Optimal Kernel-Based Dynamic Mode Decomposition

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ABSTRACT

The state-of-the-art algorithm known as kernel-based dynamic mode decomposition (K-DMD) provides a sub-optimal solution to the problem of reduced modeling of a dynamical system based on a finite approximation of the Koopman operator. It relies on crude approximations and on restrictive assumptions. The purpose of this work is to propose a kernel-based algorithm solving exactly this low-rank approximation problem in a general setting.

CONTEXT AND PROBLEM

• Intractable high-dimensional systems:

$$\begin{cases} x_t(\theta) = f_t(x_{t-1}(\theta)), \\ x_1(\theta) = \theta, \end{cases} \quad (1)$$

where $x_t \in \mathbb{R}^p$ is the state variable, $f_t : \mathbb{R}^p \rightarrow \mathbb{R}^p$, and $\theta \in \Theta \subseteq \mathbb{R}^p$ denotes an initial condition.

• Idealised reduced model:

- * Assume $\Psi \in (\mathcal{L}^2(\mathbb{R}^p))^n$ such that its image is an invariant vector space of the Koopman operator.
- * A finite approximation of the Koopman operator of rank $k \leq p$ approximates $x_t(\theta)$ by

$$\tilde{x}_t(\theta) = \Psi^{-1} \left(\sum_{i=1}^k \lambda_i^{t-1} \xi_i^\top \Psi(\theta) \zeta_i \right), \quad (2)$$

where $(\xi_i, \zeta_i, \lambda_i) \in \mathbb{C}^n \times \mathbb{C}^n \times \mathbb{C}$ target the left/right eigen-vectors and eigen-values of

$$\arg \min_{A: \text{rank}(A) \leq k} \int_{\Theta} \sum_{t \geq 1} \|\Psi(x_t(\theta)) - A^{t-1} \Psi(x_1(\theta))\|_2^2 d\theta.$$

• Data-driven reduced model:

- * Snapshots $\{x_t(\theta_\ell)\}_{t=1}^T$, $\ell = 1, \dots, N$, of (1) for initial conditions $\theta_\ell \in \Theta$.
- * Matrices $\Psi_{\mathbf{X}} = (\Psi_{1:T-1}^1 \cdots \Psi_{1:T-1}^N)$ and $\Psi_{\mathbf{Y}} = (\Psi_{2:T}^1 \cdots \Psi_{2:T}^N)$, in $\mathbb{R}^{n \times m}$ with $m = N(T-1)$ and $\Psi_{t_1:t_2}^\ell = (\Psi(x_{t_1}(\theta_\ell)) \cdots \Psi(x_{t_2}(\theta_\ell)))$.
- * Matrices $\mathbf{Y} = \Psi^{-1}(\Psi_{\mathbf{Y}})$ and $\mathbf{X} = \Psi^{-1}(\Psi_{\mathbf{X}})$ in $\mathbb{R}^{p \times m}$, where Ψ is the identity operator.

Problem 1. Assume A_k^* is diagonalisable. Given the snapshots $x_t(\theta_i)$'s and $\theta \in \Theta$, compute $\tilde{x}_t(\theta)$ solution of the reduced model (2), where $(\xi_i, \zeta_i, \lambda_i)$'s target the eigen-vectors and eigen-values of

$$A_k^* \in \arg \min_{A: \text{rank}(A) \leq k} \|\Psi_{\mathbf{Y}} - A \Psi_{\mathbf{X}}\|_F^2.$$

STATE-OF-THE-ART

- In the low-rank DMD algorithm of [Heas17], exact computation of $\tilde{x}_t(\theta)$ is obtained from the eigen-decomposition of the optimal solution

$$A_k^* = \mathcal{P} \mathcal{P}^\top \Psi_{\mathbf{Y}} \Psi_{\mathbf{X}}^\dagger, \quad (3)$$

where columns of $\mathcal{P} \in \mathbb{R}^{n \times k}$ are the k -first left singular vectors of matrix $\Psi_{\mathbf{Y}} \mathbb{P} \Psi_{\mathbf{X}}^\top \in \mathbb{R}^{n \times m}$.
 $\Rightarrow$ complexity scales in $\mathcal{O}(n)$, which is prohibitive for large (possibly infinite) $n \gg p$.

- In [Williams14], the K-DMD algorithm approximates $\tilde{x}_t(\theta)$ using the “kernel trick” with a complexity in $\mathcal{O}(p)$, independent of n . $\Rightarrow$ sub-optimal solution of $\tilde{x}_t(\theta)$ because it assumes that:
 - i)* Ψ^{-1} is linear; *ii)* $\Psi_{\mathbf{X}}$ is full-rank; *iii)* eigen-mode $\Psi^{-1} \zeta_i$ belongs to the span of the $x_t(\theta_i)$'s; *iv)* low-rank constraint can be ignored.

UPGRADING K-DMD

• The “kernel trick”:

- * $\Psi_{\mathbf{X}}^\top \Psi_{\mathbf{Y}}$, $\Psi_{\mathbf{Y}}^\top \Psi_{\mathbf{Y}}$, $\Psi_{\mathbf{Y}}^\top \Psi_{\mathbf{X}}$ and $\Psi_{\mathbf{X}}^\top \Psi(\theta)$ for any $\theta \in \Theta$ are computable from $\mathbf{X}$ and $\mathbf{Y}$ in $\mathcal{O}(p)$ if there exists

$$h : \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}; \quad (y, z) \rightarrow h(y, z) = \Psi(y)^\top \Psi(z).$$

• Kernel-based representation of eigen-vectors:

- * $\{(\tilde{\xi}_i, \tilde{\lambda}_{\ell,i})\}_{i=1}^k$ and $\{(\tilde{\zeta}_i, \tilde{\lambda}_{r,i})\}_{i=1}^k$ are two sets of eigen-vectors/values of well-chosen matrices $(\tilde{A}_{\ell,k})^\top$ and $\tilde{A}_{r,k}$ in $\mathbb{R}^{m \times m}$, computed in $\mathcal{O}(p)$ using the kernel trick.

- * The following proposition exhibits a kernel-based low-dimensional representation of the eigen-decomposition of A_k^* relying on the factorisation (3).

Proposition 1. For $i = 1, \dots, k$, the left and right eigen-vectors of A_k^* and its eigen-values satisfy $\xi_i = U_{\Psi_{\mathbf{X}}} \tilde{\xi}_i$ and $\zeta_i = \mathcal{P} \tilde{\zeta}_i$ with $\lambda_i = \tilde{\lambda}_{\ell,i} = \tilde{\lambda}_{r,i}$, where columns of $U_{\Psi_{\mathbf{X}}}$ are the right eigen-vectors of $\Psi_{\mathbf{X}}$.

• Kernel-based inversion:

- * From Proposition 1, we show that (2) is equivalent to $\tilde{x}_t(\theta) = \Psi^{-1}(\Psi_{\mathbf{Y}} G(\theta))$,

- * $G(\theta) \in \mathbb{R}^{m \times k}$ depends on $\tilde{\zeta}_i$'s on λ_i 's and $\tilde{\varphi}_i(\theta)$'s, where the latter are eigen-functions derived in $\mathcal{O}(p)$ operations from $\tilde{\xi}_i$'s and $\Psi_{\mathbf{X}}^\top \Psi(\theta)$.

- * Computation of $\Psi^{-1}(\Psi_{\mathbf{Y}} G(\theta))$ in $\mathcal{O}(p)$:

1. *Polynomial kernels.*
 - $h(y, z) = (1 + y^\top z)^\gamma$ is a scalar product in $(\mathcal{L}^2(\mathbb{R}^p))^n$ with $n < \infty$
 - $\Psi^{-1}(\Psi_{\mathbf{Y}} G(\theta)) = \mathbf{Y} G(\theta)$ (linear)
2. *Gaussian kernels.*
 - $h(y, z) = \exp\left(-\frac{\|y-z\|_2^2}{2\sigma^2}\right)$ is a scalar product in $(\mathcal{L}^2(\mathbb{R}^p))^n$ with $n = \infty$
 - $\Psi^{-1}(\Psi_{\mathbf{Y}} G(\theta)) =$ weighted sum of entries of $\mathbf{Y}$.
3. *Logarithmic kernel.*
 - $h(y, z) = (\log(y+1))^\top \log(z+1)$ is a scalar product in $(\mathcal{L}^2(\mathbb{R}^p))^n$ with $n = p$.
 - $\Psi^{-1}(\Psi_{\mathbf{Y}} G(\theta)) =$ product of exponentials of entries of $\mathbf{Y}$.

• Optimal K-DMD algorithm (OK-DMD):

- inputs:** The $x_t(\theta_i)$'s and some θ
- 1) Compute $\Psi_{\mathbf{X}}^\top \Psi_{\mathbf{X}}$, $\Psi_{\mathbf{Y}}^\top \Psi_{\mathbf{Y}}$, $\Psi_{\mathbf{Y}}^\top \Psi_{\mathbf{X}}$ and $\Psi_{\mathbf{X}}^\top \Psi(\theta)$ with the kernel trick
 - 2) Derive matrices $(\tilde{A}_{\ell,k})^\top$ and $\tilde{A}_{r,k}$.
 - 3) Compute their eigen-vectors/values $\{(\tilde{\xi}_i, \tilde{\lambda}_{\ell,i})\}_{i=1}^k$ and $\{(\tilde{\zeta}_i, \tilde{\lambda}_{r,i})\}_{i=1}^k$.
 - 4) Compute the eigen-functions $\{\tilde{\varphi}_i(\theta)\}_{i=1}^k$.
 - 5) Derive $G(\theta)$ and compute $\tilde{x}_t(\theta) = \Psi^{-1}(\Psi(\mathbf{Y}) G(\theta))$ using the kernel-based inversion formulae.
- output:** $\tilde{x}_t(\theta)$'s.

NUMERICAL EVALUATION

• Toy model:

- * Snapshots of a balanced mixture of trajectories of a linear and a quadratic model.

$$f(x_{t-1}(\theta_\ell)) = (x_{t-1}(\theta_\ell) + 1)^\beta - 1, \quad \beta \in \{1, 2\},$$

with an identical initial condition (i.i.d. realisations of the standard normal distribution).

- * Normalised approximation error norm $\|\mathbf{Y} - \tilde{\mathbf{Y}}\|_F / \|\mathbf{Y}\|_F$, with the i -th column of $\tilde{\mathbf{Y}} \in \mathbb{R}^{p \times m}$ defined as $\tilde{x}_2(\theta)$ where θ is identified to the i -th column of $\mathbf{X}$.

Remark: for low-rank DMD, this criterion simplifies into $\|\mathbf{Y} - A_k^* \mathbf{X}\|_F / \|\mathbf{Y}\|_F$.

• Results:

ArXiv reference:

Patrick Héas, Cédric Herzet, “Optimal Kernel-Based Dynamic Mode Decomposition”, arXiv:1610.02962, 2017