Data-Driven Science and Engineering

Data-driven discovery is revolutionizing the modeling, prediction, and control of complex systems. This textbook brings together machine learning, engineering mathematics, and mathematical physics to integrate modeling and control of dynamical systems with modern methods in data science. It highlights many of the recent advances in scientific computing that enable data-driven methods to be applied to a diverse range of complex systems such as turbulence, the brain, climate, epidemiology, finance, robotics, and autonomy.

Aimed at advanced undergraduate and beginning graduate students in the engineering and physical sciences, the text presents a range of topics and methods from introductory to state of the art.

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Data-Driven Science and Engineering

Machine Learning, Dynamical Systems, and Control

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Contents

	Pref	<i>lace</i>	<i>page</i> ix
	Con	nmon Optimization Techniques, Equations, Symbols, and Acronyms	xiii
Part I	Dime	nsionality Reduction and Transforms	1
1	Sing	ular Value Decomposition (SVD)	3
	1.1	Overview	3
	1.2	Matrix Approximation	7
	1.3	Mathematical Properties and Manipulations	10
	1.4	Pseudo-Inverse, Least-Squares, and Regression	15
	1.5	Principal Component Analysis (PCA)	21
	1.6	Eigenfaces Example	25
	1.7	Truncation and Alignment	30
	1.8	Randomized Singular Value Decomposition	37
	1.9	Tensor Decompositions and N-Way Data Arrays	41
2	Fourier and Wavelet Transforms		47
	2.1	Fourier Series and Fourier Transforms	47
	2.2	Discrete Fourier Transform (DFT) and Fast Fourier Transform (FFT)	56
	2.3	Transforming Partial Differential Equations	63
	2.4	Gabor Transform and the Spectrogram	69
	2.5	Wavelets and Multi-Resolution Analysis	75
	2.6	2D Transforms and Image Processing	77
3	Sparsity and Compressed Sensing		
	3.1	Sparsity and Compression	84
	3.2	Compressed Sensing	88
	3.3	Compressed Sensing Examples	92
	3.4	The Geometry of Compression	95
	3.5	Sparse Regression	98
	3.6	Sparse Representation	103
	3.7	Robust Principal Component Analysis (RPCA)	107
	3.8	Sparse Sensor Placement	110

vi

Contents

Part	II Machine Learning and Data Analysis	115
4	Regression and Model Selection	117
	4.1 Classic Curve Fitting	118
	4.2 Nonlinear Regression and Gradient Descent	123
	4.3 Regression and $Ax = b$: Over- and Under-Determined Systems	130
	4.4 Optimization as the Cornerstone of Regression	136
	4.5 The Pareto Front and <i>Lex Parsimoniae</i>	140
	4.6 Model Selection: Cross-Validation	143
	4.7 Model Selection: Information Criteria	148
5	Clustering and Classification	154
	5.1 Feature Selection and Data Mining	155
	5.2 Supervised versus Unsupervised Learning	160
	5.3 Unsupervised Learning: <i>k</i> -means Clustering	164
	5.4 Unsupervised Hierarchical Clustering: Dendrogram	168
	5.5 Mixture Models and the Expectation-Maximization Algorithm	172
	5.6 Supervised Learning and Linear Discriminants	176
	5.7 Support Vector Machines (SVM)	180
	5.8 Classification Trees and Random Forest	185
	5.9 Top 10 Algorithms in Data Mining 2008	190
6	Neural Networks and Deep Learning	
	6.1 Neural Networks: 1-Layer Networks	196
	6.2 Multi-Layer Networks and Activation Functions	199
	6.3 The Backpropagation Algorithm	204
	6.4 The Stochastic Gradient Descent Algorithm	209
	6.5 Deep Convolutional Neural Networks	212
	6.6 Neural Networks for Dynamical Systems	216
	6.7 The Diversity of Neural Networks	220
	5	
Part	III Dynamics and Control	227
Part 7	III Dynamics and Control Data-Driven Dynamical Systems	227 229
Part 7	 III Dynamics and Control Data-Driven Dynamical Systems 7.1 Overview, Motivations, and Challenges 	227 229 230
Part 7	 III Dynamics and Control Data-Driven Dynamical Systems 7.1 Overview, Motivations, and Challenges 7.2 Dynamic Mode Decomposition (DMD) 	227 229 230 235
Part 7	 III Dynamics and Control Data-Driven Dynamical Systems 7.1 Overview, Motivations, and Challenges 7.2 Dynamic Mode Decomposition (DMD) 7.3 Sparse Identification of Nonlinear Dynamics (SINDy) 	227 229 230 235 247
Part 7	 III Dynamics and Control Data-Driven Dynamical Systems 7.1 Overview, Motivations, and Challenges 7.2 Dynamic Mode Decomposition (DMD) 7.3 Sparse Identification of Nonlinear Dynamics (SINDy) 7.4 Koopman Operator Theory 	227 229 230 235 247 257
Part 7	 III Dynamics and Control Data-Driven Dynamical Systems 7.1 Overview, Motivations, and Challenges 7.2 Dynamic Mode Decomposition (DMD) 7.3 Sparse Identification of Nonlinear Dynamics (SINDy) 7.4 Koopman Operator Theory 7.5 Data-Driven Koopman Analysis 	227 229 230 235 247 257 266
Part 7 8	 III Dynamics and Control Data-Driven Dynamical Systems 7.1 Overview, Motivations, and Challenges 7.2 Dynamic Mode Decomposition (DMD) 7.3 Sparse Identification of Nonlinear Dynamics (SINDy) 7.4 Koopman Operator Theory 7.5 Data-Driven Koopman Analysis Linear Control Theory 	227 229 230 235 247 257 266 276
Part 7 8	 III Dynamics and Control Data-Driven Dynamical Systems 7.1 Overview, Motivations, and Challenges 7.2 Dynamic Mode Decomposition (DMD) 7.3 Sparse Identification of Nonlinear Dynamics (SINDy) 7.4 Koopman Operator Theory 7.5 Data-Driven Koopman Analysis Linear Control Theory 8.1 Closed-Loop Feedback Control 	227 229 230 235 247 257 266 276 277
Part 7 8	 III Dynamics and Control Data-Driven Dynamical Systems 7.1 Overview, Motivations, and Challenges 7.2 Dynamic Mode Decomposition (DMD) 7.3 Sparse Identification of Nonlinear Dynamics (SINDy) 7.4 Koopman Operator Theory 7.5 Data-Driven Koopman Analysis Linear Control Theory 8.1 Closed-Loop Feedback Control 8.2 Linear Time-Invariant Systems 	227 229 230 235 247 257 266 276 277 281

8.4 Optimal Full-State Control: Linear Quadratic Regulator (LQR)

Cambridge University Press 978-1-108-42209-3 — Data-Driven Science and Engineering Steven L. Brunton , J. Nathan Kutz Frontmatter <u>More Information</u>

		Contents	vi	
			204	
	8.5 Optimal Full-State Estimation: The Kalman Filter		296	
	8.6 Optimal Sensor-Based Control: Linear Quadratic Gaussian	(LQG)	299	
	8.7 Case Study: Inverted Pendulum on a Cart		300	
	8.8 Robust Control and Frequency Domain Techniques		508	
9	Balanced Models for Control			
	9.1 Model Reduction and System Identification		321	
	9.2 Balanced Model Reduction		322	
	9.3 System identification		336	
10	Data-Driven Control		345	
	10.1 Nonlinear System Identification for Control		346	
	10.2 Machine Learning Control		352	
	10.3 Adaptive Extremum-Seeking Control		362	
Part I	IV Reduced Order Models		373	
11	Reduced Order Models (ROMs)		375	
	11.1 POD for Partial Differential Equations		375	
	11.2 Optimal Basis Elements: The POD Expansion		381	
	11.3 POD and Soliton Dynamics		387	
	11.4 Continuous Formulation of POD		391	
	11.5 POD with Symmetries: Rotations and Translations		396	
12	Interpolation for Parametric ROMs		403	
	12.1 Gappy POD		403	
	12.2 Error and Convergence of Gappy POD		409	
	12.3 Gappy Measurements: Minimize Condition Number		413	
	12.4 Gappy Measurements: Maximal Variance		418	
	12.5 POD and the Discrete Empirical Interpolation Method (DE	IM)	423	
	12.6 DEIM Algorithm Implementation		426	
	12.7 Machine Learning ROMs		429	
	Glossary		436	
	Bibliography		443	
	Index		471	

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Preface

This book is about the growing intersection of data-driven methods, applied optimization, and the classical fields of engineering mathematics and mathematical physics. We have been developing this material over a number of years, primarily to educate our advanced undergrad and beginning graduate students from engineering and physical science departments. Typically, such students have backgrounds in linear algebra, differential equations, and scientific computing, with engineers often having some exposure to control theory and/or partial differential equations. However, most undergraduate curricula in engineering and science fields have little or no exposure to data methods and/or optimization. Likewise, computer scientists and statisticians have little exposure to dynamical systems and control. Our goal is to provide a broad entry point to applied data science for both of these groups of students. We have chosen the methods discussed in this book for their (1) relevance, (2) simplicity, and (3) generality, and we have attempted to present a range of topics, from basic introductory material up to research-level techniques.

Data-driven discovery is currently revolutionizing how we model, predict, and control complex systems. The most pressing scientific and engineering problems of the modern era are not amenable to empirical models or derivations based on first-principles. Increasingly, researchers are turning to data-driven approaches for a diverse range of complex systems, such as turbulence, the brain, climate, epidemiology, finance, robotics, and autonomy. These systems are typically nonlinear, dynamic, multi-scale in space and time, high-dimensional, with dominant underlying patterns that should be characterized and modeled for the eventual goal of sensing, prediction, estimation, and control. With modern mathematical methods, enabled by unprecedented availability of data and computational resources, we are now able to tackle previously unattainable challenge problems. A small handful of these new techniques include robust image reconstruction from sparse and noisy random pixel measurements, turbulence control with machine learning, optimal sensor and actuator placement, discovering interpretable nonlinear dynamical systems purely from data, and reduced order models to accelerate the study and optimization of systems with complex multi-scale physics.

Driving modern data science is the availability of vast and increasing quantities of data, enabled by remarkable innovations in low-cost sensors, orders-of-magnitudes increases in computational power, and virtually unlimited data storage and transfer capabilities. Such vast quantities of data are affording engineers and scientists across all disciplines new opportunities for data-driven discovery, which has been referred to as the fourth paradigm of scientific discovery [245]. This fourth paradigm is the natural culmination of the first three paradigms: empirical experimentation, analytical derivation, and computational investigation. The integration of these techniques provides a transformative framework for

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X Preface

data-driven discovery efforts. This process of scientific discovery is not new, and indeed mimics the efforts of leading figures of the scientific revolution: Johannes Kepler (1571–1630) and Sir Isaac Newton (1642–1727). Each played a critical role in developing the theoretical underpinnings of celestial mechanics, based on a combination of empirical data-driven and analytical approaches. Data science is not replacing mathematical physics and engineering, but is instead augmenting it for the twenty-first century, resulting in more of a renaissance than a revolution.

Data science itself is not new, having been proposed more than 50 years ago by John Tukey who envisioned the existence of a scientific effort focused on learning from data, or *data analysis* [152]. Since that time, data science has been largely dominated by two distinct cultural outlooks on data [78]. The *machine learning* community, which is predominantly comprised of computer scientists, is typically centered on prediction quality and scalable, fast algorithms. Although not necessarily in contrast, the *statistical learning* community, often centered in statistics departments, focuses on the inference of interpretable models. Both methodologies have achieved significant success and have provided the mathematical and computational foundations for data-science methods. For engineers and scientists, the goal is to leverage these broad techniques to infer and compute models (typically nonlinear) from observations that correctly identify the underlying dynamics *and* generalize qualitatively and quantitatively to unmeasured parts of phase, parameter, or application space. Our goal in this book is to leverage the power of both statistical and machine learning to solve engineering problems.

Themes of This Book

There are a number of key themes that have emerged throughout this book. First, many complex systems exhibit dominant low-dimensional patterns in the data, despite the rapidly increasing resolution of measurements and computations. This underlying structure enables efficient sensing, and compact representations for modeling and control. Pattern extraction is related to the second theme of finding *coordinate transforms* that simplify the system. Indeed, the rich history of mathematical physics is centered around coordinate transformations (e.g., spectral decompositions, the Fourier transform, generalized functions, etc.), although these techniques have largely been limited to simple idealized geometries and linear dynamics. The ability to derive *data-driven* transformations opens up opportunities to generalize these techniques to new research problems with more complex geometries and boundary conditions. We also take the perspective of dynamical systems and control throughout the book, applying data-driven techniques to model and control systems that evolve in time. Perhaps the most pervasive theme is that of data-driven applied optimization, as nearly every topic discussed is related to optimization (e.g., finding optimal lowdimensional patterns, optimal sensor placement, machine learning optimization, optimal control, etc.). Even more fundamentally, most data is organized into arrays for analysis, where the extensive development of numerical linear algebra tools from the early 1960s onward provides many of the foundational mathematical underpinnings for matrix decompositions and solution strategies used throughout this text.

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We would also like to thank our publisher Lauren Cowles at Cambridge University Press for being a reliable supporter throughout this process.

Online Material

We have designed this book to make extensive use of online supplementary material, including codes, data, videos, homeworks, and suggested course syllabi. All of this material can be found at the following website:

databookuw.com

In addition to course resources, all of the code and data used in the book are available. The codes online are more extensive than those presented in the book, including code used to generate publication quality figures. Data visualization was ranked as the top used data-science method in the Kaggle 2017 *The State of Data Science and Machine Learning* study, and so we highly encourage readers to download the online codes and make full use of these plotting commands.

We have also recorded and posted video lectures on YouTube for most of the topics in this book. We include supplementary videos for students to fill in gaps in their background on scientific computing and foundational applied mathematics. We have designed this text both to be a reference as well as the material for several courses at various levels of student preparation. Most chapters are also modular, and may be converted into stand-alone *boot camps*, containing roughly 10 hours of materials each.

How to Use This Book

Our intended audience includes beginning graduate students, or advanced undergraduates, in engineering and science. As such, the machine learning methods are introduced at a beginning level, whereas we assume students know how to model physical systems with differential equations and simulate them with solvers such as **ode45**. The diversity of topics covered thus range from introductory to state-of-the-art research methods. Our aim is to provide an integrated viewpoint and mathematical toolset for solving engineering and science problems. Alternatively, the book can also be useful for computer science and

xii Preface

statistics students who often have limited knowledge of dynamical systems and control. Various courses can be designed from this material, and several example syllabi may be found on the book website; this includes homework, data sets, and code.

First and foremost, we want this book to be fun, inspiring, eye-opening, and empowering for young scientists and engineers. We have attempted to make everything as simple as possible, while still providing the depth and breadth required to be useful in research. Many of the chapter topics in this text could be entire books in their own right, and many of them are. However, we also wanted to be as comprehensive as may be reasonably expected for a field that is so big and moving so fast. We hope that you enjoy this book, master these methods, and change the world with applied data science!

Common Optimization Techniques, Equations, Symbols, and Acronyms

Most Common Optimization Strategies

Least-Squares (discussed in Chapters 1 and 4) minimizes the sum of the squares of the residuals between a given fitting model and data. Linear least-squares, where the residuals are linear in the unknowns, has a closed form solution which can be computed by taking the derivative of the residual with respect to each unknown and setting it to zero. It is commonly used in the engineering and applied sciences for fitting polynomial functions. Nonlinear least-squares typically requires iterative refinement based upon approximating the nonlinear least-squares with a linear least-squares at each iteration.

Gradient Descent (discussed in Chapters 4 and 6) is the industry leading, convex optimization method for high-dimensional systems. It minimizes residuals by computing the gradient of a given fitting function. The iterative procedure updates the solution by *moving downhill* in the residual space. The Newton–Raphson method is a one-dimensional version of gradient descent. Since it is often applied in high-dimensional settings, it is prone to find only local minima. Critical innovations for big data applications include stochastic gradient descent and the backpropagation algorithm which makes the optimization amenable to computing the gradient itself.

Alternating Descent Method (ADM) (discussed in Chapter 4) avoids computations of the gradient by optimizing in one unknown at a time. Thus all unknowns are held constant while a line search (non-convex optimization) can be performed in a single variable. This variable is then updated and held constant while another of the unknowns is updated. The iterative procedure continues through all unknowns and the iteration procedure is repeated until a desired level of accuracy is achieved.

Augmented Lagrange Method (ALM) (discussed in Chapters 3 and 8) is a class of algorithms for solving constrained optimization problems. They are similar to penalty methods in that they replace a constrained optimization problem by a series of unconstrained problems and add a penalty term to the objective which helps enforce the desired constraint. ALM adds another term designed to mimic a Lagrange multiplier. The augmented Lagrangian is not the same as the method of Lagrange multipliers.

Linear Program and Simplex Method are the workhorse algorithms for convex optimization. A linear program has an objective function which is linear in the unknown and the constraints consist of linear inequalities and equalities. By computing its feasible region, which is a convex polytope, the linear programming algorithm finds a point in the polyhedron where this function has the smallest (or largest) value if such a point exists. The simplex method is a specific iterative technique for linear programs which aims to take a given basic feasible solution to another basic feasible solution for which the objective function is smaller, thus producing an iterative procedure for optimizing.

xiv Common Optimization Techniques, Equations, Symbols, and Acronyms

Most Common Equations and Symbols

Linear Algebra

Linear System of Equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}.\tag{0.1}$$

The matrix $\mathbf{A} \in \mathbb{R}^{p \times n}$ and vector $\mathbf{b} \in \mathbb{R}^p$ are generally known, and the vector $\mathbf{x} \in \mathbb{R}^n$ is unknown.

Eigenvalue Equation

$$\mathbf{AT} = \mathbf{T}\mathbf{\Lambda}.\tag{0.2}$$

The columns $\boldsymbol{\xi}_k$ of the matrix **T** are the eigenvectors of $\mathbf{A} \in \mathbb{C}^{n \times n}$ corresponding to the eigenvalue λ_k : $\mathbf{A}\boldsymbol{\xi}_k = \lambda_k \boldsymbol{\xi}_k$. The matrix $\boldsymbol{\Lambda}$ is a diagonal matrix containing these eigenvalues, in the simple case with *n* distinct eigenvalues.

Change of Coordinates

$$\mathbf{x} = \mathbf{\Psi} \mathbf{a}.\tag{0.3}$$

The vector $\mathbf{x} \in \mathbb{R}^n$ may be written as $\mathbf{a} \in \mathbb{R}^n$ in the coordinate system given by the columns of $\Psi \in \mathbb{R}^{n \times n}$.

Measurement Equation

$$\mathbf{y} = \mathbf{C}\mathbf{x}.\tag{0.4}$$

The vector $\mathbf{y} \in \mathbb{R}^p$ is a measurement of the state $\mathbf{x} \in \mathbb{R}^n$ by the measurement matrix $\mathbf{C} \in \mathbb{R}^{p \times n}$.

Singular Value Decomposition

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^* \approx \tilde{\mathbf{U}}\tilde{\mathbf{\Sigma}}\tilde{\mathbf{V}}^*. \tag{0.5}$$

The matrix $\mathbf{X} \in \mathbb{C}^{n \times m}$ may be decomposed into the product of three matrices $\mathbf{U} \in \mathbb{C}^{n \times n}$, $\mathbf{\Sigma} \in \mathbb{C}^{n \times m}$, and $\mathbf{V} \in \mathbb{C}^{m \times m}$. The matrices \mathbf{U} and \mathbf{V} are *unitary*, so that $\mathbf{U}\mathbf{U}^* = \mathbf{U}^*\mathbf{U} = \mathbf{I}_{n \times n}$ and $\mathbf{V}\mathbf{V}^* = \mathbf{V}^*\mathbf{V} = \mathbf{I}_{m \times m}$, where * denotes complex conjugate transpose. The columns of \mathbf{U} (resp. \mathbf{V}) are orthogonal, called left (resp. right) *singular vectors*. The matrix $\mathbf{\Sigma}$ contains decreasing, nonnegative diagonal entries called *singular values*.

Often, **X** is approximated with a low-rank matrix $\tilde{\mathbf{X}} = \tilde{\mathbf{U}}\tilde{\mathbf{\Sigma}}\tilde{\mathbf{V}}^*$, where $\tilde{\mathbf{U}}$ and $\tilde{\mathbf{V}}$ contain the first $r \ll n$ columns of **U** and **V**, respectively, and $\tilde{\mathbf{\Sigma}}$ contains the first $r \times r$ block of $\boldsymbol{\Sigma}$. The matrix $\tilde{\mathbf{U}}$ is often denoted Ψ in the context of spatial modes, reduced order models, and sensor placement.

XV

Regression and Optimization

Overdetermined and Underdetermined Optimization for Linear Systems

$$\underset{\mathbf{x}}{\operatorname{argmin}} \left(\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2 + \lambda g(\mathbf{x}) \right) \quad \text{or} \quad (0.6a)$$

$$\underset{\mathbf{x}}{\operatorname{argmin}} g(\mathbf{x}) \text{ subject to } \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2 \le \epsilon , \qquad (0.6b)$$

Here $g(\mathbf{x})$ is a regression penalty (with penalty parameter λ for overdetermined systems). For over- and underdetermined linear systems of equations, which result in either no solutions or an infinite number of solutions of $\mathbf{A}\mathbf{x} = \mathbf{b}$, a choice of constraint or penalty, which is also known as *regularization*, must be made in order to produce a solution.

Overdetermined and Underdetermined Optimization for Nonlinear Systems

$$\underset{\mathbf{x}}{\operatorname{argmin}} \left(f(\mathbf{A}, \mathbf{x}, \mathbf{b}) + \lambda g(\mathbf{x}) \right) \quad \text{or} \quad (0.7a)$$

$$\operatorname{argmin} g(\mathbf{x}) \text{ subject to } f(\mathbf{A}, \mathbf{x}, \mathbf{b}) \le \epsilon$$
 (0.7b)

This generalizes the linear system to a nonlinear system $f(\cdot)$ with regularization $g(\cdot)$. These over- and underdetermined systems are often solved using gradient descent algorithms.

Compositional Optimization for Neural Networks

$$\underset{\mathbf{A}_{j}}{\operatorname{argmin}}\left(f_{M}(\mathbf{A}_{M},\cdots,f_{2}(\mathbf{A}_{2},(f_{1}(\mathbf{A}_{1},\mathbf{x}))\cdots)+\lambda g(\mathbf{A}_{j})\right)$$
(0.8)

Each \mathbf{A}_k denotes the weights connecting the neural network from the *k*th to (k + 1)th layer. It is typically a massively underdetermined system which is regularized by $g(\mathbf{A}_j)$. Composition and regularization are critical for generating expressive representations of the data as well as preventing overfitting.

Dynamical Systems and Reduced Order Models

Nonlinear Ordinary Differential Equation (Dynamical System)

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), t; \boldsymbol{\beta}).$$
(0.9)

The vector $\mathbf{x}(t) \in \mathbb{R}^n$ is the state of the system evolving in time t, β are parameters, and \mathbf{f} is the vector field. Generally, \mathbf{f} is Lipschitz continuous to guarantee existence and uniqueness of solutions.

Linear Input–Output System

$$\frac{d}{dt}\mathbf{x} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u} \tag{0.10a}$$

$$\mathbf{y} = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{u}.\tag{0.10b}$$

The state of the system is $\mathbf{x} \in \mathbb{R}^n$, the inputs (actuators) are $\mathbf{u} \in \mathbb{R}^q$, and the outputs (sensors) are $\mathbf{y} \in \mathbb{R}^p$. The matrices **A**, **B**, **C**, **D** define the dynamics, the effect of actuation, the sensing strategy, and the effect of actuation feed-through, respectively.

xvi Common Optimization Techniques, Equations, Symbols, and Acronyms

Nonlinear Map (Discrete-Time Dynamical System)

$$\mathbf{x}_{k+1} = \mathbf{F}(\mathbf{x}_k). \tag{0.11}$$

The state of the system at the *k*th iteration is $\mathbf{x}_k \in \mathbb{R}^n$, and **F** is a possibly nonlinear mapping. Often, this map defines an iteration forward in time, so that $\mathbf{x}_k = \mathbf{x}(k\Delta t)$; in this case the flow map is denoted $\mathbf{F}_{\Delta t}$.

Koopman Operator Equation (Discrete-Time)

$$\mathcal{K}_t g = g \circ \mathbf{F}_t \implies \mathcal{K}_t \varphi = \lambda \varphi.$$
 (0.12)

The linear Koopman operator \mathcal{K}_t advances measurement functions of the state $g(\mathbf{x})$ with the flow \mathbf{F}_t . Eigenvalues and eigenvectors of \mathcal{K}_t are λ and $\varphi(\mathbf{x})$, respectively. The operator \mathcal{K}_t operates on a Hilbert space of measurements.

Nonlinear Partial Differential Equation

$$\mathbf{u}_t = \mathbf{N}(\mathbf{u}, \mathbf{u}_x, \mathbf{u}_{xx}, \cdots, x, t; \boldsymbol{\beta}). \tag{0.13}$$

The state of the PDE is **u**, the nonlinear evolution operator is **N**, subscripts denote partial differentiation, and x and t are the spatial and temporal variables, respectively. The PDE is parameterized by values in $\boldsymbol{\beta}$. The state **u** of the PDE may be a continuous function u(x, t), or it may be discretized at several spatial locations, $\mathbf{u}(t) = \left[u(x_1, t) \quad u(x_2, t) \quad \cdots \quad u(x_n, t)\right]^T \in \mathbb{R}^n$.

Galerkin Expansion

The continuous Galerkin expansion is:

$$u(x,t) \approx \sum_{k=1}^{r} a_k(t) \psi_k(x).$$
 (0.14)

The functions $a_k(t)$ are temporal coefficients that capture the time dynamics, and $\psi_k(x)$ are spatial modes. For a high-dimensional discretized state, the Galerkin expansion becomes: $\mathbf{u}(t) \approx \sum_{k=1}^{r} a_k(t) \boldsymbol{\psi}_k$. The spatial modes $\boldsymbol{\psi}_k \in \mathbb{R}^n$ may be the columns of $\boldsymbol{\Psi} = \tilde{\mathbf{U}}$.

Complete Symbols

Dimensions

- *K* Number of nonzero entries in a *K*-sparse vector **s**
- *m* Number of data snapshots (i.e., columns of **X**)
- *n* Dimension of the state, $\mathbf{x} \in \mathbb{R}^n$
- *p* Dimension of the measurement or output variable, $\mathbf{y} \in \mathbb{R}^p$
- q Dimension of the input variable, $\mathbf{u} \in \mathbb{R}^q$
- r Rank of truncated SVD, or other low-rank approximation

Scalars

- s Frequency in Laplace domain
- t Time
- δ learning rate in gradient descent
- Δt Time step
- *x* Spatial variable
- Δx Spatial step
 - σ Singular value
 - λ Eigenvalue
 - λ Sparsity parameter for sparse optimization (Section 7.3)
 - λ Lagrange multiplier (Sections. 3.7, 8.4, and 11.4)
 - τ Threshold

Vectors

- **a** Vector of mode amplitudes of **x** in basis Ψ , $\mathbf{a} \in \mathbb{R}^r$
- **b** Vector of measurements in linear system Ax = b
- **b** Vector of DMD mode amplitudes (Section 7.2)
- **Q** Vector containing potential function for PDE-FIND
- r Residual error vector
- **s** Sparse vector, $\mathbf{s} \in \mathbb{R}^n$
- **u** Control variable (Chapters 8, 9, and 10)
- **u** PDE state vector (Chapters 11 and 12)
- w Exogenous inputs
- \mathbf{w}_d Disturbances to system
- \mathbf{w}_n Measurement noise
- \mathbf{w}_r Reference to track
- **x** State of a system, $\mathbf{x} \in \mathbb{R}^n$
- \mathbf{x}_k Snapshot of data at time t_k
- \mathbf{x}_i Data sample $j \in Z := \{1, 2, \dots, m\}$ (Chapters 5 and 6)
- $\tilde{\mathbf{x}}$ Reduced state, $\tilde{\mathbf{x}} \in \mathbb{R}^r$, so that $\mathbf{x} \approx \tilde{\mathbf{U}}\tilde{\mathbf{x}}$
- $\hat{\mathbf{x}}$ Estimated state of a system
- **y** Vector of measurements, $\mathbf{y} \in \mathbb{R}^p$
- \mathbf{y}_j Data label $j \in Z := \{1, 2, \dots, m\}$ (Chapters 5 and 6)
- $\hat{\mathbf{y}}$ Estimated output measurement
- **z** Transformed state, $\mathbf{x} = \mathbf{T}\mathbf{z}$ (Chapters 8 and 9)
- ϵ Error vector

xvii

xviii Common Optimization Techniques, Equations, Symbols, and Acronyms

Vectors, continued

- β Bifurcation parameters
- **ξ** Eigenvector of Koopman operator (Sections 7.4 and 7.5)
- *ξ* Sparse vector of coefficients (Section 7.3)
- ϕ DMD mode
- ψ POD mode
- **Υ** Vector of PDE measurements for PDE-FIND

Matrices

- **A** Matrix for system of equations or dynamics
- $\tilde{\mathbf{A}}$ Reduced dynamics on *r*-dimensional POD subspace
- A_X Matrix representation of linear dynamics on the state x
- A_Y Matrix representation of linear dynamics on the observables y
- (A, B, C, B) Matrices for continuous-time state-space system
- $(\mathbf{A}_d, \mathbf{B}_d, \mathbf{C}_d, \mathbf{B}_d)$ Matrices for discrete-time state-space system
 - $(\hat{\mathbf{A}}, \hat{\mathbf{B}}, \hat{\mathbf{C}}, \hat{\mathbf{B}})$ Matrices for state-space system in new coordinates $\mathbf{z} = \mathbf{T}^{-1}\mathbf{x}$
 - $(\tilde{\mathbf{A}}, \tilde{\mathbf{B}}, \tilde{\mathbf{C}}, \tilde{\mathbf{B}})$ Matrices for reduced state-space system with rank r
 - **B** Actuation input matrix
 - C Linear measurement matrix from state to measurements
 - \mathcal{C} Controllability matrix
 - \mathcal{F} Discrete Fourier transform
 - **G** Matrix representation of linear dynamics on the states and inputs $[\mathbf{x}^T \mathbf{u}^T]^T$
 - H Hankel matrix
 - **H**['] Time-shifted Hankel matrix
 - I Identity matrix
 - **K** Matrix form of Koopman operator (Chapter 7)
 - **K** Closed-loop control gain (Chapter 8)
 - \mathbf{K}_f Kalman filter estimator gain
 - \mathbf{K}_r LQR control gain
 - L Low-rank portion of matrix X (Chapter 3)
 - \mathcal{O} Observability matrix
 - **P** Unitary matrix that acts on columns of **X**
 - **Q** Weight matrix for state penalty in LQR (Sec. 8.4)
 - Q Orthogonal matrix from QR factorization
 - **R** Weight matrix for actuation penalty in LQR (Sec. 8.4)
 - **R** Upper triangular matrix from QR factorization
 - **S** Sparse portion of matrix **X** (Chapter 3)
 - **T** Matrix of eigenvectors (Chapter 8)
 - T Change of coordinates (Chapters 8 and 9)
 - **U** Left singular vectors of **X**, $\mathbf{U} \in \mathbb{R}^{n \times n}$
 - $\hat{\mathbf{U}}$ Left singular vectors of economy SVD of $\mathbf{X}, \mathbf{U} \in \mathbb{R}^{n \times m}$
 - $\tilde{\mathbf{U}}$ Left singular vectors (POD modes) of truncated SVD of $\mathbf{X}, \mathbf{U} \in \mathbb{R}^{n \times r}$
 - **V** Right singular vectors of **X**, **V** $\in \mathbb{R}^{m \times m}$
 - $\tilde{\mathbf{V}}$ Right singular vectors of truncated SVD of $\mathbf{X}, \mathbf{V} \in \mathbb{R}^{m \times r}$

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Matrices, continued

- **\Sigma** Matrix of singular values of **X**, **\Sigma \in \mathbb{R}^{n \times m}**
- $\hat{\boldsymbol{\Sigma}}$ Matrix of singular values of economy SVD of $\mathbf{X}, \, \boldsymbol{\Sigma} \in \mathbb{R}^{m \times m}$
- $\tilde{\Sigma}$ Matrix of singular values of truncated SVD of **X**, $\Sigma \in \mathbb{R}^{r \times r}$
- W Eigenvectors of A
- **W**_c Controllability Gramian
- **W**_o Observability Gramian
- **X** Data matrix, $\mathbf{X} \in \mathbb{R}^{n \times m}$
- \mathbf{X}' Time-shifted data matrix, $\mathbf{X}' \in \mathbb{R}^{n \times m}$
- Y Projection of X matrix onto orthogonal basis in randomized SVD (Sec. 1.8)
- **Y** Data matrix of observables, $\mathbf{Y} = \mathbf{g}(\mathbf{X}), \mathbf{Y} \in \mathbb{R}^{p \times m}$ (Chapter 7)
- **Y**' Shifted data matrix of observables, $\mathbf{Y}' = \mathbf{g}(\mathbf{X}'), \mathbf{Y}' \in \mathbb{R}^{p \times m}$ (Chapter 7)
- **Z** Sketch matrix for randomized SVD, $\mathbf{Z} \in \mathbb{R}^{n \times r}$ (Sec. 1.8)
- Θ Measurement matrix times sparsifying basis, $\Theta = C\Psi$ (Chapter 3)
- **Θ** Matrix of candidate functions for SINDy (Sec. 7.3)
- Γ Matrix of derivatives of candidate functions for SINDy (Sec. 7.3)
- **Ξ** Matrix of coefficients of candidate functions for SINDy (Sec. 7.3)
- **Ξ** Matrix of nonlinear snapshots for DEIM (Sec. 12.5)
- Λ Diagonal matrix of eigenvalues
- **Υ** Input snapshot matrix, **Υ** $\in \mathbb{R}^{q \times m}$
- $\Phi \quad \text{Matrix of DMD modes, } \Phi \triangleq \mathbf{X}' \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{W}$
- Ψ Orthonormal basis (e.g., Fourier or POD modes)

Tensors

 $(\mathcal{A}, \mathcal{B}, \mathcal{M})$ N-way array tensors of size $I_1 \times I_2 \times \cdots \times I_N$

Norms

- $\|\cdot\|_0 = \ell_0$ pseudo-norm of a vector **x** the number of nonzero elements in **x**
- $\|\cdot\|_1 \quad \ell_1 \text{ norm of a vector } \mathbf{x} \text{ given by } \|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i|$
- $\|\cdot\|_2 \quad \ell_2 \text{ norm of a vector } \mathbf{x} \text{ given by } \|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^n (x_i^2)}$
- $\|\cdot\|_2$ 2-norm of a matrix **X** given by $\|\mathbf{X}\|_2 = \max_{\mathbf{X}} \frac{\|\mathbf{X}\|_2}{\|\mathbf{x}\|_2}$
- $\|\cdot\|_F$ Frobenius norm of a matrix **X** given by $\|\mathbf{X}\|_F = \sqrt{\sum_{i=1}^n \sum_{j=1}^m |X_{ij}|^2}$
- $\|\cdot\|_*$ Nuclear norm of a matrix **X** given by $\|\mathbf{X}\|_* = \operatorname{trace}\left(\sqrt{\mathbf{X}^*\mathbf{X}}\right) = \sum_{i=1}^m \sigma_i$ (for m < n)
 - $\langle \cdot, \cdot \rangle$ Inner product. For functions, $\langle f(x), g(x) \rangle = \int_{-\infty}^{\infty} f(x)g^*(x)dx$.
 - $\langle \cdot, \cdot \rangle$ Inner product. For vectors, $\langle u, v \rangle = u^* v$.

Operators, Functions, and Maps

- \mathcal{F} Fourier transform
- F Discrete-time dynamical system map
- \mathbf{F}_t Discrete-time flow map of dynamical system through time t
- f Continuous-time dynamical system
- \mathcal{G} Gabor transform

хіх

xx Common Optimization Techniques, Equations, Symbols, and Acronyms

Operators, Functions, and Maps, continued

- **G** Transfer function from inputs to outputs (Chapter 8)
- g Scalar measurement function on x
- g Vector-valued measurement functions on x
- J Cost function for control
- ℓ Loss function for support vector machines (Chapter 5)
- \mathcal{K} Koopman operator (continuous time)
- \mathcal{K}_t Koopman operator associated with time *t* flow map
- \mathcal{L} Laplace transform
- L Loop transfer function (Chapter 8)
- L Linear partial differential equation (Chapters 11 and 12)
- N Nonlinear partial differential equation
- \mathcal{O} Order of magnitude
- **S** Sensitivity function (Chapter 8)
- T Complementary sensitivity function (Chapter 8)
- W Wavelet transform
- μ Incoherence between measurement matrix C and basis Ψ
- κ Condition number
- φ Koopman eigenfunction
- ∇ Gradient operator
- * Convolution operator

Most Common Acronyms

- CNN Convolutional neural network
- DL Deep learning
- DMD Dynamic mode decomposition
- FFT Fast Fourier transform
- ODE Ordinary differential equation
- PCA Principal components analysis
- PDE Partial differential equation
- POD Proper orthogonal decomposition
- ROM Reduced order model
- SVD Singular value decomposition

Other Acronyms

- ADM Alternating directions method
- AIC Akaike information criterion
- ALM Augmented Lagrange multiplier
- ANN Artificial neural network
- ARMA Autoregressive moving average
- ARMAX Autoregressive moving average with exogenous input
 - BIC Bayesian information criterion
 - BPOD Balanced proper orthogonal decomposition
 - DMDc Dynamic mode decomposition with control
 - CCA Canonical correlation analysis
 - CFD Computational fluid dynamics
- CoSaMP Compressive sampling matching pursuit
 - CWT Continuous wavelet transform
 - DEIM Discrete empirical interpolation method
 - DCT Discrete cosine transform
 - DFT Discrete Fourier transform
 - DMDc Dynamic mode decomposition with control
 - DNS Direct numerical simulation
 - DWT Discrete wavelet transform
 - ECOG Electrocorticography
 - eDMD Extended DMD
 - EIM Empirical interpolation method
 - EM Expectation maximization
 - EOF Empirical orthogonal functions
 - ERA Eigensystem realization algorithm
 - ESC Extremum-seeking control
 - GMM Gaussian mixture model
- HAVOK Hankel alternative view of Koopman
 - JL Johnson-Lindenstrauss
 - KL Kullback-Leibler
 - ICA Independent component analysis

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xxii Common Optimization Techniques, Equations, Symbols, and Acronyms

Other Acronyms, continued

KLT	Karhunen–Loève transform
LAD	Least absolute deviations
LASSO	Least absolute shrinkage and selection operator
LDA	Linear discriminant analysis
LQE	Linear quadratic estimator
LQG	Linear quadratic Gaussian controller
LQR	Linear quadratic regulator
LTI	Linear time invariant system
MIMO	Multiple input, multiple output
MLC	Machine learning control
MPE	Missing point estimation
mrDMD	Multi-resolution dynamic mode decomposition
NARMAX	Nonlinear autoregressive model with exogenous inputs
NLS	Nonlinear Schrödinger equation
OKID	Observer Kalman filter identification
PBH	Popov–Belevitch–Hautus test
PCP	Principal component pursuit
PDE-FIND	Partial differential equation functional identification
	of nonlinear dynamics
PDF	Probability distribution function
PID	Proportional-integral-derivative control
PIV	Particle image velocimetry
RIP	Restricted isometry property
rSVD	Randomized SVD
RKHS	Reproducing kernel Hilbert space
RNN	Recurrent neural network
RPCA	Robust principal components analysis
SGD	Stochastic gradient descent
SINDy	Sparse identification of nonlinear dynamics
SISO	Single input, single output
SRC	Sparse representation for classification
SSA	Singular spectrum analysis
STFT	Short time Fourier transform
STLS	Sequential thresholded least-squares
SVM	Support vector machine

- TICA Time-lagged independent component analysis
- VAC Variational approach of conformation dynamics