Study	276
9.6	Summary and Conclusions	282
9.7	Notes for Further Reading	283
9.8	Exercises	284
10	Simultaneous Methods for Dynamic Optimization	287
10.1	Introduction	287
10.2	Derivation of Collocation Methods	288
10.2.1	Polynomial Representation for ODE Solutions	289
10.2.2	Collocation with Orthogonal Polynomials	290
10.3	NLP Formulations and Solution	295
10.3.1	Treatment of Finite Elements	296
10.3.2	Treatment of Unstable Dynamic Systems	299
10.3.3	Large-Scale NLP Solution Strategies	302
10.3.4	Parameter Estimation for Low-Density Polyethylene Reactors	304
10.4	Convergence Properties of Simultaneous Approach	309
10.4.1	Optimality with Gauss–Legendre Collocation	312
10.4.2	Optimality with Radau Collocation	313
10.4.3	Convergence Orders for NLP Solutions	314
10.4.4	Singular Optimal Controls	315
10.4.5	High-Index Inequality Path Constraints	317
10.5	Summary and Conclusions	322
10.6	Notes for Further Reading	322
10.7	Exercises	323
11	Process Optimization with Complementarity Constraints	325
11.1	Introduction	325
11.2	MPCC Properties and Formulations	327
11.2.1	Solution Strategies	331
11.2.2	Comparison of MPCC Formulations	333

11.3	Complementary Models for Process Optimization	336
11.4	Distillation Case Studies	343
11.4.1	Multicomponent Column Optimization with Phase Changes	343
11.4.2	Tray Optimization	345
11.5	Optimization of Hybrid Dynamic Systems	349
11.6	Dynamic MPC Case Studies	352
11.6.1	Reformulation of a Differential Inclusion	352
11.6.2	Cascading Tank Problem	356
11.7	Summary and Conclusions	359
11.8	Notes for Further Reading	360
11.9	Exercises	361
	Bibliography	363
	Index	391