

# Contents

<b>1</b>	<b>Introduction to Optimization</b>	<b>1</b>
1.1	Definition of Optimization	1
1.1.1	Mathematical Formulation	1
1.1.2	Convex Optimization	3
1.1.3	Quasi-convex Function	4
1.1.4	Global and Local Optima	4
1.2	Types of Optimization Problems	5
1.2.1	Continuous Versus Discrete Optimization	5
1.2.2	Unconstrained Versus Constrained Optimization	7
1.2.3	Single Versus Multi-objective Optimization	7
1.2.4	Deterministic Versus Stochastic Optimization	8
1.2.5	Black-Box and Data-Driven Optimization	8
1.3	Multi-objective Optimization	9
1.3.1	Mathematical Formulation	9
1.3.2	Pareto Optimality	10
1.3.3	Preference Modeling	14
1.3.4	Preference Articulation	16
1.4	Handling Uncertainty in Optimization	17
1.4.1	Noise in Evaluations	18
1.4.2	Robust Optimization	19
1.4.3	Multi-scenario Optimization	21
1.4.4	Dynamic Optimization	22
1.4.5	Robust Optimization Over Time	24
1.5	Comparison of Optimization Algorithms	27
1.5.1	Algorithmic Efficiency	27
1.5.2	Performance Indicators	28
1.5.3	Reliability Assessment	34
1.5.4	Statistical Tests	35
1.5.5	Benchmark Problems	36
1.6	Summary	38
	References	38

<b>2</b>	<b>Classical Optimization Algorithms</b> .....	41
2.1	Unconstrained Optimization .....	41
2.1.1	The Gradient Based Method .....	42
2.1.2	Newton's Method .....	43
2.1.3	Quasi-Newton Method .....	44
2.2	Constrained Optimization .....	44
2.2.1	Penalty and Barriers .....	45
2.2.2	Lagrangian Multipliers .....	46
2.3	Derivative-Free Search Methods .....	47
2.3.1	Line Search and Pattern Search .....	47
2.3.2	Nelder-Mead Simplex Method .....	47
2.3.3	Model-Based Derivative-Free Search Methods .....	48
2.4	Deterministic Global Optimization .....	49
2.4.1	Lipschitzian-Based Methods .....	49
2.4.2	DIRECT .....	50
2.5	Summary .....	50
	References .....	51
<b>3</b>	<b>Evolutionary and Swarm Optimization</b> .....	53
3.1	Introduction .....	53
3.2	Genetic Algorithms .....	54
3.2.1	Definitions .....	54
3.2.2	Representation .....	56
3.2.3	Crossover and Mutation .....	57
3.2.4	Environmental Selection .....	57
3.3	Real-Coded Genetic Algorithms .....	59
3.3.1	Real-Valued Representation .....	60
3.3.2	Blended Crossover .....	60
3.3.3	Simulated Binary Crossover and Polynomial Mutation .....	61
3.4	Evolution Strategies .....	62
3.4.1	(1 + 1)-ES .....	63
3.4.2	Evolution Strategies with One Global Step Size .....	63
3.4.3	Evolution Strategies with Individual Step Sizes .....	64
3.4.4	Reproduction and Environmental Selection .....	64
3.4.5	Covariance Matrix Adaptation Evolution Strategy .....	65
3.5	Genetic Programming .....	67
3.5.1	Tree-Based Genetic Programming .....	67
3.5.2	Initialization .....	69
3.5.3	Crossover and Mutation .....	70
3.6	Ant Colony Optimization .....	70
3.6.1	Overall Framework .....	72
3.6.2	Extensions .....	73
3.7	Differential Evolution .....	73
3.7.1	Initialization .....	74

3.7.2	Differential Mutation .....	74
3.7.3	Differential Crossover .....	75
3.7.4	Environmental Selection .....	76
3.8	Particle Swarm Optimization .....	76
3.8.1	Canonical Particle Swarm Optimization .....	76
3.8.2	Competitive Swarm Optimizer .....	78
3.8.3	Social Learning Particle Swarm Optimizer .....	80
3.9	Memetic Algorithms .....	83
3.9.1	Basic Concepts .....	83
3.9.2	Lamarckian Versus Baldwinian Approaches .....	84
3.9.3	Multi-objective Memetic Algorithms .....	85
3.9.4	Baldwin Effect Versus Hiding Effect .....	86
3.10	Estimation of Distribution Algorithms .....	88
3.10.1	A Simple EDA .....	88
3.10.2	EDAs for Discrete Optimization .....	90
3.10.3	EDAs for Continuous Optimization .....	91
3.10.4	Multi-objective EDAs .....	92
3.11	Parameter Adaptation and Algorithm Selection .....	94
3.11.1	Automated Parameter Tuning .....	94
3.11.2	Hyper-heuristics .....	95
3.11.3	Fitness Landscape Analysis .....	97
3.11.4	Automated Recommendation Systems .....	97
3.12	Summary .....	99
	References .....	99
<b>4</b>	<b>Introduction to Machine Learning .....</b>	<b>103</b>
4.1	Machine Learning Problems .....	103
4.1.1	Clustering .....	103
4.1.2	Dimension Reduction .....	106
4.1.3	Regression .....	108
4.1.4	Classification .....	109
4.2	Machine Learning Models .....	110
4.2.1	Polynomials .....	110
4.2.2	Multi-layer Perceptrons .....	110
4.2.3	Radial-Basis-Function Networks .....	112
4.2.4	Support Vector Machines .....	113
4.2.5	Gaussian Processes .....	114
4.2.6	Decision Trees .....	115
4.2.7	Fuzzy Rule Systems .....	116
4.2.8	Ensembles .....	118
4.3	Learning Algorithms .....	120
4.3.1	Supervised Learning .....	120
4.3.2	Unsupervised Learning .....	122
4.3.3	Reinforcement Learning .....	125
4.3.4	Advanced Learning Algorithms .....	126

4.4	Multi-objective Machine Learning .....	130
4.4.1	Single- and Multi-objective Learning .....	130
4.4.2	Multi-objective Clustering, Feature Selection and Extraction .....	132
4.4.3	Multi-objective Ensemble Generation .....	135
4.5	Deep Learning Models .....	135
4.5.1	Convolutional Neural Networks .....	136
4.5.2	Long Short-Term Memory Networks .....	136
4.5.3	Autoassociative Neural Networks and Autoencoder .....	137
4.5.4	Generative Adversarial Networks .....	139
4.6	Synergies Between Evolution and Learning .....	140
4.6.1	Evolutionary Learning .....	141
4.6.2	Learning for Evolutionary Optimization .....	142
4.7	Summary .....	143
	References .....	143
<b>5</b>	<b>Data-Driven Surrogate-Assisted Evolutionary Optimization .....</b>	<b>147</b>
5.1	Introduction .....	147
5.2	Offline and Online Data-Driven Optimization .....	149
5.2.1	Offline Data-Driven Optimization .....	149
5.2.2	Online Data-Driven Optimization .....	150
5.3	Online Surrogate Management Methods .....	151
5.3.1	Population-Based Model Management .....	151
5.3.2	Generation-Based Model Management .....	152
5.3.3	Individual-Based Model Management .....	154
5.3.4	Trust Region Method for Memetic Algorithms .....	156
5.4	Bayesian Model Management .....	157
5.4.1	Acquisition Functions .....	158
5.4.2	Evolutionary Bayesian Optimization .....	159
5.4.3	Bayesian Evolutionary Optimization .....	161
5.5	Bayesian Constrained Optimization .....	162
5.5.1	Acquisition Function for Constrained Optimization .....	163
5.5.2	Two-Stage Acquisition Functions .....	165
5.6	Surrogate-Assisted Robust Optimization .....	166
5.6.1	Bi-objective Formulation of Robust Optimization .....	166
5.6.2	Surrogate Construction .....	167
5.7	Performance Indicators for Surrogates .....	167
5.7.1	Accuracy .....	168
5.7.2	Selection-based Performance Indicator .....	168
5.7.3	Rank Correlation .....	170
5.7.4	Fitness Correlation .....	170
5.8	Summary .....	171
	References .....	171

<b>6</b>	<b>Multi-surrogate-Assisted Single-objective Optimization</b> .....	173
6.1	Introduction .....	173
6.2	Local and Global Surrogates Assisted Optimization .....	174
6.2.1	Ensemble Surrogate Model .....	175
6.2.2	Multi-surrogate for Single-objective Memetic Optimization .....	176
6.2.3	Multi-surrogate for Multi-objective Memetic Optimization .....	176
6.2.4	Trust Region Method Assisted Local Search .....	178
6.2.5	Experimental Results .....	180
6.3	Two-Layer Surrogate-Assisted Particle Swarm Optimization .....	181
6.3.1	Global Surrogate Model .....	182
6.3.2	Local Surrogate Model .....	183
6.3.3	Fitness Estimation .....	184
6.3.4	Surrogate Management .....	185
6.3.5	Experimental Results and Discussions .....	185
6.4	Committee Surrogate Assisted Particle Swarm Optimization .....	186
6.4.1	Committee of Surrogate Models .....	187
6.4.2	Infill Sampling Criteria .....	188
6.4.3	Overall Framework .....	188
6.4.4	Experimental Results on Benchmark Problems .....	189
6.5	Hierarchical Surrogate-Assisted Multi-scenario Optimization .....	190
6.5.1	Multi-scenario Airfoil Optimization .....	190
6.5.2	Hierarchical Surrogates for Multi-scenario Optimization .....	192
6.6	Adaptive Surrogate Selection .....	195
6.6.1	Basic Idea .....	195
6.6.2	Probabilistic Model for Surrogate Selection .....	196
6.7	Summary .....	199
	References .....	199
<b>7</b>	<b>Surrogate-Assisted Multi-objective Evolutionary Optimization</b> .....	201
7.1	Evolutionary Multi-objective Optimization .....	201
7.1.1	Hypothesis and Methodologies .....	201
7.1.2	Decomposition Approaches .....	203
7.1.3	Dominance Based Approaches .....	205
7.1.4	Performance Indicator Based Approaches .....	211
7.2	Gaussian Process Assisted Randomized Weighted Aggregation .....	212
7.2.1	Challenges for Surrogate-Assisted Multi-objective Optimization .....	212

7.2.2	Efficient Global Optimization Algorithm .....	214
7.2.3	Extension to Multi-objective Optimization .....	214
7.3	Gaussian Process Assisted Decomposition-Based Multi-objective Optimization .....	216
7.3.1	MOEA/D .....	216
7.3.2	Main Framework .....	218
7.3.3	Local Surrogate Models .....	218
7.3.4	Surrogate Management .....	219
7.3.5	Discussions .....	221
7.4	High-Dimensional Multi-objective Bayesian Optimization .....	221
7.4.1	Main Challenges .....	221
7.4.2	Heterogeneous Ensemble Construction .....	222
7.4.3	Pareto Approach to Multi-objective Bayesian Optimization .....	223
7.4.4	Overall Framework .....	224
7.5	Summary .....	228
	References .....	228
<b>8</b>	<b>Surrogate-Assisted Many-Objective Evolutionary Optimization .....</b>	<b>231</b>
8.1	New Challenges in Many-Objective Optimization .....	231
8.1.1	Introduction .....	231
8.1.2	Diversity Versus Preferences .....	232
8.1.3	Search for Knee Solutions .....	233
8.1.4	Solving Problems with Irregular Pareto Fronts .....	235
8.2	Evolutionary Many-Objective Optimization Algorithms .....	236
8.2.1	Reference Vector Guided Many-Objective Optimization .....	236
8.2.2	A Knee-Driven Many-Objective Optimization Algorithm .....	240
8.2.3	A Two-Archive Algorithm for Many-Objective Optimization .....	243
8.2.4	Corner Sort for Many-Objective Optimization .....	245
8.3	Gaussian Process Assisted Reference Vector Guided Many-Objective Optimization .....	248
8.3.1	Surrogate Management .....	250
8.3.2	Archive Maintenance .....	250
8.4	Classification Surrogate Assisted Many-Objective Optimization .....	252
8.4.1	Main Framework .....	252
8.4.2	Radial Projection Based Selection .....	254
8.4.3	Reference Set Based Dominance Relationship Prediction .....	254
8.4.4	Surrogate Management .....	256
8.4.5	Surrogate-Assisted Environmental Selection .....	258

8.5	Dropout Neural Network Assisted Many-Objective Optimization .....	259
8.5.1	AR-MOEA .....	259
8.5.2	Efficient Deep Dropout Neural Networks .....	262
8.5.3	Model Management .....	264
8.5.4	Overall Framework of EDN-ARMOEA .....	265
8.5.5	Operational Optimization in Crude Oil Distillation Units .....	266
8.6	Summary .....	269
	References .....	269
<b>9</b>	<b>Knowledge Transfer in Data-Driven Evolutionary Optimization .....</b>	<b>273</b>
9.1	Introduction .....	273
9.2	Co-Training for Surrogate-Assisted Interactive Optimization .....	274
9.2.1	Overall Framework .....	275
9.2.2	Surrogate for Interval Prediction .....	276
9.2.3	Fitness Estimation .....	278
9.2.4	An Improved CSSL .....	279
9.2.5	Surrogate Management .....	280
9.3	Semi-Supervised Learning Assisted Particle Swarm Optimization .....	280
9.3.1	Algorithm Framework .....	281
9.3.2	Social Learning Particle Swarm Optimization .....	281
9.3.3	Surrogate Management Strategy .....	283
9.3.4	Selection of Unlabeled Data .....	284
9.3.5	Experimental Results and Discussions .....	285
9.4	Knowledge Transfer between Problems in Multi-objective Optimization .....	286
9.4.1	Domain Adaptation for Transfer Learning .....	286
9.4.2	Knowledge Transfer from Cheap to Expensive Problems .....	290
9.4.3	CE-BDA for Data Augmentation .....	292
9.4.4	Evolutionary Multi-Objective Bayesian Optimization .....	293
9.5	Knowledge Transfer between Objectives in Multi-objective Optimization .....	294
9.5.1	Motivation .....	294
9.5.2	Parameter Based Transfer Learning .....	294
9.5.3	Overall Framework .....	295
9.6	Data-Driven Multi-fidelity Transfer Optimization .....	296
9.6.1	Transfer Learning for Bi-Fidelity Optimization .....	297
9.6.2	Transfer Stacking .....	297

9.6.3	Surrogate-Assisted Bi-Fidelity Evolutionary Optimization .....	298
9.6.4	Experimental Results .....	300
9.7	Surrogate-Assisted Multitasking Multi-Scenario Optimization .....	301
9.7.1	Multi-Scenario Minimax Optimization .....	301
9.7.2	Surrogate-Assisted Minimax Multifactorial Evolutionary Optimization .....	302
9.7.3	Experiment Results .....	304
9.8	Summary .....	306
	References .....	306
<b>10</b>	<b>Surrogate-Assisted High-Dimensional Evolutionary Optimization</b> .....	<b>309</b>
10.1	Surrogate-Assisted Cooperative Optimization for High-Dimensional Optimization .....	309
10.1.1	RBF-Assisted SL-PSO .....	311
10.1.2	FES-Assisted PSO .....	312
10.1.3	Archive Update .....	316
10.1.4	Experimental Results and Discussions .....	317
10.2	A Multi-objective Infill Criterion for High-Dimensional Optimization .....	320
10.2.1	Main Framework .....	321
10.2.2	Multiobjective Infill Criterion .....	322
10.2.3	Experimental Results and Discussions .....	325
10.3	Multi-surrogate Multi-tasking Optimization of Expensive problems .....	327
10.3.1	Multi-factorial Evolutionary Algorithms .....	327
10.3.2	Main Framework .....	328
10.3.3	Global and Local Surrogates .....	329
10.3.4	Multi-tasking Optimization Based on Global and Local Surrogates .....	331
10.3.5	Experimental Results and Discussions .....	331
10.4	Surrogate-Assisted Large Optimization with Random Feature Selection .....	333
10.4.1	Main Framework .....	335
10.4.2	Sub-problem Formation and Optimization .....	335
10.4.3	Global Best Position Update .....	337
10.4.4	Experimental Results and Discussions .....	338
10.5	Summary .....	340
	References .....	340
<b>11</b>	<b>Offline Big or Small Data-Driven Optimization and Applications</b> .....	<b>343</b>
11.1	Adaptive Clustering for Offline Big-Data Driven Optimization ... ..	343



11.1.1	Problem Formulation .....	343
11.1.2	Adaptive Clustering for Offline Data-Driven Optimization .....	345
11.1.3	Empirical Results .....	346
11.1.4	Discussions .....	347
11.2	Small Data-Driven Multi-objective Magnesium Furnace Optimization .....	348
11.2.1	Model Management Based on a Global Surrogate .....	348
11.2.2	Empirical Verification on Benchmark Problems .....	349
11.2.3	Optimization of Fused Magnesium Furnaces .....	350
11.3	Selective Ensemble for Offline Airfoil Optimization .....	354
11.3.1	Problem Formulation .....	354
11.3.2	Selective Ensemble for Offline Data-Driven Optimization .....	355
11.3.3	Comparative Results .....	356
11.4	Knowledge Transfer in Offline Data-Driven Beneficiation Process ... ..	358
11.4.1	Introduction .....	358
11.4.2	Knowledge Transfer by Multi-surrogate Optimization .....	359
11.4.3	Reference Vector Based Final Solution Selection .....	360
11.4.4	Optimization of Beneficiation Process .....	361
11.5	Transfer Learning for Offline Data-Driven Dynamic Optimization .....	364
11.5.1	Dynamic Data-Driven Optimization .....	364
11.5.2	Data Stream Ensemble for Incremental Learning .....	365
11.5.3	Ensemble Based Transfer Optimization .....	367
11.5.4	Support Vector Domain Description for Final Solution Selection .....	367
11.5.5	Empirical Results .....	368
11.6	Summary .....	370
	References .....	370
<b>12</b>	<b>Surrogate-Assisted Evolutionary Neural Architecture Search .....</b>	<b>373</b>
12.1	Challenges in Neural Architecture Search .....	373
12.1.1	Architecture Representation .....	374
12.1.2	Search Strategies .....	376
12.1.3	Performance Evaluation .....	377
12.2	Bayesian Optimization for Neural Architecture Search .....	377
12.2.1	Architecture Encoding .....	379
12.2.2	Kernel Functions .....	379
12.2.3	Discussions .....	380
12.3	Random Forest Assisted Neural Architecture Search .....	380
12.3.1	Block-Based Architecture Representation .....	381
12.3.2	Offline Data Generation .....	382

12.3.3 Random Forest Construction ..... 383

12.3.4 Search Methodology ..... 383

12.3.5 Experimental Results ..... 384

12.4 Summary ..... 385

References ..... 385

**Index** ..... 389

11.1.1 Model Management Based on Global Statistics ..... 378

11.2.1 Empirical Verification on Classification Problems ..... 368

11.2.2 Optimization of Batch Management ..... 368

11.2.3 Selective Ensemble for Online Active Optimization ..... 354

11.3.1 Problem Formulation ..... 354

11.3.2 Selective Ensemble for Online Data-Driven ..... 352

Optimization ..... 352

11.3.3 Comparative Results ..... 350

11.4 Knowledge Transfer in Online Data-Driven ..... 348

Process ..... 348

11.4.1 Introduction ..... 348

11.4.2 Knowledge Transfer by Multi-Instance ..... 348

Optimization ..... 348

11.4.3 Reinforce Vector Based Trial Solution Selection ..... 340

11.4.4 Optimization of Bandwidth Process ..... 340

11.5 Transfer Learning for Online Data-Driven Training ..... 304

Optimization ..... 304

11.5.1 Dynamic Data-Driven Optimization ..... 304

11.5.2 Data Stream Ensemble for Incremental Learning ..... 302

11.5.3 Ensemble Based Transfer Optimization ..... 302

11.5.4 Reinforce Vector Dynamic Transfer for Band ..... 302

Solution Selection ..... 302

11.5.5 Empirical Results ..... 302

11.6 Summary ..... 300

References ..... 300

12.1.1 Challenges in Neural Architecture Search ..... 373

12.1.2 Search Space ..... 374

12.1.3 Performance Evaluation ..... 374

12.1.4 Bayesian Optimization for Neural Architecture Search ..... 373

12.2.1 Architecture Enriching ..... 370

12.2.2 Kernel Functions ..... 370

12.2.3 Discussion ..... 380

12.3 Random Forest Assisted Neural Architecture Search ..... 380

12.3.1 Block-Based Architecture Representation ..... 381

12.3.2 Online Data Curation ..... 382