Data-Driven Science and Engineering

Machine Learning, Dynamical Systems, and Control Second Edition

STEVEN L. BRUNTON

University of Washington

J. NATHAN KUTZ University of Washington



Contents

| | Preface | <i>page</i> ix | |
|----------|---|----------------|--|
| | Acknowledgments | | |
| | Common Optimization Techniques, Equations, Symbols, and Acronyms | xv | |
| Part I I | Dimensionality Reduction and Transforms | 1 | |
| 1 | Singular Value Decomposition (SVD) | 3 | |
| | 1.1 Overview | 3 | |
| | 1.2 Matrix Approximation | 7 | |
| | 1.3 Mathematical Properties and Manipulations | 12 | |
| | 1.4 Pseudo-Inverse, Least-Squares, and Regression | 16 | |
| | 1.5 Principal Component Analysis (PCA) | 23 | |
| | 1.6 Eigenfaces Example | 28 | |
| | 1.7 Truncation and Alignment | 35 | |
| | 1.8 Randomized Singular Value Decomposition | 40 | |
| | 1.9 Tensor Decompositions and N-Way Data Arrays | 46 | |
| 2 | Fourier and Wavelet Transforms | 53 | |
| | 2.1 Fourier Series and Fourier Transforms | 53 | |
| | 2.2 Discrete Fourier Transform (DFT) and Fast Fourier Transform (FFT) | 63 | |
| | 2.3 Transforming Partial Differential Equations | 70 | |
| | 2.4 Gabor Transform and the Spectrogram | 76 | |
| | 2.5 Laplace Transform | 81 | |
| | 2.6 Wavelets and Multi-Resolution Analysis | 85 | |
| | 2.7 Two-Dimensional Transforms and Image Processing | 87 | |
| 3 | Sparsity and Compressed Sensing | 97 | |
| | 3.1 Sparsity and Compression | 97 | |
| | 3.2 Compressed Sensing | 101 | |
| | 3.3 Compressed Sensing Examples | 105 | |
| | 3.4 The Geometry of Compression | 109 | |
| | 3.5 Sparse Regression | 113 | |
| | 3.6 Sparse Representation | 117 | |
| | 3.7 Robust Principal Component Analysis (RPCA) | 120 | |
| | 3.8 Sparse Sensor Placement | 123 | |

| Part II | Machin | e Learning and Data Analysis | 131 |
|----------|-------------------------------|--|-----|
| 4 | Reg | ression and Model Selection | 133 |
| | 4.1 | Classic Curve Fitting | 134 |
| | 4.2 | Nonlinear Regression and Gradient Descent | 140 |
| | 4.3 | Regression and $Ax = b$: Over- and Under-Determined Systems | 145 |
| | 4.4 | Optimization as the Cornerstone of Regression | 151 |
| | 4.5 | The Pareto Front and Lex Parsimoniae | 155 |
| | 4.6 | Model Selection: Cross-Validation | 158 |
| | 4.7 | Model Selection: Information Criteria | 162 |
| 5 | Clus | stering and Classification | 168 |
| | 5.1 | Feature Selection and Data Mining | 169 |
| | 5.2 | Supervised versus Unsupervised Learning | 174 |
| | 5.3 | Unsupervised Learning: k-Means Clustering | 178 |
| | 5.4 | Unsupervised Hierarchical Clustering: Dendrogram | 182 |
| | 5.5 | Mixture Models and the Expectation-Maximization Algorithm | 186 |
| | 5.6 | Supervised Learning and Linear Discriminants | 189 |
| | 5.7 | Support Vector Machines (SVM) | 193 |
| | 5.8 | Classification Trees and Random Forest | 198 |
| | 5.9 | Top 10 Algorithms of Data Mining circa 2008 (Before the Deep | |
| | | Learning Revolution) | 203 |
| 6 | Neu | ral Networks and Deep Learning | 208 |
| | 6.1 | Neural Networks: Single-Layer Networks | 209 |
| | 6.2 | Multi-Layer Networks and Activation Functions | 214 |
| | 6.3 | The Backpropagation Algorithm | 219 |
| | 6.4 | The Stochastic Gradient Descent Algorithm | 222 |
| | 6.5 | Deep Convolutional Neural Networks | 224 |
| | 6.6 | Neural Networks for Dynamical Systems | 228 |
| | 6.7 | Recurrent Neural Networks | 233 |
| | 6.8 | Autoencoders | 236 |
| | 6.9 | Generative Adversarial Networks (GANs) | 240 |
| | 6.10 | The Diversity of Neural Networks | 242 |
| Part III | Part III Dynamics and Control | | |
| 7 | Data | -Driven Dynamical Systems | 253 |
| | 7.1 | Overview, Motivations, and Challenges | 254 |
| | 7.2 | Dynamic Mode Decomposition (DMD) | 260 |
| | 7.3 | Sparse Identification of Nonlinear Dynamics (SINDy) | 275 |
| | 7.4 | Koopman Operator Theory | 286 |
| | 7.5 | Data-Driven Koopman Analysis | 296 |

| 8 | Linear Control Theory | 311 |
|-----------|---|-----|
| | 8.1 Closed-Loop Feedback Control | 312 |
| | 8.2 Linear Time-Invariant Systems | 317 |
| | 8.3 Controllability and Observability | 322 |
| | 8.4 Optimal Full-State Control: Linear–Quadratic Regulator (LQR) | 328 |
| | 8.5 Optimal Full-State Estimation: the Kalman Filter | 332 |
| | 8.6 Optimal Sensor-Based Control: Linear–Quadratic Gaussian (LQG) | 335 |
| | 8.7 Case Study: Inverted Pendulum on a Cart | 336 |
| | 8.8 Robust Control and Frequency-Domain Techniques | 346 |
| 9 | Balanced Models for Control | 360 |
| | 9.1 Model Reduction and System Identification | 360 |
| | 9.2 Balanced Model Reduction | 361 |
| | 9.3 System Identification | 375 |
| Part IV A | Ivanced Data-Driven Modeling and Control | 387 |
| 10 | Data-Driven Control | 389 |
| | 10.1 Model Predictive Control (MPC) | 390 |
| | 10.2 Nonlinear System Identification for Control | 392 |
| | 10.3 Machine Learning Control | 398 |
| | 10.4 Adaptive Extremum-Seeking Control | 408 |
| 11 | Reinforcement Learning | 419 |
| | 11.1 Overview and Mathematical Formulation | 419 |
| | 11.2 Model-Based Optimization and Control | 426 |
| | 11.3 Model-Free Reinforcement Learning and <i>Q</i> -Learning | 429 |
| | 11.4 Deep Reinforcement Learning | 436 |
| | 11.5 Applications and Environments | 440 |
| | 11.6 Optimal Nonlinear Control | 444 |
| 12 | Reduced-Order Models (ROMs) | 449 |
| | 12.1 Proper Orthogonal Decomposition (POD) for Partial Differential Equations | 449 |
| | 12.2 Optimal Basis Elements: the POD Expansion | 455 |
| | 12.3 POD and Soliton Dynamics | 461 |
| | 12.4 Continuous Formulation of POD | 465 |
| | 12.5 POD with Symmetries: Rotations and Translations | 470 |
| | 12.6 Neural Networks for Time-Stepping with POD | 475 |
| | 12.7 Leveraging DMD and SINDy for Galerkin–POD | 479 |
| 13 | Interpolation for Parametric Reduced-Order Models | 485 |
| | 13.1 Gappy POD | 485 |
| | 13.2 Error and Convergence of Gappy POD | 490 |
| | 13.3 Gappy Measurements: Minimize Condition Number | 493 |
| | 13.4 Gappy Measurements: Maximal Variance | 497 |

| 13.5 POD and the Discrete Empirical Interpolation Method (DEIM) | 500 |
|---|-----|
| 13.6 DEIM Algorithm Implementation | 504 |
| 13.7 Decoder Networks for Interpolation | 508 |
| 13.8 Randomization and Compression for ROMs | 512 |
| 13.9 Machine Learning ROMs | 513 |
| Physics-Informed Machine Learning | 520 |
| 14.1 Mathematical Foundations | 520 |
| 14.2 SINDy Autoencoder: Coordinates and Dynamics | 523 |
| 14.3 Koopman Forecasting | 526 |
| 14.4 Learning Nonlinear Operators | 529 |
| 14.5 Physics-Informed Neural Networks (PINNs) | 533 |
| 14.6 Learning Coarse-Graining for PDEs | 535 |
| 14.7 Deep Learning and Boundary Value Problems | 539 |
| Glossary | 542 |
| References | 552 |
| Index | 588 |