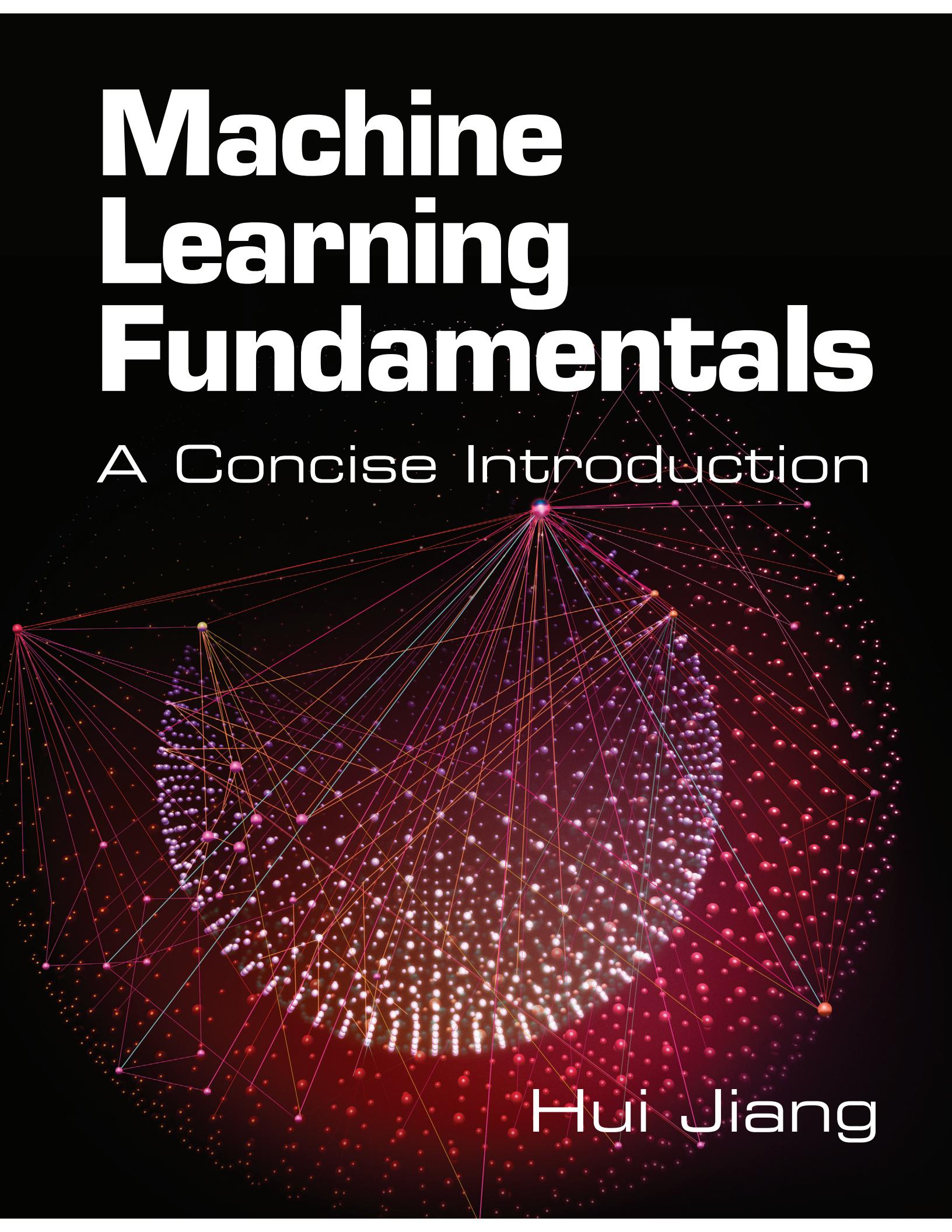


# Machine Learning Fundamentals

A Concise Introduction

A complex, abstract network graph serves as the background for the entire cover. It consists of numerous small, semi-transparent spheres of various colors (pink, purple, blue, yellow, orange) connected by thin, translucent lines of the same colors. The spheres are densely packed in several large, roughly triangular clusters that radiate from a central point at the bottom right. The overall effect is a futuristic, data-oriented, and organic design.

Hui Jiang

# **Machine Learning Fundamentals**

**A Concise Introduction**

Hui Jiang

*York University, Toronto*



# Contents

<b>Preface</b>	<b>xi</b>
<b>Notation</b>	<b>xvii</b>
<b>1 Introduction</b>	<b>1</b>
1.1 What Is Machine Learning? . . . . .	1
1.2 Basic Concepts in Machine Learning . . . . .	4
1.2.1 Classification versus Regression . . . . .	4
1.2.2 Supervised versus Unsupervised Learning . . . . .	5
1.2.3 Simple versus Complex Models . . . . .	5
1.2.4 Parametric versus Nonparametric Models . . . . .	7
1.2.5 Overfitting versus Underfitting . . . . .	8
1.2.6 Bias–Variance Trade-Off . . . . .	10
1.3 General Principles in Machine Learning . . . . .	11
1.3.1 Occam’s Razor . . . . .	11
1.3.2 No-Free-Lunch Theorem . . . . .	11
1.3.3 Law of the Smooth World . . . . .	12
1.3.4 Curse of Dimensionality . . . . .	14
1.4 Advanced Topics in Machine Learning . . . . .	15
1.4.1 Reinforcement Learning . . . . .	15
1.4.2 Meta-Learning . . . . .	16
1.4.3 Causal Inference . . . . .	16
1.4.4 Other Advanced Topics . . . . .	16
Exercises . . . . .	18
<b>2 Mathematical Foundation</b>	<b>19</b>
2.1 Linear Algebra . . . . .	19
2.1.1 Vectors and Matrices . . . . .	19
2.1.2 Linear Transformation as Matrix Multiplication . . . . .	20
2.1.3 Basic Matrix Operations . . . . .	21

2.1.4	Eigenvalues and Eigenvectors . . . . .	23
2.1.5	Matrix Calculus . . . . .	25
2.2	<b>Probability and Statistics</b> . . . . .	27
2.2.1	Random Variables and Distributions . . . . .	27
2.2.2	Expectation: Mean, Variance, and Moments . . . . .	28
2.2.3	Joint, Marginal, and Conditional Distributions . . . . .	30
2.2.4	Common Probability Distributions . . . . .	33
2.2.5	Transformation of Random Variables . . . . .	40
2.3	<b>Information Theory</b> . . . . .	41
2.3.1	Information and Entropy . . . . .	41
2.3.2	Mutual Information . . . . .	43
2.3.3	KL Divergence . . . . .	46
2.4	<b>Mathematical Optimization</b> . . . . .	48
2.4.1	General Formulation . . . . .	49
2.4.2	Optimality Conditions . . . . .	50
2.4.3	Numerical Optimization Methods . . . . .	59
	Exercises . . . . .	64
3	<b>Supervised Machine Learning (in a Nutshell)</b>	67
3.1	<b>Overview</b> . . . . .	67
3.2	<b>Case Studies</b> . . . . .	72
4	<b>Feature Extraction</b>	77
4.1	<b>Feature Extraction: Concepts</b> . . . . .	77
4.1.1	Feature Engineering . . . . .	77
4.1.2	Feature Selection . . . . .	78
4.1.3	Dimensionality Reduction . . . . .	79
4.2	<b>Linear Dimension Reduction</b> . . . . .	79
4.2.1	Principal Component Analysis . . . . .	80
4.2.2	Linear Discriminant Analysis . . . . .	84
4.3	<b>Nonlinear Dimension Reduction (I): Manifold Learning</b> . . . . .	86
4.3.1	Locally Linear Embedding . . . . .	87
4.3.2	Multidimensional Scaling . . . . .	88
4.3.3	Stochastic Neighborhood Embedding . . . . .	89
4.4	<b>Nonlinear Dimension Reduction (II): Neural Networks</b> . . . . .	90
4.4.1	Autoencoder . . . . .	90
4.4.2	Bottleneck Features . . . . .	91
	Lab Project I . . . . .	92
	Exercises . . . . .	93

<b>DISCRIMINATIVE MODELS</b>	<b>95</b>
<b>5 Statistical Learning Theory</b>	<b>97</b>
5.1 Formulation of Discriminative Models . . . . .	97
5.2 Learnability . . . . .	99
5.3 Generalization Bounds . . . . .	100
5.3.1 Finite Model Space: $ H $ . . . . .	100
5.3.2 Infinite Model Space: VC Dimension . . . . .	102
Exercises . . . . .	105
<b>6 Linear Models</b>	<b>107</b>
6.1 Perceptron . . . . .	108
6.2 Linear Regression . . . . .	112
6.3 Minimum Classification Error . . . . .	113
6.4 Logistic Regression . . . . .	114
6.5 Support Vector Machines . . . . .	116
6.5.1 Linear SVM . . . . .	116
6.5.2 Soft SVM . . . . .	121
6.5.3 Nonlinear SVM: The Kernel Trick . . . . .	123
6.5.4 Solving Quadratic Programming . . . . .	126
6.5.5 Multiclass SVM . . . . .	127
Lab Project II . . . . .	129
Exercises . . . . .	130
<b>7 Learning Discriminative Models in General</b>	<b>133</b>
7.1 A General Framework to Learn Discriminative Models . . . . .	133
7.1.1 Common Loss Functions in Machine Learning . . . . .	135
7.1.2 Regularization Based on $L_p$ Norm . . . . .	136
7.2 Ridge Regression and LASSO . . . . .	139
7.3 Matrix Factorization . . . . .	140
7.4 Dictionary Learning . . . . .	145
Lab Project III . . . . .	149
Exercises . . . . .	150
<b>8 Neural Networks</b>	<b>151</b>
8.1 Artificial Neural Networks . . . . .	152
8.1.1 Basic Formulation of Artificial Neural Networks . . . . .	152
8.1.2 Mathematical Justification: Universal Approximator . . . . .	154
8.2 Neural Network Structures . . . . .	156
8.2.1 Basic Building Blocks to Connect Layers . . . . .	156
8.2.2 Case Study I: Fully Connected Deep Neural Networks . . . . .	165
8.2.3 Case Study II: Convolutional Neural Networks . . . . .	166
8.2.4 Case Study III: Recurrent Neural Networks (RNNs) . . . . .	170

8.2.5	Case Study IV: Transformer . . . . .	172
8.3	<b>Learning Algorithms for Neural Networks</b> . . . . .	174
8.3.1	Loss Function . . . . .	175
8.3.2	Automatic Differentiation . . . . .	176
8.3.3	Optimization Using Stochastic Gradient Descent . . . . .	188
8.4	<b>Heuristics and Tricks for Optimization</b> . . . . .	189
8.4.1	Other SGD Variant Optimization Methods: ADAM . . . . .	192
8.4.2	Regularization . . . . .	194
8.4.3	Fine-Tuning Tricks . . . . .	196
8.5	<b>End-to-End Learning</b> . . . . .	197
8.5.1	Sequence-to-Sequence Learning . . . . .	198
	Lab Project IV . . . . .	200
	Exercises . . . . .	201
<b>9</b>	<b>Ensemble Learning</b>	<b>203</b>
9.1	<b>Formulation of Ensemble Learning</b> . . . . .	203
9.1.1	Decision Trees . . . . .	205
9.2	<b>Bagging</b> . . . . .	208
9.2.1	Random Forests . . . . .	208
9.3	<b>Boosting</b> . . . . .	209
9.3.1	Gradient Boosting . . . . .	210
9.3.2	AdaBoost . . . . .	212
9.3.3	Gradient Tree Boosting . . . . .	214
	Lab Project V . . . . .	216
	Exercises . . . . .	217
	<b>GENERATIVE MODELS</b>	<b>219</b>
<b>10</b>	<b>Overview of Generative Models</b>	<b>221</b>
10.1	<b>Formulation of Generative Models</b> . . . . .	221
10.2	<b>Bayesian Decision Theory</b> . . . . .	222
10.2.1	Generative Models for Classification . . . . .	223
10.2.2	Generative Models for Regression . . . . .	227
10.3	<b>Statistical Data Modeling</b> . . . . .	228
10.3.1	Plug-In MAP Decision Rule . . . . .	229
10.4	<b>Density Estimation</b> . . . . .	231
10.4.1	Maximum-Likelihood Estimation . . . . .	231
10.4.2	Maximum-Likelihood Classifier . . . . .	234
10.5	<b>Generative Models (in a Nutshell)</b> . . . . .	234
10.5.1	Generative versus Discriminative Models . . . . .	236
	Exercises . . . . .	237

<b>11 Unimodal Models</b>	<b>239</b>
11.1 Gaussian Models . . . . .	240
11.2 Multinomial Models . . . . .	243
11.3 Markov Chain Models . . . . .	245
11.4 Generalized Linear Models . . . . .	250
11.4.1 Probit Regression . . . . .	252
11.4.2 Poisson Regression . . . . .	252
11.4.3 Log-Linear Models . . . . .	253
Exercises . . . . .	256
<b>12 Mixture Models</b>	<b>257</b>
12.1 Formulation of Mixture Models . . . . .	257
12.1.1 Exponential Family (e-Family) . . . . .	259
12.1.2 Formal Definition of Mixture Models . . . . .	261
12.2 Expectation-Maximization Method . . . . .	261
12.2.1 Auxiliary Function: Eliminating Log-Sum . . . . .	262
12.2.2 Expectation-Maximization Algorithm . . . . .	265
12.3 Gaussian Mixture Models . . . . .	268
12.3.1 K-Means Clustering for Initialization . . . . .	270
12.4 Hidden Markov Models . . . . .	271
12.4.1 HMMs: Mixture Models for Sequences . . . . .	272
12.4.2 Evaluation Problem: Forward–Backward Algorithm . . . . .	276
12.4.3 Decoding Problem: Viterbi Algorithm . . . . .	279
12.4.4 Training Problem: Baum–Welch Algorithm . . . . .	280
Lab Project VI . . . . .	287
Exercises . . . . .	288
<b>13 Entangled Models</b>	<b>291</b>
13.1 Formulation of Entangled Models . . . . .	291
13.1.1 Framework of Entangled Models . . . . .	292
13.1.2 Learning of Entangled Models in General . . . . .	294
13.2 Linear Gaussian Models . . . . .	296
13.2.1 Probabilistic PCA . . . . .	296
13.2.2 Factor Analysis . . . . .	298
13.3 Non-Gaussian Models . . . . .	300
13.3.1 Independent Component Analysis (ICA) . . . . .	300
13.3.2 Independent Factor Analysis (IFA) . . . . .	301
13.3.3 Hybrid Orthogonal Projection and Estimation (HOPE) . . . . .	302
13.4 Deep Generative Models . . . . .	303
13.4.1 Variational Autoencoders (VAE) . . . . .	304
13.4.2 Generative Adversarial Nets (GAN) . . . . .	307
Exercises . . . . .	309

<b>14 Bayesian Learning</b>	<b>311</b>
14.1 Formulation of Bayesian Learning . . . . .	311
14.1.1 Bayesian Inference . . . . .	313
14.1.2 Maximum a Posterior Estimation . . . . .	314
14.1.3 Sequential Bayesian Learning . . . . .	315
14.2 Conjugate Priors . . . . .	318
14.2.1 Maximum-Marginal-Likelihood Estimation . . . . .	323
14.3 Approximate Inference . . . . .	324
14.3.1 Laplace's Method . . . . .	324
14.3.2 Variational Bayesian (VB) Methods . . . . .	326
14.4 Gaussian Processes . . . . .	332
14.4.1 Gaussian Processes as Nonparametric Priors . . . . .	333
14.4.2 Gaussian Processes for Regression . . . . .	335
14.4.3 Gaussian Processes for Classification . . . . .	338
Exercises . . . . .	340
<b>15 Graphical Models</b>	<b>343</b>
15.1 Concepts of Graphical Models . . . . .	343
15.2 Bayesian Networks . . . . .	346
15.2.1 Conditional Independence . . . . .	346
15.2.2 Representing Generative Models as Bayesian Networks .	351
15.2.3 Learning Bayesian Networks . . . . .	353
15.2.4 Inference Algorithms . . . . .	355
15.2.5 Case Study I: Naive Bayes Classifier . . . . .	361
15.2.6 Case Study II: Latent Dirichlet Allocation . . . . .	362
15.3 Markov Random Fields . . . . .	366
15.3.1 Formulation: Potential and Partition Functions . . . . .	366
15.3.2 Case Study III: Conditional Random Fields . . . . .	368
15.3.3 Case Study IV: Restricted Boltzmann Machines . . . . .	370
Exercises . . . . .	372
<b>APPENDIX</b>	<b>375</b>
<b>A Other Probability Distributions</b>	<b>377</b>
<b>Bibliography</b>	<b>381</b>
<b>Index</b>	<b>397</b>