Dynamic Mode Decomposition Theory and Applications

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Abstract

This document provides a comprehensive theoretical foundation for Dynamic Mode Decomposition (DMD), a data-driven technique for analyzing complex dynamical systems. We develop the mathematics from first principles, starting with the basic formulation and extending to advanced variants. The document covers standard DMD, exact DMD, time-delay embeddings, sparsity-promoting techniques, multi-resolution DMD, and connections to Koopman operator theory. Each section includes the mathematical formulation, practical implementation considerations, and insights into interpretation of results.

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1 Introduction

Dynamic Mode Decomposition (DMD) has emerged as a powerful tool for analyzing complex, high-dimensional, and time-evolving systems across nu-

merous scientific disciplines. Originally developed in the fluid dynamics community by Schmid (2010) (1), DMD has since found applications in fields ranging from neuroscience to financial market analysis.

The primary appeal of DMD lies in its ability to decompose complex dynamics into coherent spatiotemporal modes with specific oscillation frequencies and growth/decay rates, without requiring knowledge of the governing equations. This purely data-driven approach makes DMD particularly valuable for systems where first-principles modeling is challenging or impossible.

At its core, DMD approximates the nonlinear dynamics of a system using a best-fit linear operator that advances the system forward in time. Through spectral analysis of this operator, DMD extracts coherent modes and their temporal evolution, effectively separating spatial and temporal components of the dynamics.

In this document, we develop the mathematical foundations of DMD from first principles and explore its various extensions, interpretations, and applications. We aim to provide both theoretical rigor and practical insights to help researchers and practitioners effectively apply DMD to their specific domains.

2 Mathematical Foundations

2.1 Problem Formulation

Consider a dynamical system whose state $\mathbf{x}(t) \in \mathbb{R}^n$ evolves in time according to:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) \tag{1}$$

where \mathbf{f} is generally a nonlinear function. In many practical scenarios, we do not know the function \mathbf{f} explicitly, but we have access to measurement data.

Let us collect a sequence of state snapshots at times t_1, t_2, \ldots, t_m :

$$\mathbf{X} = \begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_m \\ | & | & & | \end{bmatrix}$$
 (2)

where $\mathbf{x}_j = \mathbf{x}(t_j)$ and m is the number of snapshots. We also define a time-shifted data matrix:

$$\mathbf{X}' = \begin{bmatrix} | & | & & | \\ \mathbf{x}_2 & \mathbf{x}_3 & \cdots & \mathbf{x}_{m+1} \\ | & | & & | \end{bmatrix}$$
 (3)

DMD seeks to find a linear operator **A** that best approximates the dynamics by mapping each snapshot to the next:

$$\mathbf{x}_{i+1} \approx \mathbf{A}\mathbf{x}_i \tag{4}$$

or in matrix form:

$$\mathbf{X}' \approx \mathbf{A}\mathbf{X} \tag{5}$$

The optimal solution in the least-squares sense is:

$$\mathbf{A} = \mathbf{X}'\mathbf{X}^{\dagger} \tag{6}$$

where \mathbf{X}^{\dagger} is the Moore-Penrose pseudoinverse of \mathbf{X} .

2.2 Singular Value Decomposition (SVD) Approach

Computing the full $n \times n$ matrix **A** is often impractical for high-dimensional systems where n could be millions or billions. Instead, DMD typically employs a reduced-order approach using the Singular Value Decomposition (SVD).

We first compute the SVD of the data matrix:

$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^* \tag{7}$$

where $\mathbf{U} \in \mathbb{C}^{n \times r}$, $\mathbf{\Sigma} \in \mathbb{C}^{r \times r}$, and $\mathbf{V} \in \mathbb{C}^{m \times r}$, with r being the rank of \mathbf{X} . The pseudoinverse of \mathbf{X} is then:

$$\mathbf{X}^{\dagger} = \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{U}^* \tag{8}$$

Instead of computing the full matrix A, we project onto the POD modes (columns of U) to obtain a reduced matrix:

$$\tilde{\mathbf{A}} = \mathbf{U}^* \mathbf{A} \mathbf{U} = \mathbf{U}^* \mathbf{X}' \mathbf{V} \mathbf{\Sigma}^{-1} \tag{9}$$

This $r \times r$ matrix **A** captures the same eigenvalue dynamics as the full matrix **A**, but at a much lower computational cost.

2.3 Eigendecomposition and DMD Modes

The eigendecomposition of $\tilde{\mathbf{A}}$ gives:

$$\tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\mathbf{\Lambda} \tag{10}$$

where Λ is a diagonal matrix of eigenvalues and \mathbf{W} is a matrix whose columns are the corresponding eigenvectors.

The DMD eigenvalues λ_i (diagonal elements of Λ) characterize the temporal dynamics:

- $|\lambda_i| < 1$: Decaying mode
- $|\lambda_i| = 1$: Neutral (marginal) mode
- $|\lambda_i| > 1$: Growing mode
- angle(λ_i): Oscillation frequency

The DMD modes, which represent the spatial structures, are computed as:

$$\mathbf{\Phi} = \mathbf{X}' \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{W} \tag{11}$$

These modes are the eigenvectors of the full matrix \mathbf{A} , and they correspond to the spatial patterns that evolve coherently with fixed frequency and growth/decay rate.

2.4 Continuous-Time Formulation

The DMD eigenvalues exist in discrete time. To obtain continuous-time dynamics, we compute:

$$\omega_i = \frac{\ln(\lambda_i)}{\Delta t} \tag{12}$$

where Δt is the time step between snapshots. The real part of ω_i represents the growth/decay rate, and the imaginary part represents the oscillation frequency in continuous time.

The time evolution of the system can then be expressed as:

$$\mathbf{x}(t) = \sum_{i=1}^{r} b_i \phi_i e^{\omega_i t} \tag{13}$$

where b_i are the initial amplitudes of each mode, calculated by projecting the initial condition onto the modes:

$$\mathbf{b} = \mathbf{\Phi}^{\dagger} \mathbf{x}(0) \tag{14}$$

3 Algorithm Implementation

3.1 Standard DMD Algorithm

The standard DMD algorithm can be summarized as follows:

Algorithm 1 Standard DMD

- 1: Arrange the data into matrices X and X'
- 2: Compute the SVD: $\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^*$
- 3: Compute the reduced matrix: $\tilde{\mathbf{A}} = \mathbf{U}^* \mathbf{X}' \mathbf{V} \mathbf{\Sigma}^{-1}$
- 4: Compute eigendecomposition: $\tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\mathbf{\Lambda}$
- 5: Compute DMD modes: $\Phi = \mathbf{X}'\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{W}$
- 6: Compute mode amplitudes: $\mathbf{b} = \mathbf{\Phi}^{\dagger} \mathbf{x}_1$

3.2 Exact DMD

The "exact" DMD algorithm, introduced by Tu et al. (2014) (2), modifies step 5 to compute modes that exactly fit the data:

$$\mathbf{\Phi} = \mathbf{X}' \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{W} \tag{15}$$

This formulation ensures that the reconstructed data exactly matches the original snapshots at the sampled time points.

3.3 Rank Truncation

In practice, we often truncate the SVD to retain only the k most significant singular values and vectors:

$$\mathbf{X} \approx \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^* \tag{16}$$

where k < r. This truncation serves two purposes:

- It reduces computational cost
- It acts as a filter to remove noise and small-scale dynamics

The choice of k is critical and can be guided by examining the decay of singular values or using methods like the optimal hard threshold.

3.4 DMD with Control

For systems with external inputs or control, the dynamics can be modeled as:

$$\mathbf{x}_{j+1} = \mathbf{A}\mathbf{x}_j + \mathbf{B}\mathbf{u}_j \tag{17}$$

where \mathbf{u}_j is the control input at time j and \mathbf{B} is the control matrix. DMD with control (DMDc) extends the standard algorithm to identify both \mathbf{A} and \mathbf{B} from data.

4 Advanced DMD Variants

4.1 Multi-Resolution DMD

Multi-resolution DMD (mrDMD) decomposes the dynamics across multiple time scales. The algorithm recursively applies DMD to residuals from coarser time scales, effectively creating a hierarchical decomposition.

This approach is particularly useful for systems with dynamics spanning multiple time scales, as it allows separate identification and analysis of slow and fast processes.

4.2 Compressed DMD

For extremely large datasets, compressed DMD applies random projections to reduce the dimensionality before performing DMD:

$$Y = PX \tag{18}$$

where \mathbf{P} is a random projection matrix. DMD is then performed on the compressed data \mathbf{Y} , and the results are lifted back to the original space.

4.3 Sparsity-Promoting DMD

Sparsity-promoting DMD (spDMD) adds a sparsity constraint on the mode amplitudes to select only the most important modes:

$$\min_{\mathbf{b}} \|\mathbf{X} - \mathbf{\Phi} \mathbf{D}_b \mathbf{V}_{and}\|_F^2 + \gamma \|\mathbf{b}\|_1 \tag{19}$$

where \mathbf{D}_b is a diagonal matrix of amplitudes, \mathbf{V}_{and} is the Vandermonde matrix of temporal dynamics, and γ controls the level of sparsity.

4.4 Optimized DMD

Optimized DMD modifies the objective function to minimize the total reconstruction error over all snapshots:

$$\min_{\mathbf{\Phi}, \mathbf{\Lambda}, \mathbf{b}} \sum_{i=1}^{m} \|\mathbf{x}_{j} - \sum_{i=1}^{r} b_{i} \phi_{i} \lambda_{i}^{j-1} \|_{2}^{2}$$

$$(20)$$

This non-convex optimization problem can be solved using techniques like variable projection.

5 Koopman Operator Theory and DMD

5.1 The Koopman Operator

The Koopman operator \mathcal{K} is an infinite-dimensional linear operator that evolves observables (functions of the state) forward in time:

$$\mathcal{K}g(\mathbf{x}) = g(\mathbf{F}(\mathbf{x})) \tag{21}$$

where g is an observable function and \mathbf{F} is the flow map of the dynamical system. The key insight is that the Koopman operator is linear even when the underlying dynamics are nonlinear.

5.2 DMD as Koopman Approximation

DMD can be interpreted as computing a finite-dimensional approximation of the Koopman operator. The DMD modes correspond to Koopman modes, and the DMD eigenvalues correspond to Koopman eigenvalues.

This connection is profound, as it provides a theoretical foundation for DMD and explains why a linear method can effectively analyze nonlinear systems.

5.3 Extended DMD (EDMD)

Extended DMD expands the state space using a dictionary of observable functions:

$$\mathbf{g}(\mathbf{x}) = \begin{bmatrix} g_1(\mathbf{x}) \\ g_2(\mathbf{x}) \\ \vdots \\ g_p(\mathbf{x}) \end{bmatrix}$$
(22)

DMD is then applied to the expanded state, potentially capturing more complex nonlinear dynamics.

5.4 Kernel DMD

Kernel DMD leverages the kernel trick to implicitly work in a high-dimensional (potentially infinite-dimensional) feature space:

$$\tilde{\mathbf{A}} = \mathbf{G}^{\prime *} \mathbf{G} (\mathbf{G}^* \mathbf{G})^{-1} \tag{23}$$

where ${\bf G}$ and ${\bf G}'$ are matrices of observable functions evaluated at the snapshots.

6 Applications and Case Studies

6.1 Fluid Dynamics

DMD has been extensively used in fluid dynamics for:

- Identifying coherent structures in turbulent flows
- Analyzing instabilities and transition to turbulence
- Predicting flow evolution and separation
- Reduced-order modeling for computational efficiency

6.2 Neuroscience

In neuroscience, DMD has been applied to:

- Extracting oscillatory patterns from neural recordings
- Identifying functional connectivity in brain networks
- Characterizing neural responses to stimuli
- Denoising and dimensionality reduction of neural data

6.3 Financial Markets

In financial applications, DMD has been used for:

- Identifying market modes and cycles
- Forecasting price movements
- Risk assessment and regime detection
- Anomaly detection in trading patterns

6.4 Video Processing

In video analysis, DMD serves for:

- Background subtraction and moving object detection
- Compression and dimensionality reduction
- Pattern recognition in spatiotemporal data
- Identifying recurring events and anomalies

7 Practical Considerations

7.1 Data Preprocessing

Several preprocessing steps can significantly improve DMD results:

- Mean subtraction: Removing the time average to focus on dynamics
- Normalization: Scaling features to comparable ranges
- Detrending: Removing long-term trends to focus on oscillatory dynamics
- Smoothing: Applying filters to reduce noise

7.2 Parameter Selection

Critical parameters in DMD include:

- Rank truncation: Determining how many SVD modes to retain
- Time delay: Choosing the sampling interval between snapshots
- Embedding dimension: For time-delay embeddings
- Sparsity parameter: For sparsity-promoting variants

7.3 Validation and Error Assessment

Methods for validating DMD results include:

- Cross-validation: Splitting data into training and testing sets
- Reconstruction error analysis: Comparing original and reconstructed data
- Eigenvalue sensitivity: Assessing stability of eigenvalues to perturbations
- Physical interpretation: Ensuring modes have meaningful physical interpretation

7.4 Numerical Stability

Techniques to improve numerical stability include:

- SVD truncation: Removing small singular values
- Regularization: Adding small diagonal terms to ill-conditioned matrices
- Scaling: Proper normalization of data
- Robust SVD algorithms: Using techniques like randomized SVD for large datasets

8 Theoretical Insights

8.1 Spectral Analysis of DMD

The DMD spectrum provides valuable insights into the system dynamics:

- Eigenvalues on the unit circle indicate neutral (persistent) modes
- Eigenvalues inside the unit circle indicate decaying modes
- Eigenvalues outside the unit circle indicate growing modes
- The distance from the unit circle indicates the growth/decay rate
- The angle from the positive real axis indicates the oscillation frequency

8.2 DMD for Linear Systems

For a linear system $\dot{\mathbf{x}} = \mathbf{A}_c \mathbf{x}$, DMD exactly recovers the dynamics:

- DMD eigenvalues are exactly $e^{\lambda_i \Delta t}$ where λ_i are eigenvalues of \mathbf{A}_c
- DMD modes coincide with eigenvectors of \mathbf{A}_c

8.3 DMD for Nonlinear Systems

For nonlinear systems, DMD provides a linear approximation that:

- Is exact for Koopman-invariant observables
- Captures locally linearized dynamics around attractors
- Can represent nonlinear dynamics through superposition of modes
- May require extended observables to fully capture nonlinearity

8.4 Connections to Other Methods

DMD has connections to several other analysis techniques:

- Proper Orthogonal Decomposition (POD): DMD modes are not orthogonal but temporal dynamics are simpler
- Fourier Analysis: DMD can be viewed as a generalization that allows for growth/decay

- Linear Systems Identification: DMD is related to the Eigensystem Realization Algorithm (ERA)
- Machine Learning: DMD has connections to regression, dimensionality reduction, and spectral methods

9 Future Directions

9.1 Theoretical Developments

Active areas of theoretical research include:

- Convergence guarantees for DMD approximations
- Optimal sampling strategies for DMD
- Connections to information theory and maximum entropy principles
- Unified frameworks for data-driven operator approximation

9.2 Algorithmic Innovations

Emerging algorithmic approaches include:

- Neural network representations of Koopman operators
- Probabilistic DMD formulations
- Online/streaming DMD algorithms
- Hardware-accelerated implementations for massive datasets

9.3 Applications in Emerging Fields

DMD is finding applications in new areas:

- Climate science and Earth system modeling
- Epidemiological forecasting
- Social network dynamics
- Quantum system identification

10 Conclusion

Dynamic Mode Decomposition represents a powerful bridge between datadriven methods and dynamical systems theory. Its ability to extract coherent structures and temporal patterns from high-dimensional data without prior knowledge of the governing equations makes it an invaluable tool across scientific disciplines.

The connection to Koopman operator theory provides a rigorous mathematical foundation, while practical variants and extensions make DMD adaptable to a wide range of applications and data types.

As computational capabilities continue to advance and data availability increases, DMD is poised to play an increasingly important role in understanding and modeling complex dynamical systems in science and engineering.

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