Dynamic Mode Decomposition

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Data-Driven Modeling of Complex Systems

J. Nathan Kutz
University of Washington
Seattle, Washington

Steven L. Brunton
University of Washington
Seattle, Washington

Bingni W. Brunton
University of Washington
Seattle, Washington

Joshua L. Proctor
Institute for Disease Modeling
Bellevue, Washington

Society for Industrial and Applied Mathematics
Philadelphia

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Preface

The integration of data and scientific computation is driving a paradigm shift across the engineering, natural, and physical sciences. Indeed, there exists an unprecedented availability of high-fidelity measurements from time-series recordings, numerical simulations, and experimental data. When data is coupled with readily available algorithms and innovations in machine (statistical) learning, it is possible to extract meaningful spatiotemporal patterns that dominate dynamic activity. A direct implication of such data-driven modeling strategies is that we can gain traction on understanding fundamental scientific processes and also enhance our capabilities for prediction, state estimation, and control of complex systems. The ability to discover underlying principles from data has been called the *fourth paradigm of scientific discovery* [131]. Mathematical techniques geared toward characterizing patterns in data and capitalizing on the observed low-dimensional structures fall clearly within this fourth paradigm and are in ever-growing demand.

The focus of this book is on the emerging method of *dynamic mode decomposition (DMD)*. DMD is a matrix decomposition technique that is highly versatile and builds upon the power of singular value decomposition (SVD). The low-rank structures extracted from DMD, however, are associated with temporal features as well as correlated spatial activity. One only need consider the impact of principal component analysis (PCA) and Fourier transforms to understand the importance of versatile matrix decomposition methods and time-series characterizations for data analysis.

From a conceptional viewpoint, the DMD method has a rich history stemming from the seminal work of Bernard Koopman in 1931 [162] on nonlinear dynamical systems. But due to the lack of computational resources during his era, the theoretical developments were largely limited. Interest in Koopman theory was revived in 2004/05 by Mezić et al. [196, 194], with Schmid and Sesterhenn [250] and Schmid [247], in 2008 and 2010, respectively, first defining DMD as an algorithm. Rowley et al. [235] quickly realized that the DMD algorithm was directly connected to the underlying nonlinear dynamics through the Koopman operator, opening up the theoretical underpinnings for DMD theory. Thus, a great deal of credit for the success of DMD can be directly attributed to the seminal contributions of Igor Mezić (University of California, Santa Barbara), Peter Schmid (Imperial College), and Clancy Rowley (Princeton University).

This book develops the fundamental theoretical foundations of DMD and the Koopman operator. It further highlights many new innovations and algorithms that extend the range of applicability of the method. We also demonstrate how DMD can be applied in a variety of discipline-specific settings. These exemplar fields show how DMD can be used successfully for prediction, state estimation, and control of complex systems. By providing a suite of algorithms for DMD and its variants, we hope to help the practitioner quickly become fluent in this emerging method. Our aim is also to augment a traditional training in dynamical systems with a data-driven viewpoint of the field.

To aid in demonstrating the key concepts of this book, we have made extensive use of the scientific computing software MATLAB. MATLAB is one of the leading scientific computing software packages and is used across universities in the United States for teaching and learning. It is easy to use, provides high-level programming functionality, and greatly reduces the time to produce example code. The built-in algorithms developed by MATLAB allow us to easily use many of the key workhorse routines of scientific computing. Given that DMD was originally defined as an algorithm, it is fitting that the book is strongly focused on implementation and algorithm development. We are confident that the codes provided in MATLAB will not only allow for reproducible research but also enhance the learning experience for both those committed to its research implementation and those curious to dabble in a new mathematical subject. All the codes are available at www.siam.org/books/ot149.

J. Nathan Kutz
Steven L. Brunton
Bingni W. Brunton
Joshua L. Proctor

Seattle, WA
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Notation

$\mathbf{A}$	Matrix representation of discrete-time linear dynamics
$\tilde{\mathbf{A}}$	Reduced dynamics on POD subspace
$\mathcal{A}$	Matrix representation of continuous-time linear dynamics
$\mathbf{A}^{\mathrm{b}}$	Matrix representation of backward-time dynamics
$\mathbf{A}_r$	Rank-r approximation of linear dynamics from ERA
$\mathbf{A}_{\mathbf{X}}$	Matrix representation of linear dynamics on the state $\mathbf{x}$
$\mathbf{A}_{\mathbf{Y}}$	Matrix representation of linear dynamics on the observables $\mathbf{y}$
$\mathbf{B}$	Input matrix
$\mathbf{B}_r$	Input matrix for rank-r ERA system
$\mathbf{b}$	Vector of DMD mode amplitudes
$\mathbf{C}$	Linear measurement matrix from state to outputs
$\mathbf{C}_r$	Linear measurement matrix for rank-r ERA system
D	Cylinder diameter
$\mathbf{F}$	Discrete-time flow map of dynamical system
$\mathbf{F}_t$	Discrete-time flow map of dynamical system through time t
$\mathbf{f}$	Continuous-time dynamical system
$\mathbf{G}$	Matrix representation of linear dynamics on the states and inputs $[\mathbf{x}^T \mathbf{u}^T]^T$
G	Implicit measurement function
$\mathbf{g}$	Vector-valued observable functions on $\mathbf{x}$
g	Scalar observable function on $\mathbf{x}$
$\mathcal{H}$	Hilbert space of scalar-valued functions on state-space
J	Number of time bins in mrDMD
$\mathcal{K}$	Koopman operator
$\mathbf{K}$	Finite-dimensional approximation to Koopman operator
$\mathbf{L}$	Low-rank portion of matrix $\mathbf{X}$
L	Number of levels in mrDMD
ℓ	Current level in mrDMD
m	Number of data snapshots
m_f	Number of days in the future for DMD prediction
m_p	Number of past days taken into account in DMD prediction
$\mathbf{N}$	Nonlinear partial differential equation
$\tilde{\mathbf{N}}$	Macroscale nonlinearity
n	Dimension of the state, $\mathbf{x} \in \mathbb{R}^n$
$\mathbf{P}$	Unitary matrix that acts on columns of $\mathbf{X}$
p	Dimension of the measurement or output variable, $\mathbf{y} \in \mathbb{R}^p$
$\mathbf{q}$	Continuous-time state of partial differential equation
q	Dimension of the input variable, $\mathbf{u} \in \mathbb{R}^q$
Re	Reynolds number

$\mathbf{r}$	Residual error vector
r	Rank of truncated SVD
$\tilde{r}$	Rank of truncated SVD of $\mathbf{\Omega}$
$\mathbf{S}$	Sparse portion of matrix $\mathbf{X}$
$\mathbf{s}$	Sparse vector
s	Number of times to shift-stack data for ERA
t	Time
t_k	kth discrete time step
Δt	Time step
$\mathbf{U}$	Left singular vectors (POD modes) of $\mathbf{X}$
$\hat{\mathbf{U}}$	Left singular vectors (POD modes) of $\mathbf{\Omega}$
$\tilde{\mathbf{U}}$	Left singular vectors (POD modes) of $\mathbf{X}'$
U_∞	Free-stream fluid velocity
$\mathbf{u}$	Control variable
$\mathbf{V}$	Right singular vectors of $\mathbf{X}$
$\hat{\mathbf{V}}$	Right singular vectors (POD modes) of $\mathbf{\Omega}$
$\tilde{\mathbf{V}}$	Right singular vectors (POD modes) of $\mathbf{X}'$
$\mathbf{W}$	Eigenvectors of $\tilde{\mathbf{A}}$
$\mathbf{X}$	Data matrix, $\mathbf{X} \in \mathbb{R}^{n \times (m-1)}$
$\mathbf{X}'$	Shifted data matrix, $\mathbf{X}' \in \mathbb{R}^{n \times (m-1)}$
$\mathbf{X}_j^k$	Data matrix containing snapshots j through k
$\mathbf{x}_k$	Snapshot of data at time t_k
$\mathbf{Y}$	Data matrix of observables, $\mathbf{Y} = \mathbf{g}(\mathbf{X})$, $\mathbf{Y} \in \mathbb{R}^{p \times (m-1)}$
$\mathbf{Y}'$	Shifted data matrix of observables, $\mathbf{Y}' = \mathbf{g}(\mathbf{X}')$, $\mathbf{Y}' \in \mathbb{R}^{p \times (m-1)}$
$\mathbf{y}$	Vector of measurements, $\mathbf{y} \in \mathbb{R}^p$
η	Noise magnitude
$\mathbf{\Theta}$	Measurement matrix times sparsifying basis, $\mathbf{\Theta} = \mathbf{C}\mathbf{\Psi}$
$\mathbf{\Lambda}$	Diagonal matrix of DMD eigenvalues (discrete-time)
λ	DMD eigenvalue
μ	Bifurcation parameters
ν	Kinematic viscosity of fluid
ξ	Spatial variable
ρ	Radius of eigenvalue threshold for fast/slow separation in mrDMD
$\mathbf{\Sigma}$	Matrix of singular values
$\hat{\mathbf{\Sigma}}$	Matrix of singular values of $\mathbf{\Omega}$
$\tilde{\mathbf{\Sigma}}$	Matrix of singular values of $\mathbf{X}'$
σ_k	kth singular value
$\mathbf{\Upsilon}$	Input snapshot matrix, $\mathbf{\Upsilon} \in \mathbb{R}^{q \times (m-1)}$
$\mathbf{\Phi}$	Matrix of DMD modes, $\mathbf{\Phi} \triangleq \mathbf{X}'\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{W}$
$\mathbf{\Phi}_{\mathbf{X}}$	DMD modes on $\mathbf{X}$
$\mathbf{\Phi}_{\mathbf{Y}}$	DMD modes on $\mathbf{Y}$
$\boldsymbol{\phi}$	DMD mode
φ	Koopman eigenfunction

$\mathbf{\Psi}$	Orthonormal basis (e.g., Fourier or POD modes)
$\mathbf{\Omega}$	State and input snapshot matrix, $\mathbf{\Omega} \in \mathbb{R}^{(q+n)\times(m-1)}$
ω	Continuous-time DMD eigenvalue, $\omega \triangleq \log(\lambda)/\Delta t$
$\lvert\lvert\cdot\rvert\rvert_0$	ℓ_0 pseudonorm of a vector $\mathbf{x}$: the number of nonzero elements in $\mathbf{x}$
$\lvert\lvert\cdot\rvert\rvert_1$	ℓ_1-norm of a vector $\mathbf{x}$ given by $\lvert\lvert\mathbf{x}\rvert\rvert_1 = \sum_{i=1}^n \lvert x_i\rvert$
$\lvert\lvert\cdot\rvert\rvert_2$	ℓ_2-norm of a vector $\mathbf{x}$ given by $\lvert\lvert\mathbf{x}\rvert\rvert_2 = \sqrt{\sum_{i=1}^n (x_i^2)}$
$\lvert\lvert\cdot\rvert\rvert_F$	Frobenius norm of a matrix $\mathbf{X}$ given by $\lvert\lvert\mathbf{X}\rvert\rvert_F = \sqrt{\sum_{i=1}^n \sum_{j=1}^m \lvert X_{ij}\rvert^2}$
$\lvert\lvert\cdot\rvert\rvert_*$	Nuclear norm of a matrix $\mathbf{X}$ given by $\lvert\lvert\mathbf{X}\rvert\rvert_* = \mathrm{trace}\left(\sqrt{\mathbf{X}^*\mathbf{X}}\right) = \sum_{i=1}^m \sigma_i$ (for $m \leq n$)
$\langle\cdot,\cdot\rangle$	Inner product. For functions, $\langle f(x), g(x)\rangle = \int_{-\infty}^{\infty} f(x) g^*(x)dx$.

Acronyms

ALM	Augmented Lagrange multiplier
ARIMA	Autoregressive integrated moving average
ARMA	Autoregressive moving average
ARX	Autoregressive exogenous
BPOD	Balanced proper orthogonal decomposition
cDMD	Compressed dynamic mode decomposition
csDMD	Compressed sensing dynamic mode decomposition
CFD	Computational fluid dynamics
CWT	Continuous wavelet transform
DEIM	Discrete empirical interpolation method
DMD	Dynamic mode decomposition
DMDc	Dynamic mode decomposition with control
DNS	Direct numerical simulation
ECoG	Electrocorticography
EEG	Electroencephalography
EFM	Equation-free method
EOF	Empirical orthogonal functions
ERA	Eigensystem realization algorithm
fbDMD	Forward/backward DMD
FFT	Fast Fourier transform
GPFA	Gaussian process factor analysis
HMM	Hidden Markov model
ICA	Independent component analysis
KIC	Koopman with inputs and control
LDS	Linear dynamical system
LDV	Laser Doppler velocimetry
LIM	Linear inverse modeling
MRA	Multiresolution analysis
mrDMD	Multiresolution dynamic mode decomposition
NLDS	Nonlinear dynamical systems
NLS	Nonlinear Schrödinger
NLSA	Nonlinear Laplacian spectral analysis
NNMF	Nonnegative matrix factorization
OKID	Observer Kalman filter identification
PCA	Principal component analysis

PCP	Principal component pursuit
PCR	Principal component regression
PIV	Particle image velocimetry
POD	Proper orthogonal decomposition
RIP	Restricted isometry property
ROM	Reduced-order model
RPCA	Robust principal component analysis
SARIMA	Seasonal autoregressive integrated moving average
SIR	Susceptible, infected, recovered
SSA	Singular spectrum analysis
STBLI	Shock turbulent boundary layer interaction
STFT	Short-time Fourier transform
SVD	Singular value decomposition
SVM	Support vector machine
tlsDMD	Total-least-squares DMD
VARIMA	Vector autoregressive integrated moving average