

Contents

Part I Theory

Overview of Stochastic Optimization Algorithms

0	General Remarks	3
0.1	Why Optimize Things?	3
0.2	Moral Aspects of Optimization	4
0.3	How To Think About It	5
0.4	Minima, Maxima, and Extrema	6
0.5	What Is So Hard About Optimization?	6
0.6	Algorithms, Heuristics, Metaheuristics	7
1	Exact Optimization Algorithms for Simple Problems	9
1.1	A Simple Example—Exact Optimization in One Dimension ..	9
1.2	Newton–Raphson Method	10
1.3	Descent Methods in More Than One Dimension	12
1.4	Conjugate Gradients	13
2	Exact Optimization Algorithms for Complex Problems ...	15
2.1	Simplex Algorithm	15
2.2	Integer Optimization	20
2.3	Branch & Bound	21
2.4	Branch & Cut	24
3	Monte Carlo	31
3.1	Pseudorandom Numbers	31
3.2	Random Number Generation and Random Number Tests	32
3.3	Transformation of Random Numbers	37
3.4	Example: Calculation of π with MC	42
4	Overview of Optimization Heuristics	43
4.1	Necessity of Heuristics	43
4.2	Construction Heuristics	44
4.3	Markovian Improvement Heuristics	45
4.4	Set-Based Improvement Heuristics	46

5	Implementation of Constraints	49
5.1	Moves, Constraints, Deadlines.....	49
5.2	Incorporation into the Configurations.....	49
5.3	Consideration of Feasible Solutions Only.....	50
5.4	Penalty Functions.....	50
6	Parallelization Strategies	53
6.1	Parallelization Models and Computer Architectures.....	53
6.2	Running Several Copies.....	54
6.3	Divide et Impera.....	54
6.4	Information Exchange.....	56
7	Construction Heuristics	59
7.1	General Outline of Construction Heuristics.....	59
7.2	Insertion Heuristics.....	60
7.3	Savings Heuristics.....	61
7.4	More Intelligent Ways of Construction.....	61
8	Markovian Improvement Heuristics	63
8.1	Constructing a Markov Chain.....	63
8.2	Trivial Acceptance Functions.....	64
8.3	Introduction of a Control Parameter.....	65
8.4	Heat Bath Approach.....	66
9	Local Search	69
9.1	Classic Local Search Approach.....	69
9.2	Problems of the Local Search Approach.....	70
9.3	Larger Moves.....	70
9.4	Jumping Between Different Move Sizes.....	71
10	Ruin & Recreate	73
10.1	The Philosophy of Building One's Own Castle.....	73
10.2	Outline of Approach.....	73
10.3	Discussion of Ruin & Recreate.....	76
10.4	Ruin & Recreate as a Self-Contained Optimization Algorithm.....	77
11	Simulated Annealing	79
11.1	Physical and Historical Background.....	79
11.2	Derivation of Simulated Annealing.....	81
11.3	Thermal Expectation Values.....	85
11.4	Inverse Simulated Annealing.....	88
12	Threshold Accepting and Other Algorithms Related to Simulated Annealing	89
12.1	Threshold Accepting.....	89

12.2	The Steady-State Equilibrium Characteristics of TA	91
12.3	Methods Based on the Tsallis Statistics	96
12.4	The Great Deluge Algorithm	100
13	Changing the Energy Landscape	103
13.1	Search Space Smoothing	103
13.2	Ant Lion Heuristics and Activation Relaxation Technique	108
13.3	Noising or Permutation of System Parts	111
13.4	Weight Annealing	112
14	Estimation of Expectation Values	115
14.1	Simple Sampling	115
14.2	Biased Sampling	115
14.3	Importance Sampling	116
14.4	Parallel Sampling	117
15	Cooling Techniques	119
15.1	Standard Cooling Schedules	119
15.2	Nonmonotonic Cooling Schedules	122
15.3	Ensemble Based Schedules	126
15.4	Simulated Tempering and Parallel Tempering	130
16	Estimation of Calculation Time Needed	135
16.1	Exponentially Growing Space Size	135
16.2	Polynomial Approach	135
16.3	Grest Hypothesis	135
17	Weakening the Pure Markovian Approach	137
17.1	Saving the Best-So-Far Solution and Spinoffs at Good Solutions	137
17.2	Record-to-Record Travel	138
17.3	Stochastic Tunneling	139
17.4	Changing the Cooling Schedule Due to Intermediate Results	139
18	Neural Networks	143
18.1	Biological Motivation	143
18.2	Artificial Neural Networks	145
18.3	The Hopfield Model	149
18.4	Kohonen Networks	154
19	Genetic Algorithms and Evolution Strategies	157
19.1	Charles Darwin's Natural Selection	157
19.2	Mutations and Crossovers	158
19.3	Application to Optimization Problems	161
19.4	Parallel Applications	166

20	Optimization Algorithms Inspired by Social Animals	169
20.1	Inspiration by the Behavior of Animals	169
20.2	Ant Colony Optimization	169
20.3	Particle Swarm Optimization	171
20.4	Fighting and Ranking	172
21	Optimization Algorithms Based on Multiagent Systems	175
21.1	Motivation	175
21.2	Simulated Trading	176
21.3	Selfish vs. Global Optimization	178
21.4	Introduction of a Social Temperature	179
22	Tabu Search	181
22.1	Tabu	181
22.2	Use of Memory	182
22.3	Aspiration	183
22.4	Intensification and Diversification	183
23	Histogram Algorithms	185
23.1	Guided Local Search	185
23.2	Multicanonical Algorithm	186
23.3	MUCAREM and REMUCA	192
23.4	Multicanonical Annealing	192
24	Searching for Backbones	193
24.1	Comparing Different Good Solutions	193
24.2	Determining the Backbone	194
24.3	Outline of the SFB Algorithm	195
24.4	Discussion of the Algorithm	196

Part II Applications

0	General Remarks	201
0.1	Dealing with a Proposed Optimization Problem	201
0.2	Programming Languages and Parallelization Libraries	202
0.3	Optimization Libraries	204
0.4	Difficulty of Comparing Various Algorithms	205

Applications A
The Traveling Salesman Problem

1	The Traveling Salesman Problem	211
1.1	The Task of the Traveling Salesman	211
1.2	Distance Metrics	211

1.3	The Dijkstra Algorithm	212
1.4	Various Possible Codings	215
1.5	Four Approaches to the TSP	218
1.6	Benchmark Instances	219
1.7	Bounds for the Optimum Solution	223
1.8	The Misfit: A Frustration Measure	225
1.9	Order Parameters for the TSP	226
1.10	Short History of TSP	229
2	Extensions of Traveling Salesman Problem	233
2.1	Temporal Constraints	233
2.2	Vehicle Routing Problems	234
2.3	Probabilistic Models and Online Optimization	239
2.4	Supply Chain Management	240
3	Application of Construction Heuristics to TSP	243
3.1	Nearest Neighbor Heuristic	243
3.2	Insertion Heuristics	246
3.3	Using Deeper Insight into the Problem	251
3.4	The Savings Heuristic	255
4	Local Search Concepts Applied to TSP	263
4.1	Initialization Routine	263
4.2	Small Moves	265
4.3	Computational Results for Greedy Algorithm	269
4.4	Local Search as Afterburner for Construction Heuristics	272
5	Next Larger Moves Applied to TSP	275
5.1	Lin-3-Opts	275
5.2	Higher-Order Lin- n -Opts	277
5.3	Computational Results for the Greedy Algorithm	283
5.4	Combination of Moves of Various Sizes	285
6	Ruin & Recreate Applied to TSP	287
6.1	Application of Ruin & Recreate	287
6.2	Analysis of R & R Moves in RW and GRE Modes	290
6.3	Ruin & Recreate as Self-Contained Algorithm	294
6.4	Discussion of Application Possibilities of Ruin & Recreate	296
7	Application of Simulated Annealing to TSP	299
7.1	Simulated Annealing for the TSP	299
7.2	Computational Results for Observables of Interest	302
7.3	Computational Results for Acceptance Rates	306
7.4	Quality of the Results Achieved with Various Computing Times	310

8	Dependencies of SA Results on Moves and Cooling Process	315
8.1	Results for Various Small Moves	315
8.2	Results for Monotonous Cooling Schedules	318
8.3	Results for Bouncing	324
8.4	Results for Parallel Tempering	334
9	Application to TSP of Algorithms Related to Simulated Annealing	341
9.1	Computational Results for Threshold Accepting	341
9.2	Computational Results for Penna Criterion	347
9.3	Computational Results for Great Deluge Algorithm	350
9.4	Computational Results for Record-to-Record Travel	359
10	Application of Search Space Smoothing to TSP	367
10.1	A Small Toy Problem	367
10.2	Gu and Huang Approach	369
10.3	Effect of Numerical Precision on Smoothing	383
10.4	Smoothing with Finite Numerical Precision Only	386
11	Further Techniques Changing the Energy Landscape of a TSP	389
11.1	The Convex-Concave Approach to Search Space Smoothing	389
11.2	Noising the System	397
11.3	Weight Annealing	399
11.4	Final Remarks on Application of Changing Techniques	403
12	Application of Neural Networks to TSP	405
12.1	Application of a Hopfield Network	405
12.2	Computational Results for the Hopfield Network	407
12.3	Application of a Kohonen Network	408
12.4	Computational Results for a Kohonen Network	409
13	Application of Genetic Algorithms to TSP	415
13.1	Mutations	415
13.2	Crossovers	416
13.3	Natural Selection	419
13.4	Computational Results	420
14	Social Animal Algorithms Applied to TSP	423
14.1	Application of Ant Colony Optimization	423
14.2	Computational Results	426
14.3	Application of Bird Flock Model	428
14.4	Computational Results	429

15 Simulated Trading Applied to TSP	431
15.1 Application of Simulated Trading to the TSP	431
15.2 Computational Results	435
15.3 Discussion of Simulated Trading	438
15.4 Simulated Trading and Working	438
16 Tabu Search Applied to TSP	441
16.1 Definition of a Tabu List	441
16.2 Introduction of Short-Term Memory	444
16.3 Adding some Aspiration	445
16.4 Adding Intensification and Diversification	445
17 Application of History Algorithms to TSP	449
17.1 The Multicanonical Algorithm	449
17.2 Multicanonical Annealing	452
17.3 Acceptance Simulated Annealing	455
17.4 Guided Local Search	464
18 Application of Searching for Backbones to TSP	471
18.1 Definition of a Backbone	471
18.2 Application to the Completely Asymmetric TSP	475
18.3 Application to Partially Asymmetric TSP	477
18.4 Computational Results	478
19 Simulating Various Types of Government with Searching for Backbones	489
19.1 An Aristocratic Approach	489
19.2 A Democratic Approach	491
19.3 Solution of the PCB442 Problem	492
19.4 Can Humans Do This, Too?	496

Applications B
The Constraint Satisfaction Problem

20 The Constraint Satisfaction Problem	501
20.1 Sources of Constraint Satisfaction Problems	501
20.2 Benchmarks and Competitions	503
20.3 Randomly Generated Models and Their Complexity	504
20.4 Randomly Generated Models and Their Phase Diagrams	506
20.5 Mixtures of easy and hard CSPs	510

21 Construction Heuristics for CSP	513
21.1 Application of the Bestinsertion Heuristic to the 3-SAT Problem	513
21.2 Assertion, Decimation, and Resolution	517
21.3 Analyzable Assertion Protocols	517
21.4 Solution Space Structure of XOR-SAT	519
22 Random Local Iterative Search Heuristics	523
22.1 RWalkSAT	523
22.2 WalkSAT	524
22.3 Simulated Annealing	526
23 Belief Propagation and Survey Propagation	529
23.1 Belief Propagation, Message Passing, and Cavities	529
23.2 Message Passing as Side Information for Decimation	531
23.3 Belief Propagation and Sudoku	534

Part III Outlook

24 Future Outlook of Optimization Business	539
24.1 $\mathcal{P} = \mathcal{NP}$?	539
24.2 Quantum Computing	540
24.3 DNA Computing	541
24.4 How Will the Problems Evolve?	544
Acknowledgments	547
References	551
Index	563