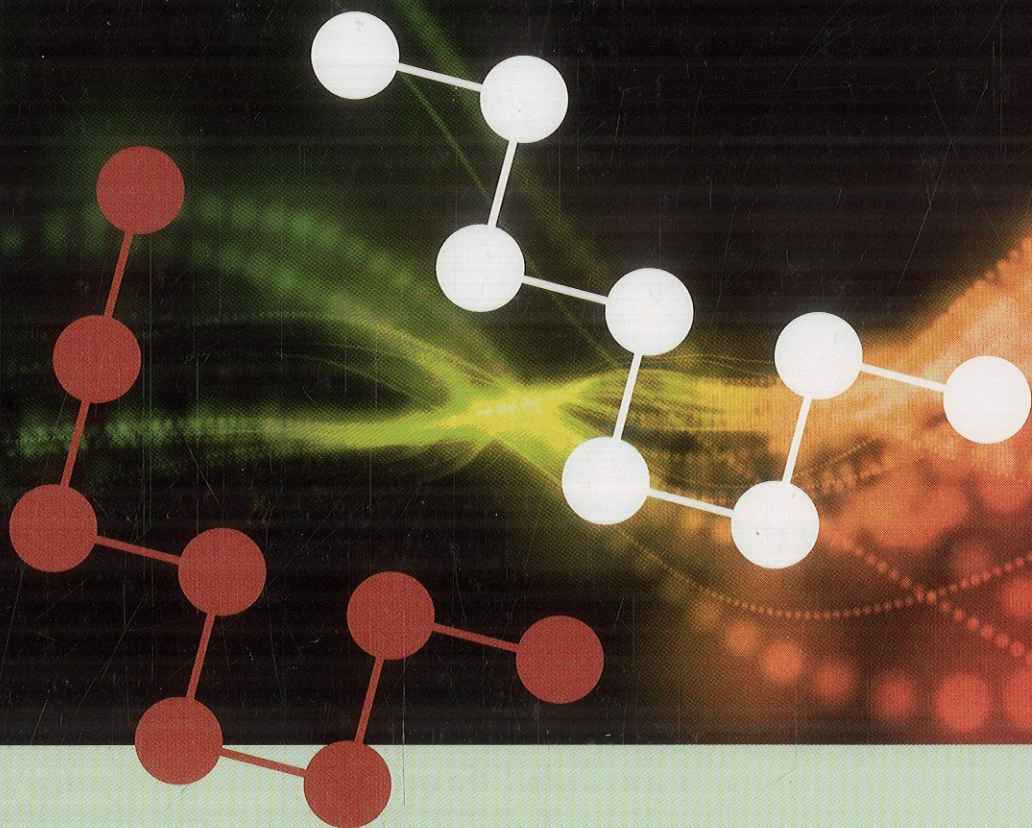


WILEY SERIES IN COMPUTATIONAL STATISTICS



Faming Liang, Chuanhai Liu, Raymond J. Carroll

ADVANCED MARKOV CHAIN MONTE CARLO METHODS

LEARNING FROM PAST SAMPLES

 WILEY

Contents

Preface	xiii
Acknowledgments	xvii
Publisher's Acknowledgments	xix
1 Bayesian Inference and Markov Chain Monte Carlo	1
1.1 Bayes	1
1.1.1 Specification of Bayesian Models	2
1.1.2 The Jeffreys Priors and Beyond	2
1.2 Bayes Output	4
1.2.1 Credible Intervals and Regions	4
1.2.2 Hypothesis Testing: Bayes Factors	5
1.3 Monte Carlo Integration	8
1.3.1 The Problem	8
1.3.2 Monte Carlo Approximation	9
1.3.3 Monte Carlo via Importance Sampling	9
1.4 Random Variable Generation	10
1.4.1 Direct or Transformation Methods	11
1.4.2 Acceptance-Rejection Methods	11
1.4.3 The Ratio-of-Uniforms Method and Beyond	14
1.4.4 Adaptive Rejection Sampling	18
1.4.5 Perfect Sampling	18
1.5 Markov Chain Monte Carlo	18
1.5.1 Markov Chains	18
1.5.2 Convergence Results	20
1.5.3 Convergence Diagnostics	23
Exercises	24
2 The Gibbs Sampler	27
2.1 The Gibbs Sampler	27
2.2 Data Augmentation	30

2.3	Implementation Strategies and Acceleration Methods	33
2.3.1	Blocking and Collapsing	33
2.3.2	Hierarchical Centering and Reparameterization	34
2.3.3	Parameter Expansion for Data Augmentation	35
2.3.4	Alternating Subspace-Spanning Resampling	43
2.4	Applications	45
2.4.1	The Student-t Model	45
2.4.2	Robit Regression or Binary Regression with the Student-t Link	47
2.4.3	Linear Regression with Interval-Censored Responses	50
	Exercises	54
	Appendix 2A: The EM and PX-EM Algorithms	56
3	The Metropolis-Hastings Algorithm	59
3.1	The Metropolis-Hastings Algorithm	59
3.1.1	Independence Sampler	62
3.1.2	Random Walk Chains	63
3.1.3	Problems with Metropolis-Hastings Simulations	63
3.2	Variants of the Metropolis-Hastings Algorithm	65
3.2.1	The Hit-and-Run Algorithm	65
3.2.2	The Langevin Algorithm	65
3.2.3	The Multiple-Try MH Algorithm	66
3.3	Reversible Jump MCMC Algorithm for Bayesian Model Selection Problems	67
3.3.1	Reversible Jump MCMC Algorithm	67
3.3.2	Change-Point Identification	70
3.4	Metropolis-Within-Gibbs Sampler for ChIP-chip Data Analysis	75
3.4.1	Metropolis-Within-Gibbs Sampler	75
3.4.2	Bayesian Analysis for ChIP-chip Data	76
	Exercises	83
4	Auxiliary Variable MCMC Methods	85
4.1	Simulated Annealing	86
4.2	Simulated Tempering	88
4.3	The Slice Sampler	90
4.4	The Swendsen-Wang Algorithm	91
4.5	The Wolff Algorithm	93
4.6	The Møller Algorithm	95
4.7	The Exchange Algorithm	97
4.8	The Double MH Sampler	98
4.8.1	Spatial Autologistic Models	99
4.9	Monte Carlo MH Sampler	103
4.9.1	Monte Carlo MH Algorithm	103
4.9.2	Convergence	107

4.9.3	Spatial Autologistic Models (Revisited)	110
4.9.4	Marginal Inference	111
4.10	Applications	113
4.10.1	Autonormal Models	114
4.10.2	Social Networks	116
	Exercises	121
5	Population-Based MCMC Methods	123
5.1	Adaptive Direction Sampling	124
5.2	Conjugate Gradient Monte Carlo	125
5.3	Sample Metropolis-Hastings Algorithm	126
5.4	Parallel Tempering	127
5.5	Evolutionary Monte Carlo	128
5.5.1	Evolutionary Monte Carlo in Binary-Coded Space	129
5.5.2	Evolutionary Monte Carlo in Continuous Space	132
5.5.3	Implementation Issues	133
5.5.4	Two Illustrative Examples	134
5.5.5	Discussion	139
5.6	Sequential Parallel Tempering for Simulation of High Dimensional Systems	140
5.6.1	Build-up Ladder Construction	141
5.6.2	Sequential Parallel Tempering	142
5.6.3	An Illustrative Example: the Witch's Hat Distribution	142
5.6.4	Discussion	145
5.7	Equi-Energy Sampler	146
5.8	Applications	148
5.8.1	Bayesian Curve Fitting	148
5.8.2	Protein Folding Simulations: 2D HP Model	153
5.8.3	Bayesian Neural Networks for Nonlinear Time Series Forecasting	156
	Exercises	162
	Appendix 5A: Protein Sequences for 2D HP Models	163
6	Dynamic Weighting	165
6.1	Dynamic Weighting	165
6.1.1	The IWIW Principle	165
6.1.2	Tempering Dynamic Weighting Algorithm	167
6.1.3	Dynamic Weighting in Optimization	171
6.2	Dynamically Weighted Importance Sampling	173
6.2.1	The Basic Idea	173
6.2.2	A Theory of DWIS	174
6.2.3	Some IWIW _p Transition Rules	176
6.2.4	Two DWIS Schemes	179
6.2.5	Weight Behavior Analysis	180

6.2.6	A Numerical Example	183
6.3	Monte Carlo Dynamically Weighted Importance Sampling	185
6.3.1	Sampling from Distributions with Intractable Normalizing Constants	185
6.3.2	Monte Carlo Dynamically Weighted Importance Sampling	186
6.3.3	Bayesian Analysis for Spatial Autologistic Models	191
6.4	Sequentially Dynamically Weighted Importance Sampling	195
	Exercises	197
7	Stochastic Approximation Monte Carlo	199
7.1	Multicanonical Monte Carlo	200
7.2	$1/k$ -Ensemble Sampling	202
7.3	The Wang-Landau Algorithm	204
7.4	Stochastic Approximation Monte Carlo	207
7.5	Applications of Stochastic Approximation Monte Carlo	218
7.5.1	Efficient p -Value Evaluation for Resampling- Based Tests	218
7.5.2	Bayesian Phylogeny Inference	222
7.5.3	Bayesian Network Learning	227
7.6	Variants of Stochastic Approximation Monte Carlo	233
7.6.1	Smoothing SAMC for Model Selection Problems	233
7.6.2	Continuous SAMC for Marginal Density Estimation	239
7.6.3	Annealing SAMC for Global Optimization	244
7.7	Theory of Stochastic Approximation Monte Carlo	253
7.7.1	Convergence	253
7.7.2	Convergence Rate	267
7.7.3	Ergodicity and its IWIW Property	271
7.8	Trajectory Averaging: Toward the Optimal Convergence Rate	275
7.8.1	Trajectory Averaging for a SAMCMC Algorithm	277
7.8.2	Trajectory Averaging for SAMC	279
7.8.3	Proof of Theorems 7.8.2 and 7.8.3.	281
	Exercises	296
	Appendix 7A: Test Functions for Global Optimization	298
8	Markov Chain Monte Carlo with Adaptive Proposals	305
8.1	Stochastic Approximation-Based Adaptive Algorithms	306
8.1.1	Ergodicity and Weak Law of Large Numbers	307
8.1.2	Adaptive Metropolis Algorithms	309
8.2	Adaptive Independent Metropolis-Hastings Algorithms	312
8.3	Regeneration-Based Adaptive Algorithms	315
8.3.1	Identification of Regeneration Times	315
8.3.2	Proposal Adaptation at Regeneration Times	317

8.4	Population-Based Adaptive Algorithms	317
8.4.1	ADS, EMC, NKC and More	317
8.4.2	Adaptive EMC	318
8.4.3	Application to Sensor Placement Problems	323
	Exercises	324

References	327
-------------------	------------

Index	353
--------------	------------