Utilizing Koopman Theory and Extended DMD to find Linear Representations of Nonlinear Systems

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Abstract

Solving Nonlinear Systems is a central challenge in almost every physics discipline. These systems typically generate complex dynamics and they do not have a closed-form solution. Utilizing the Koopman Operator Framework, we instead identify certain nonlinear transformations that allow to develop an equivalent linear coordinate system where the dynamics can be analyzed using standard methods applicable to linear systems. In exchange for the linearity of the Koopman Operator approach, the dimensionality of the original low-dimensional nonlinear system often becomes infinite in the Koopman linear coordinates. Finding these coordinate transformations is a core challenge of the theory, and the task is seldom easy. To resolve this problem, we rely on data-driven techniques such as Extended Dynamic Mode Decomposition (eDMD) which takes in time-series data and constructs a linear approximation of the nonlinear system. The power of this methodology is that it is completely agnostic to the equations of motion, and takes in purely data which is extremely useful when these equations are highly complex or unknown.

Koopman and eDMD Theory

Dynamics Mode Decomposition (DMD):

Schematic for DMD Algorithm. First, collect time-series data into two large matrices. Second, perform a regression analysis based purely on singular value decomposition and matrix multiplication. Third, test your linear model against the true dynamics.

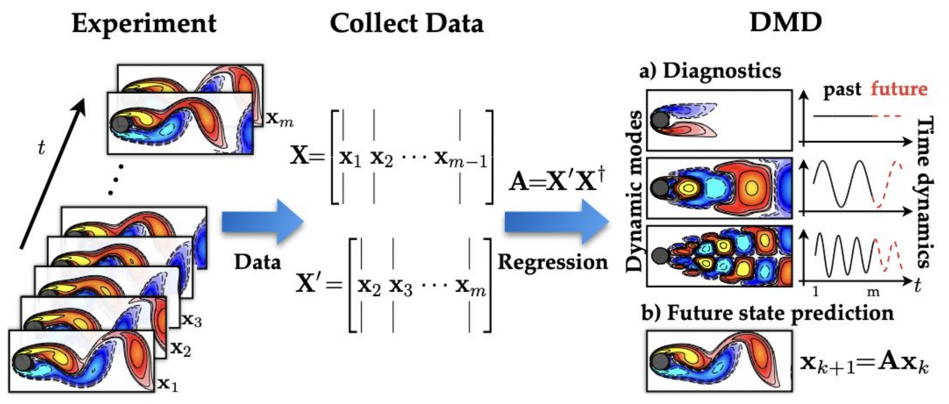


Image Credit: Brunton, Steven L., and J. Nathan Kutz. *Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control*. Cambridge University Press, 2024.

$$\mathbf{X} = \begin{bmatrix} | & | & & | \\ \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_{m-1} \\ | & | & & | \end{bmatrix} \quad \mathbf{X}' = \begin{bmatrix} | & | & & | \\ \mathbf{x}_2 & \mathbf{x}_3 & \cdots & \mathbf{x}_m \\ | & | & & | \end{bmatrix}$$

Time-Series Data Matrices

$$\mathbf{X}' \approx \mathbf{A}\mathbf{X} \rightarrow \mathbf{A} = \mathbf{X}'\mathbf{X}^\dagger$$

$$\mathbf{X} \approx \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^* \rightarrow \mathbf{A} = \mathbf{X}'\mathbf{V}\boldsymbol{\Sigma}^{-1}\mathbf{U}^*.$$

Singular Value Decomposition — Approximate Linear Evolution Operator

Low Rank Approximation:

$$\tilde{\mathbf{A}} = \mathbf{U}^*\mathbf{A}\mathbf{U} = \mathbf{U}^*\mathbf{X}'\mathbf{V}\boldsymbol{\Sigma}^{-1}. \rightarrow \tilde{\mathbf{x}}_{k+1} = \tilde{\mathbf{A}}\tilde{\mathbf{x}}_k, \quad \mathbf{x}_k = \mathbf{U}\tilde{\mathbf{x}}_k$$

Time Evolution of Low Rank Dynamics and Transformation between low and high rank dynamics

$$\tilde{\mathbf{A}}\mathbf{W} = \mathbf{W}\boldsymbol{\Lambda} \rightarrow \boldsymbol{\Phi} = \mathbf{X}'\mathbf{V}\boldsymbol{\Sigma}^{-1}\mathbf{W} \rightarrow \mathbf{x}(t) \approx \sum_{k=1}^{r} \boldsymbol{\phi}_k \exp(\omega_k t) b_k = \boldsymbol{\Phi}\exp(\boldsymbol{\Omega}t)\mathbf{b}, \quad \mathbf{b} = \boldsymbol{\Phi}^\dagger \mathbf{x}_1$$

Eigendecomposition — Spectral Expansion

Koopman Theory:

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t)), \rightarrow \mathbf{z} = \boldsymbol{\varphi}(\mathbf{x}), \rightarrow \frac{d}{dt}\mathbf{z} = \mathbf{L}\mathbf{z}.$$

Standard form of arbitrary dynamics system — Coordinate Transformation — Linearized Dynamics

Future of the System is determined by the spectral decomposition of L

Properties:

$$\mathcal{K}g(\mathbf{x}_k) := g(\mathbf{F}(\mathbf{x}_k)) = g(\mathbf{x}_{k+1}).$$

By definition the Koopman Operator advances a measurement function one time step

$$\mathcal{K}\varphi(\mathbf{x}_k) = \lambda\varphi(\mathbf{x}_k) = \varphi(\mathbf{x}_{k+1})$$

Eigenfunctions evolve linearly

$$\mathcal{K}^t(\alpha_1 g_1(\mathbf{x}) + \alpha_2 g_2(\mathbf{x})) = \alpha_1 g_1(\mathbf{F}^t(\mathbf{x})) + \alpha_2 g_2(\mathbf{F}^t(\mathbf{x})) = \alpha_1 \mathcal{K}^t g_1(\mathbf{x}) + \alpha_2 \mathcal{K}^t g_2(\mathbf{x}).$$

The Koopman Operator inherits linearity from the linearity of the measurement space regardless of whether the dynamics are linear

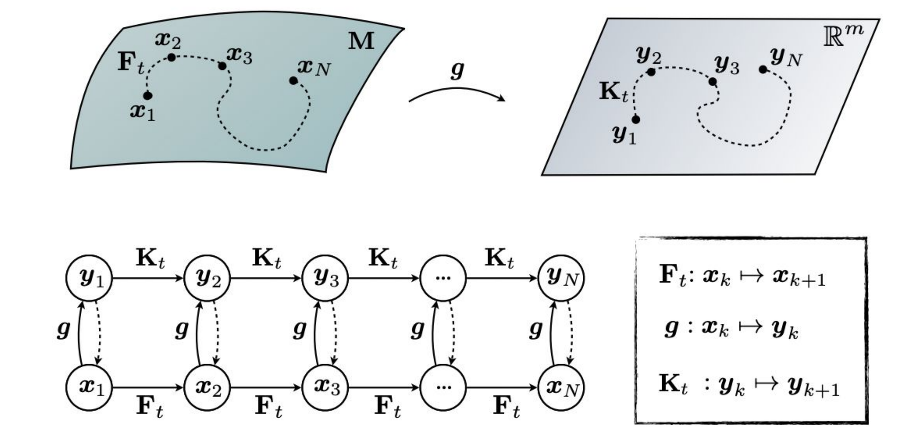


Image Credit: Brunton, Steven L., and J. Nathan Kutz. *Data-Driven Science and Engineering: Machine Learning, Dynamical Systems, and Control*. Cambridge University Press, 2024.

Extended DMD (eDMD):

Instead of considering state measurement of a system, we instead consider scalar measurement function and then do DMD the same way to get a spectral expansion in terms of out measurement functions

$$\mathbf{y} = \boldsymbol{\Theta}^T(\mathbf{x}) = \begin{bmatrix} \theta_1(\mathbf{x}) \\ \theta_2(\mathbf{x}) \\ \vdots \\ \theta_p(\mathbf{x}) \end{bmatrix} \rightarrow \mathbf{Y} = \begin{bmatrix} | & | & & | \\ \mathbf{y}_1 & \mathbf{y}_2 & \cdots & \mathbf{y}_m \\ | & | & & | \end{bmatrix} \quad \mathbf{Y}' = \begin{bmatrix} | & | & & | \\ \mathbf{y}_2 & \mathbf{y}_3 & \cdots & \mathbf{y}_{m+1} \\ | & | & & | \end{bmatrix}$$

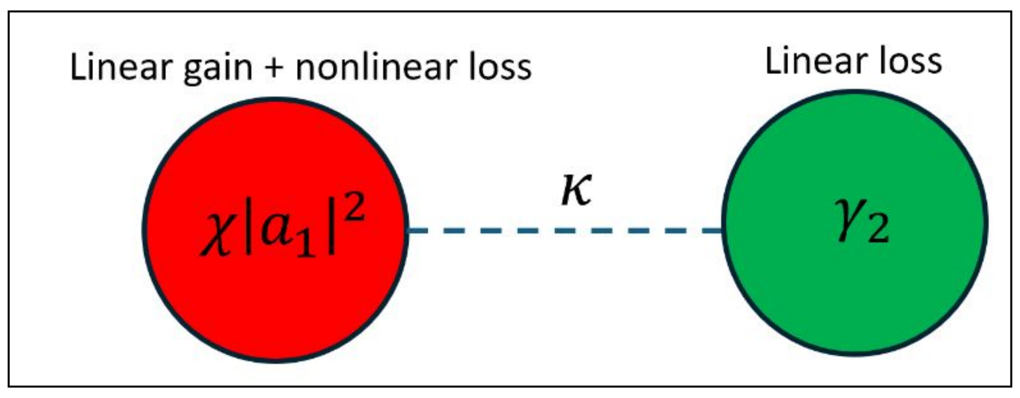
Construct Data Matrices

$$\rightarrow \mathbf{A}_\mathbf{Y} = \underset{\mathbf{A}_\mathbf{Y}}{\operatorname{argmin}} \|\mathbf{Y}' - \mathbf{A}_\mathbf{Y}\mathbf{Y}\| = \mathbf{Y}'\mathbf{Y}^\dagger$$

Regression

$$\mathbf{g}(\mathbf{x}) = \begin{bmatrix} g_1(\mathbf{x}) \\ g_2(\mathbf{x}) \\ \vdots \\ g_p(\mathbf{x}) \end{bmatrix} = \sum_{j=1}^{\infty} \varphi_j(\mathbf{x})\mathbf{v}_j \rightarrow \mathbf{g}(\mathbf{x}_k) = \mathcal{K}_{\Delta t}^k \mathbf{g}(\mathbf{x}_0) = \mathcal{K}_{\Delta t}^k \sum_{j=0}^{\infty} \varphi_j(\mathbf{x}_0)\mathbf{v}_j = \sum_{j=0}^{\infty} \lambda_j^k \varphi_j(\mathbf{x}_0)\mathbf{v}_j$$

Nonlinear Dimer



- ω_1 resonant frequency of 1st resonator (1)
- ω_2 resonant frequency of 2nd resonator (1)
- κ coupling between resonators (0.22)
- $\tilde{\gamma}_1$ linear gain of 1st resonator (0.21)
- $\tilde{\gamma}_2$ linear loss of 2nd resonator (0.2)
- χ nonlinearity strength (0.01)

Equations of Motion:

$$i|\dot{\psi}\rangle = H_{eff}|\psi\rangle \qquad |\psi\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \qquad H_{eff} = \begin{pmatrix} \omega_1 + i\gamma_1 - i\chi|a_1|^2 - i\gamma_e & \kappa \\ \kappa & \omega_2 - i\gamma_2 - i\gamma_e \end{pmatrix}$$

Decompose the Real and Imaginary Parts of the Fields:

$$a_1 = u_1 + iv_1 \qquad a_2 = u_2 + iv_2$$

$$\begin{aligned} \dot{u}_1 &= \tilde{\gamma}_1 u_1 - \chi u_1^3 - \chi u_1 v_1^2 + \epsilon v_1 + \kappa v_2 \\ \dot{v}_1 &= -\epsilon u_1 + \tilde{\gamma}_1 v_1 - \chi u_1^2 v_1 - \chi v_1^3 - \kappa u_2 \\ \dot{u}_2 &= \kappa v_1 - \tilde{\gamma}_2 u_2 - \epsilon v_2 \\ \dot{v}_2 &= -\kappa u_1 + \epsilon u_2 - \tilde{\gamma}_2 v_2 \end{aligned}$$

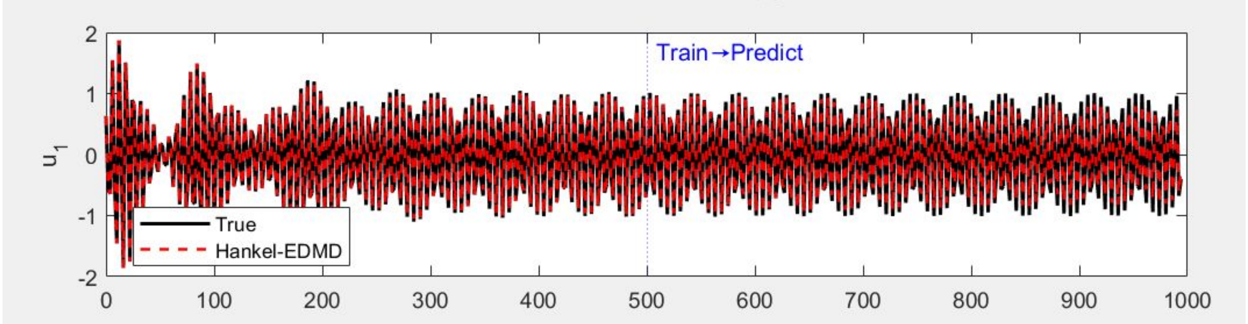
Dictionary of Observables:

$$\vec{\theta}(\vec{x}) = [1, u_1, u_2, v_1, v_2, u_1^2, u_1u_2, u_1v_1, u_1v_2, u_2^2, \ldots]$$

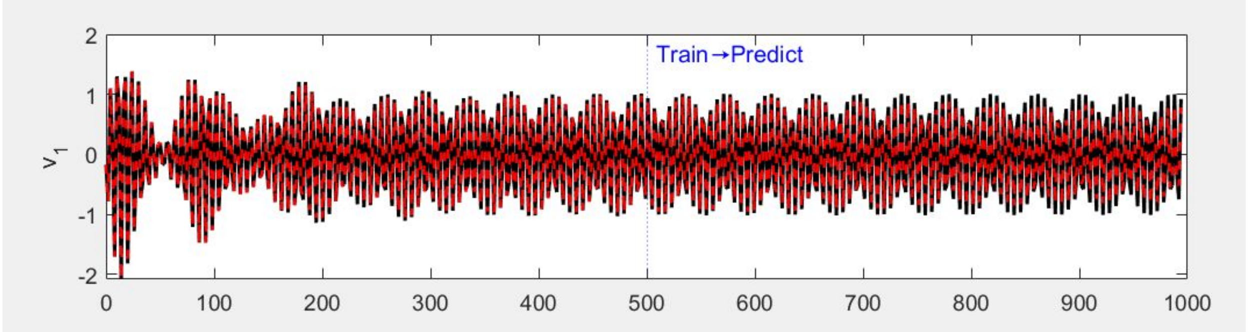
Polynomials of the state variables upto degree 6, so a total of 210 observables.

Results:

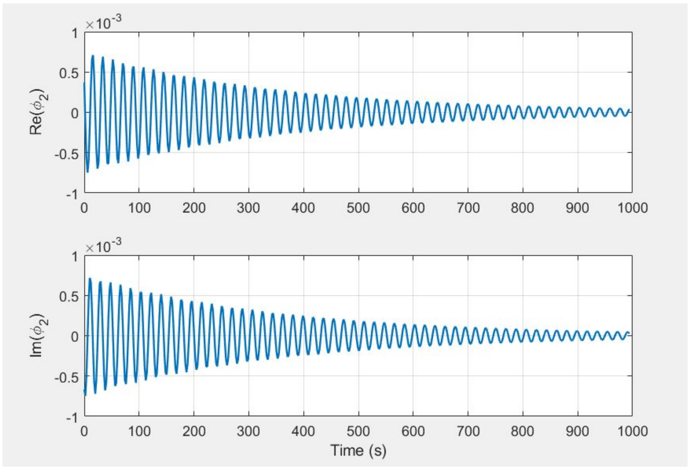
Real Part of Field Amplitude of First Resonator



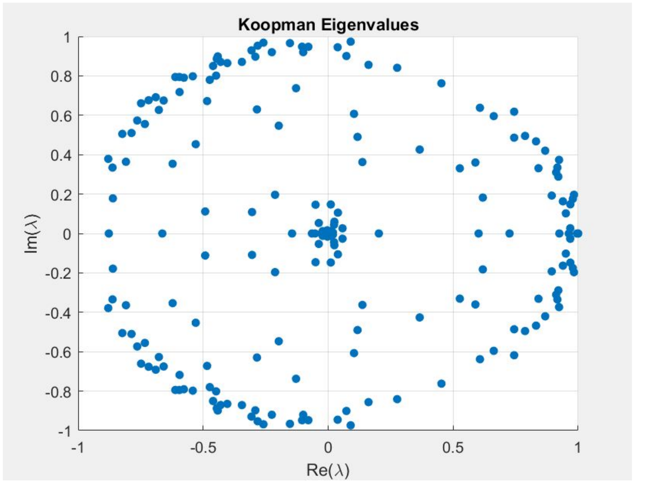
Imaginary Part of Field Amplitude of First Resonator



The eDMD model is trained on 500 seconds of the dimer dynamics, and then predicts the future of the system up until 1000 seconds. The red curve indicates the eDMD trajectory, and the black curve is the true dynamics.

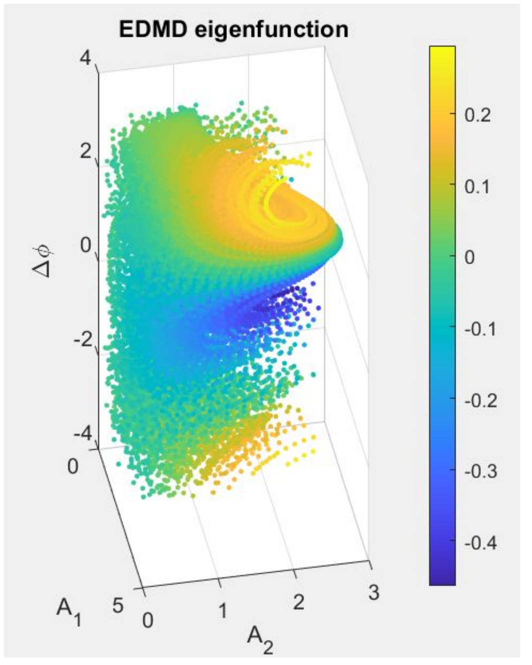


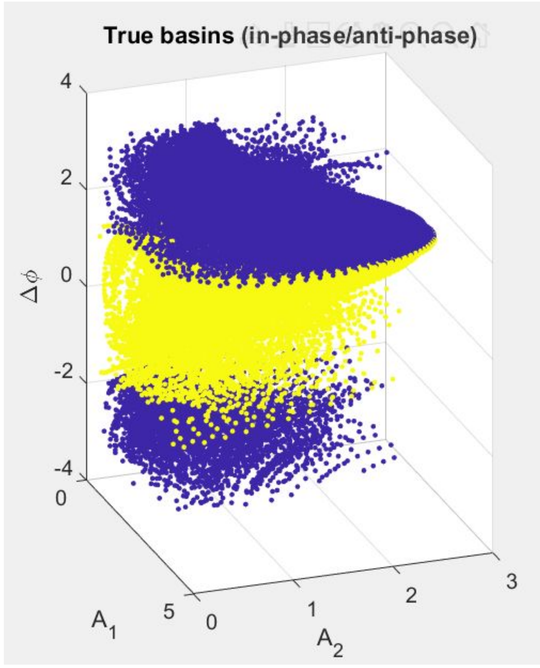
Plot of the 2nd eigenfunction which exhibits a linear evolution through time

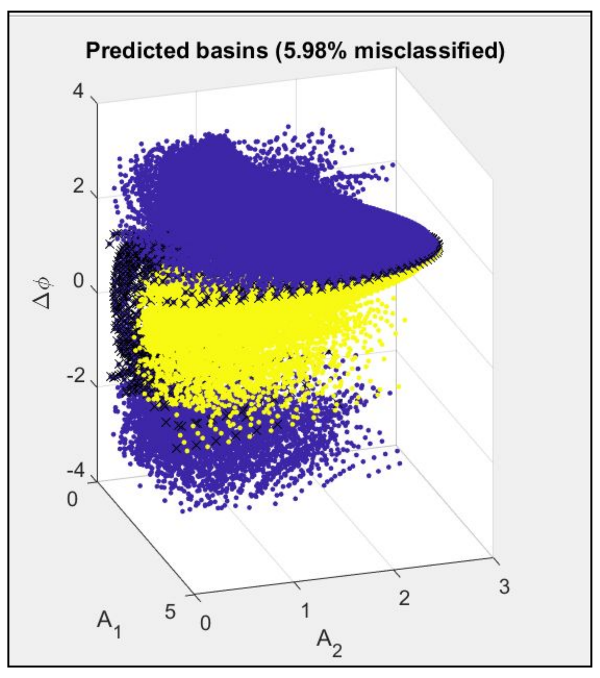


Plot of Koopman Matrix eigenvalues

Phase Space:







The eigenfunction with eigenvalue closest to 1, maps out the "basins of attraction" on the system, i.e characterized the long term behaviour. Even in a model with 1000 observables (which is small compared to infinity), we can extract information about the topology of the phase space from our finite truncation of the Koopman Operator. The left plot shows this eigenfunction. The middle plot shows the true basins of attraction from the dynamics. The right plot shows how the value of the eigenfunction can predict these true basins.

References

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