Data driven identification and model reduction for nonlinear dynamics ⋆

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1. INTRODUCTION

The Dynamic Mode Decomposition (DMD) Schmid and Sesterhenn (2008), Schmid (2010) is a versatile computational tool for data driven analysis of nonlinear dynamical systems, with applications in e.g. computational fluid dynamics, aeroacoustics, robotics. It can be used for model order reduction, analysis of latent structures in the dynamics, and e.g. for data driven identification, forecasting and control. The theoretical underpinning of the DMD is in the framework of the Koopman (composition) operator theory Rowley et al. (2009), Mezić (2013).

The Koopman (composition) operator provides an infinitely dimensional linearization of nonlinear dynamical systems, and it is a tool of the trade for computational data driven analysis (identification, prediction, control) of nonlinear dynamics. For instance, consider the discrete dynamical system

$$\mathbf{x}_{i+1} = \mathbf{T}(\mathbf{x}_i), \qquad (1)$$

where $\mathbf{T} : \mathcal{X} \longrightarrow \mathcal{X}$ is a map on a state space $\mathcal{X} \subseteq \mathbb{R}^n$ and $i \in \mathbb{Z}$. The $\mathbf{x}_i$'s are e.g. obtained by numerical simulations of a continuous system (i.e. system of differential equations), or by measuring experimental data. Further, the mapping $\mathbf{T}$ might be unknown, but an abundance of data snapshots $\mathbf{x}_i$ is available. The Koopman operator $\mathcal{K} \equiv \mathcal{K}_{\mathbf{T}}$ for the discrete system (1) is defined on a suitable (Hilbert) space of observables $\mathcal{F}$ by

$$\mathcal{K}f = f \circ \mathbf{T}, \quad f \in \mathcal{F}. \qquad (2)$$

The key observation is that for a vector valued observable $\mathbf{f} = (f_1, \ldots, f_n)^T$ of interest, its value along the trajectory of (1) can be represented as $\mathbf{f}(\mathbf{x}_1) = (\mathcal{K}^0\mathbf{f})(\mathbf{x}_1)$, $\mathbf{f}(\mathbf{x}_2) = (\mathcal{K}\mathbf{f})(\mathbf{x}_1)$, $\mathbf{f}(\mathbf{x}_3) = (\mathcal{K}^2\mathbf{f})(\mathbf{x}_1)$, …, $\mathbf{f}(\mathbf{x}_{m+1}) = (\mathcal{K}^m\mathbf{f})(\mathbf{x}_1)$, where the action of $\mathcal{K}$ defined component-wise. Hence, to reveal the latent structure of (1) and to develop forecasting skills, or to identify $\mathbf{T}$, it is plausible to try to identify $\mathcal{K}$ (based on the data only) and compute its approximate eigenvalues and eigenvectors (using a data driven compression of $\mathcal{K}$ and the well known procedures from numerical linear algebra, but adapted to the data driven scenario).

The available data are stored in the snapshot matrix F with columns $\mathbf{f}(\mathbf{x}_1), \mathbf{f}(\mathbf{x}_{k+1}) = (\mathcal{K}\mathbf{f})(\mathbf{x}_k)$, $\mathbf{x}_{k+1} = \mathbf{T}(\mathbf{x}_k)$:

$$F = \begin{pmatrix}\mathbf{f}(\mathbf{x}_1) & \ldots & \mathbf{f}(\mathbf{x}_m) & \mathbf{f}(\mathbf{x}_{m+1})\end{pmatrix} = \begin{pmatrix} f_1(\mathbf{x}_1) & \ldots & f_1(\mathbf{x}_m) & f_1(\mathbf{x}_{m+1}) \\ f_2(\mathbf{x}_1) & \ldots & f_2(\mathbf{x}_m) & f_2(\mathbf{x}_{m+1}) \\ \vdots & \vdots & \vdots & \vdots \\ f_d(\mathbf{x}_1) & \ldots & f_d(\mathbf{x}_m) & f_d(\mathbf{x}_{m+1}) \end{pmatrix}.$$

(i) The snapshots are generated by a nonlinear system.
(ii) The snapshots are a Krylov sequence $\mathbf{f}, \mathcal{K}\mathbf{f}, \mathcal{K}^2\mathbf{f}, \ldots$, driven by the linear operator $\mathcal{K}$ and evaluated along a trajectory initialized at $\mathbf{x}_1$.

It makes sense to find a matrix A that reproduces the Krylov sequence (over available data), i.e. such that

$$\mathsf{A}\mathbf{f}(\mathbf{x}_k) = (\mathcal{K}\mathbf{f})(\mathbf{x}_k) = \begin{pmatrix} (\mathcal{K}f_1)(\mathbf{x}_k) \\ \vdots \\ (\mathcal{K}f_n)(\mathbf{x}_k) \end{pmatrix} = \mathbf{f}(\mathbf{T}(\mathbf{x}_k)), \; k = 1, \ldots, m. \qquad (3)$$

The Koopman Mode Decomposition (KMD) represents the scalar observables f_i in terms of the eigenfunctions of $\mathcal{K}$, so that for an $\mathbf{x}$

$$(\mathcal{K}^k\mathbf{f})(\mathbf{x}) = \begin{pmatrix} (\mathcal{K}^k f_1)(\mathbf{x}) \\ \vdots \\ (\mathcal{K}^k f_n)(\mathbf{x}) \end{pmatrix} \approx \sum_{i=1}^{m} \mathbf{z}_i \phi_i(\mathbf{x}) \lambda_i^k, \; k = 0, 1, \ldots \qquad (4)$$

where $(\mathcal{K}\phi_i)(\mathbf{x}) \approx \lambda_i \phi_i(\mathbf{x})$. It can be shown that $(\mathbf{z}_i, \lambda_i)$'s are approximate eigenpairs of A ($\mathsf{A}\mathbf{z}_i \approx \lambda_i \mathbf{z}_i$). This requires solving the eigenvalue problem for the matrix A defined in (3).

2. THE DMD AND THE KMD: NUMERICAL ALGORITHMS

The application of the KMD introduced in §1 is based on a supplied sequence of snapshots $\mathbf{f}_i \in \mathbb{C}^n$ of an underlying dynamics, that are driven by an unaccessible *black box* linear operator A;

$$\mathbf{f}_{i+1} \approx \mathsf{A}\mathbf{f}_i, \quad i = 1, \ldots, m, \quad m < n, \qquad (5)$$

with some initial $\mathbf{f}_1$. No other information is available.

The two basic tasks are then:

(1) Identify approximate eigenpairs $(\lambda_j, \mathbf{z}_j)$ such that
$$\mathsf{A}\mathbf{z}_j \approx \lambda_j \mathbf{z}_j, \quad j = 1, \ldots, k; \quad k \le m, \qquad (6)$$
This is solved by a data driven Rayleigh–Ritz procedure introduced by Schmid (2010).

(2) Derive a spectral spatio–temporal representation of the snapshots $\mathbf{f}_{i_\ell}$ (KMD):
$$\mathbf{f}_i \approx \sum_{j=1} \mathbf{z}_{\varsigma_j} \alpha_j \lambda_{\varsigma_j}^{i-1}, \quad i = 1, \ldots, m, \qquad (7)$$

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Algorithm 1. $(\mathsf{Z}_k, \Lambda_k, \mathsf{r}_k, [\mathsf{B}_k], [\mathsf{Z}_k^{(ex)}]) = \mathrm{xGEDMD}(\mathsf{X}, \mathsf{Y}; \mathrm{tol})$

Input: $\mathsf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_m), \mathsf{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_m) \in \mathbb{C}^{N\times m}$ that define a sequence of snapshot pairs $(\mathbf{x}_i, \mathbf{y}_i)$. Tolerance tol for the numerical rank of X.

$\mathsf{D} = (\mathrm{diag}(\|\mathsf{X}(:,i)\|_2)_{i=1}^m)^\dagger$; $\mathsf{X}_c = \mathsf{X}\mathsf{D}$; $\mathsf{Y}_c = \mathsf{Y}\mathsf{D}$.

$[\mathsf{U}, \Sigma, \mathsf{V}] = svd(\mathsf{X}_c)$; {*The thin SVD:* $\mathsf{X}_c = \mathsf{U}\Sigma\mathsf{V}^*$, $\mathsf{U} \in \mathbb{C}^{n\times m}$, $\Sigma = \mathrm{diag}(\sigma_i)_{i=1}^m$.}

Determine numerical rank k, using the threshold tol.

Set $\mathsf{U}_k = \mathsf{U}(:, 1{:}k)$, $\mathsf{V}_k = V(:, 1{:}k)$, $\Sigma_k = \Sigma(1{:}k, 1{:}k)$.

$\mathsf{B}_k = \mathsf{Y}_c(\mathsf{V}_k\Sigma_k^{-1})$; {*Schmid's data driven formula for* $\mathsf{A}\mathsf{U}_k$ *[optional output].*}

$\mathsf{S}_k = \mathsf{U}_k^*\mathsf{B}_k$ {$\mathsf{S}_k = \mathsf{U}_k^*\mathsf{A}\mathsf{U}_k$ *is the Rayleigh quotient.*}

$[\mathsf{W}_k, \Lambda_k] = \mathrm{eig}(\mathsf{S}_k)$ {$\Lambda_k = \mathrm{diag}(\lambda_i)_{i=1}^k$; $\mathsf{S}_k\mathsf{W}_k(:,i) = \lambda_i\mathsf{W}_k(:,i)$; $\|\mathsf{W}_k(:,i)\|_2 = 1$.}

$\mathsf{Z}_k = \mathsf{U}_k\mathsf{W}_k$ {*The Ritz vectors.*}

$\mathsf{Z}_k^{(ex)} = \mathsf{B}_k\mathsf{W}_k$ {*The (unscaled) Exact DMD vectors [optional output].*}

$\mathsf{r}_k(i) = \|\mathsf{B}_k\mathsf{W}_k(:,i) - \lambda_i\mathsf{Z}_k(:,i)\|_2$, $i = 1, \ldots, k$. {*The residuals.*}

Output: Z_k, Λ_k, r_k, $[\mathsf{B}_k]$, $[\mathsf{Z}_k^{(ex)}]$.

for some suitable selection of the modes $\mathbf{z}_{\varsigma_j}$. The coefficients are computed by using a sparsity promoting optimization Jovanović et al. (2014), or by solving a Khatri–Rao structured least squares problem Drmač et al. (2020).

2.1 An improved DMD/KMD

The original method Schmid (2010) is considerably improved in Drmač et al. (2018), and a robust software implementation is available in the LAPACK library Drmač (2024a). One of the key features of the modified DMD is that it provides computable residuals ($r_k(\varsigma_j) = \|\mathsf{A}\mathbf{z}_{\varsigma_j} - \lambda_{\varsigma_j}\mathbf{z}_{\varsigma_j}\|_2$), that can be used to select physically meaningful eigenvalues and modes, and to guide sparse representation of the snapshot in the KMD (7).

The improved version of the DMD is summarized in Algorithm 1. In the case of physics–informed DMD, where it is known that the underlying operator is Hermitian, a Hermitian version of the DMD requires careful implementation as in Baddoo et al. (2021), Drmač (2024b).

2.2 An example

An example of DMD/KMD is illustrated in Figure 1. The data are collected by solving the two–dimensional Navier–Stokes equation for 150 discrete time steps. The grid data are reshaped into columns and arranged column–wise in the 89351×151 matrix F. The input to DMD is $\mathsf{X} = F(:, 1:150)$, $\mathsf{Y} = F(:, 2:151)$. Only nine modes (eigenvectors of A) are enough to represent the entire simulation with high fidelity, and to provide very good forecasting skill.

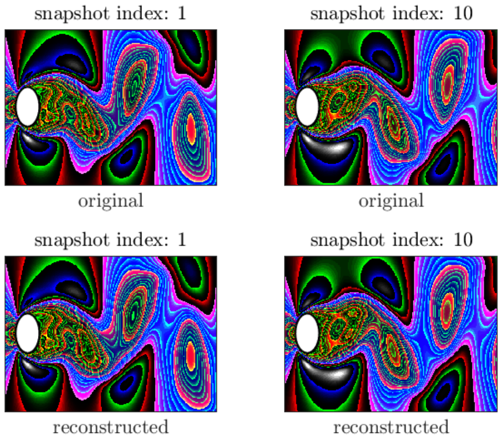

Fig. 1. Flow around a circular cylinder. The observable is the norm of the velocity. The snapshots obatined in the simulation are represented using only 9 Koopman modes. The accuracy of such representation is illustrated in the first plot for snapshots indexed as $i = 1$ and $i = 10$.

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