State-Of-The-Art Algorithms For Low-Rank Dynamic Mode Decomposition.

Patrick Héas · Cédric Herzet

Abstract. This technical note reviews state-of-the-art algorithms for linear approximation of high-dimensional dynamical systems using low-rank dynamic mode decomposition (DMD). While repeating several parts of the article [12], this work provides useful complementary details to build up an overall picture of state-of-the-art methods.

1 Introduction

1.1 Context

The numerical discretization of a partial differential equation parametrized by its initial condition often leads to a very high dimensional system of the form:

\[
\begin{align*}
    x_t(\theta) &= f_t(x_{t-1}(\theta)), & t = 2, \ldots, T, \\
    x_1(\theta) &= \theta,
\end{align*}
\]

(1)

where \( x_t(\theta) \in \mathbb{R}^n \) is the state variable, \( f_t : \mathbb{R}^n \rightarrow \mathbb{R}^n \), and \( \theta \in \mathbb{R}^n \) denotes an initial condition. In some context, e.g., for uncertainty quantification purposes, one is interested by computing a set of trajectories corresponding to different initial conditions \( \theta \in \Theta \subset \mathbb{R}^n \). This may constitute an intractable task due to the high dimensionality of the space embedding the trajectories. For instance, in the case where \( f_t \) is linear, the complexity required to compute a trajectory of model (1) scales in \( O(T n^2) \), which is prohibitive for large values of \( n \) or \( T \).

To deal with these large values, reduced models approximate the trajectories of the system for a range of regimes determined by a set of initial conditions \( \Theta \). A common assumption is that the trajectories of interest are well approximated in a low-dimensional subspace of \( \mathbb{R}^n \). In this spirit, many tractable
approximations of model (1) have been proposed, in particular the well-known Petrov-Galerkin projection [27]. However, these methods require the knowledge of the equations ruling the high-dimensional system.

Alternatively, there exist data-driven approaches. In particular, linear inverse modeling [26], principal oscillating patterns [10], or more recently, dynamic mode decomposition (DMD) [3,6,14,17,19,29,30] propose to approximate the unknown function \( f_t \) by a linear and low-rank operator. This linear framework has been extended to quadratic approximations of \( f_t \) in [5]. Although linear approximations are in appearance restrictive, they have recently sparked a new surge of interest because they are at the core of the so-called extended DMD or kernel-based DMD [2,22,31,32,34]. The latter decompositions characterize accurately non-linear behaviours under certain conditions [18].

Reduced models based on low-rank linear approximations substitute function \( f_t \) by a matrix \( \hat{A}_k \in \mathbb{R}^{n \times n} \) with \( r = \text{rank}(\hat{A}_k) \leq n \) as

\[
\begin{align*}
\tilde{x}_t(\theta) &= \hat{A}_k \tilde{x}_{t-1}(\theta), \quad t = 2, \ldots, T, \\
\tilde{x}_1(\theta) &= \theta,
\end{align*}
\]

where \( \{\tilde{x}_t(\theta)\}_{t=1}^T \) denotes an approximation of the trajectory \( \{x_t(\theta)\}_{t=1}^T \) of system (1). The complexity for the evaluation of a trajectory approximation with (2) will be referred to as on-line complexity. A low on-line complexity is obtained by exploiting the low rank of matrix \( \hat{A}_k \). A scaling in \( O(T r^2 + r n) \) is reached if the reduced model is parametrized by matrices \( R, L \in \mathbb{C}^{n \times r} \) and \( S \in \mathbb{C}^{r \times r} \) such that trajectories of (2) correspond to the recursion

\[
\begin{align*}
\tilde{x}_t(\theta) &= R z_t, \quad t = 2, \ldots, T, \\
z_t &= S z_{t-1}, \quad t = 3, \ldots, T, \\
z_2 &= L^T \theta.
\end{align*}
\]

The equivalence of systems (2) and (3) is obtained for \( T \geq 2 \) by setting \( \hat{A}_k^T = R S T^{-2} L^T \). In particular, consider a factorization of the form

\[
\hat{A}_k = PQ^T \quad \text{with} \quad P, Q \in \mathbb{R}^{n \times r}.
\]

This factorization is always possible by computing the singular value decomposition (SVD) \( \hat{A}_k = U_{\hat{A}_k} \Sigma_{\hat{A}_k} V_{\hat{A}_k}^T \) and identifying \( P = U_{\hat{A}_k} \) and \( Q^T = \Sigma_{\hat{A}_k} V_{\hat{A}_k}^T \). Factorization (4) implies that trajectories of (2) are obtained with system (3) setting \( R = P, L = Q \) and \( S = Q^T P \). Another factorization of interest relies on the eigenvalue decomposition (EVD)

\[
\hat{A}_k = D A D^{-1}, \quad \text{with} \quad D, A \in \mathbb{C}^{n \times n},
\]

where \( A \) is a Jordan-block matrix [9] of rank \( r \). Using the "economy size" EVD yields a system of the form of (3). Indeed, it is obtained by making the identification \( L = (\xi_1 \cdots \xi_r) \) and \( R = (\zeta_1 \cdots \zeta_r) \), where \( \xi_i \in \mathbb{C}^n \) and \( \zeta_i \in \mathbb{C}^n \) are the \( i \)-th left and right eigenvectors of \( \hat{A}_k \) (equivalently the \( i \)-th column of
(\(D^{-1}\) and \(D\)), and identifying \(S\) to the first \(r \times r\) block of \(A\) multiplied by \(LT\).

The on-line complexity to compute this recursion is still \(O(Tr^2 + rn)\). But assuming that \(\hat{A}_k\) is diagonalizable\(^1\), we have \(S = \text{diag}(\lambda_1, \cdots, \lambda_r)\) and system (3) becomes

\[
\begin{align*}
\tilde{x}_t(\theta) &= \sum_{i=1}^{r} \zeta_i \nu_{i,t}, \\
\nu_{i,t} &= \lambda_i^{t-1} \xi^\top \theta, \quad \text{for } i = 1, \ldots, \text{rank}(\hat{A}_k)
\end{align*}
\]

where \(\lambda_i \in \mathbb{C}\) is the \(i\)-th (non-zero) eigenvalue of \(\hat{A}_k\). This reduced-model possesses a very desirable on-line complexity of \(O(rn)\), i.e., linear in the ambient dimension \(n\), linear in the reduced-model intrinsic dimension \(r\) and independent of the trajectory length \(T\).

The key of reduced modeling is to find a “good” tradeoff between the on-line complexity and the accuracy of the approximation. As shown previously, the low on-line computational effort is obtained by a proper factorization of the low-rank matrix \(\hat{A}_k\). Thus, in an off-line stage, it remains to i) search \(\hat{A}_k\) within the family of low-rank matrices which yields the “best” approximation (2), ii) compute the SVD or EVD based factorization of \(\hat{A}_k\). We will refer to the computational cost associated to these two steps as off-line complexity.

A standard choice is to select \(\hat{A}_k\) inducing the best trajectory approximation in the \(\ell_2\)-norm sense, for initial conditions in the set \(\Theta \subset \mathbb{R}^n\): matrix \(\hat{A}_k\) in (2) targets the solution of the following minimization problem for some given \(k \leq n\):

\[
\arg \min_{A: \text{rank}(A) \leq k} \int_{\theta \in \Theta} \sum_{t=2}^{T} \|x_t(\theta) - A^{t-1} \theta\|_2^2,
\]

where \(\| \cdot \|_2\) denotes the \(\ell_2\)-norm. Since we focus on data-driven approaches, we assume that we do not know the exact form of \(f_t\) in (1) and we only have access to a set of representative trajectories \(\{x_t(\theta_i)\}_{t=1}^{T}\), \(i = 1, \ldots, N\) so-called snapshots, obtained by running the high-dimensional system for \(N\) different initial conditions \(\{\theta_i\}_{i=1}^{N}\) in the set \(\Theta\). Using these snapshots, we consider a discretized version of (7), which corresponds to the constrained optimization problem studied in [3][17][33]: matrix \(\hat{A}_k\) now targets the solution

\[
\hat{A}_k^* \in \arg \min_{A: \text{rank}(A) \leq k} \sum_{i=1}^{N} \sum_{t=2}^{T} \|x_t(\theta_i) - Ax_{t-1}(\theta_i)\|_2^2,
\]

where we have substituted \(A^{t-1} \theta_i\) in (7) by \(Ax_{t-1}(\theta_i)\) and where we have approximated the integral by an empirical average over the snapshots.

\(^1\) Diagonalizability is guaranteed if all the non-zero eigenvalues are distinct. However, this condition is only sufficient and the class of diagonalizable matrices is larger [15].
Problem (8) is non-convex due to the presence of the rank constraint 
"rank(A) ≤ k". As consequence, it has been considered as intractable in several 
contributions of the literature and numerous procedures have been proposed 
to approximate its solution (see next section). The work [12] shows that problem (8) is in fact tractable and admits a closed-form solution which can be 
evaluated in polynomial-time.

1.2 Problem Statement

The off-line construction of reduced models of the form of (3) focuses on the 
following questions:

1. Can we compute a solution of problem (8) in polynomial time?
2. How to compute efficiently a factorization of this solution, and in particular 
eits EVD?

Let us make some correspondences with the terminology used in the DMD lit-
erature [3,6,11,14,17,19,29,30] in order to reformulate these two questions in the 
gargon used in this community. The “low-rank DMD” of system (1) refers to 
the EVD of the solution $A_k^\ast$ of problem (8), or equivalently to the parameters 
of reduced model (6) in the case where $A_k = A_k^\ast$ is diagonalizable. Using this 
terminology, the two above questions can be summarized as follows: can we compute exactly and with a polynomial complexity the low-rank 
DMD of system (1)? The answer to this question is positive as proved in [12].

Solver for problem (8). In the last decade, there has been a surge of interest for low-rank solutions of linear matrix equations, see e.g., [8,16,20,21,24,28]. This class of problems includes (8) as an important particular case. 
Problems in this class are always non-convex due to the rank constraint and 
computing their solutions in polynomial time is often out of reach. Neverthe-
less, certain instances of these problems with very special structures admit 
closed-form solutions [7,23,25]. The work [12] shows that (8) belongs to this 
class of problems and provide a closed-form solution which can be computed 
in polynomial time. Prior to this work, many authors have proposed tracetable 
procedures to compute approximations of the solution to problem (8) [3,17, 
22,30,33,34] or to related problems [14]. We review these contributions in Sec-
tion 3.1 and discuss their complexity.

Factorization of the solution. The second problem concerns the com-
putation of the factorization of the form (4) or (5) of the solution $A_k^\ast \in \mathbb{R}^{n\times n}$. 
A brute-force computation of a factorization of a matrix in $\mathbb{R}^{n\times n}$, in par-
ticular an EVD, is prohibitive for large values of $n$. The paper [12] proposes 
low-complexity algorithms computing such factorization of $A_k^\ast$. This follows the 
line and extends previous works [17,30,32], as detailed in Section 3.2.

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2 The “DMD” of system (1) refers to the EVD of the solution of problem (8) without the 
low-rank constraint.
The following sections provide a review on techniques for approximating and factorizing the solution of problem (8).

2 Notations

All along the paper, we make extensive use of the economy-size SVD of a matrix $M \in \mathbb{R}^{p \times q}$ with $p \geq q$: $M = U_M \Sigma_M V_M^\top$, with $U_M \in \mathbb{R}^{p \times q}$ and $\Sigma_M \in \mathbb{R}^{q \times q}$ so that $U_M^\top U_M = V_M^\top V_M = I_q$ and $\Sigma_M$ is diagonal, where the upper script $\cdot^\top$ refers to the transpose and $I_q$ denotes the $q$-dimensional identity matrix. The columns of matrices $U_M$ and $V_M$ are denoted $U_M = (u_M^1, \ldots, u_M^q)$ and $V_M = (v_M^1, v_M^2)$. While $\Sigma_M = \text{diag}(\sigma_M, \ldots, \sigma_M)$ with $\sigma_M, i \geq \sigma_M, i+1$ for $i = 1, \ldots, q - 1$. The Moore-Penrose pseudo-inverse of matrix $M$ is then defined as $M^\dagger = V_M \Sigma_M^{-1} U_M^\top$, where $\Sigma_M^{-1} = \text{diag}(\sigma_M^1, \ldots, \sigma_M^q)$ with

$$\sigma_M^i = \begin{cases} \sigma_M^{-1} & \text{if } \sigma_M > 0 \\ 0 & \text{otherwise} \end{cases}.$$

The orthogonal projector onto the span of the columns (resp. of the rows) of matrix $M$ is denoted by $P_M = MM^\dagger = U_M \Sigma_M^{-1} U_M^\top$ (resp. $P_M^\top = M^\dagger M = V_M \Sigma_M^{-1} V_M^\top$).

We also introduce additional notations to derive a matrix formulation of the low-rank estimation problem (8). We gather consecutive elements of the $i$-th snapshot trajectory between time $t_1$ and $t_2$ in matrix $X_{1:t_2}^{(i)} = (x_{t_1}^{(i)}(\theta_i) \cdots x_{t_2}^{(i)}(\theta_i))$ and form large matrices $X, Y \in \mathbb{R}^{n \times m}$ with $m = N(T - 1)$ as

$$X = (X_{1:T-1}^{(1)} \cdots X_{1:T-1}^{(N)}) \quad \text{and} \quad Y = (X_{2:T}^{(1)} \cdots X_{2:T}^{(N)}).$$

In order to be consistent with the SVD definition and to keep the presentation as simple as possible, this work assumes that $m \leq n$. However, all the result presented in this work can be extended without any difficulty to the case where $m > n$ by using an alternative definition of the SVD.

3 Sub-Optimal Solutions

We begin by presenting state-of-the-art methods solving approximatively the low-rank minimisation problem (8). In a second part, we make an overview of state-of-the-art algorithms computing factorisations of these approximated solutions of the form of (4) or (5).

3.1 Tractable Approximations to Problem (8)

Using the notations introduced in Section 2, problem (8) can be rewritten as

$$\begin{equation}
A_k^* \in \arg \min_{A: \text{rank}(A) \leq k} \|Y - AX\|_F^2, 
\end{equation}$$

where $\| \cdot \|_F$ refers to the Frobenius norm.
3.1.1 Truncation of the Unconstrained Solution

A first approximation consists in removing the low-rank constraint in problem \( (9) \). As pointed out by Tu et al. in \( [30] \), the problem then boils down to a least-squares problem

\[
\arg \min_A \| Y - AX \|^2_F, \tag{10}
\]

admitting the closed-form solution \( YX^\dagger \). Matrix \( YX^\dagger \) also solves the constrained problem \( (9) \) in the case where \( k \geq m \) and in particular for \( k = m \), i.e.,

\[
A^*_m = YX^\dagger. \tag{11}
\]

This solution relies on the SVD of \( X \): \( A^*_m = YV_X \Sigma_X^{\dagger} U_X^\top \), which is computed with a complexity of \( O(m^2(m+n)) \) \( [9] \). An approximation of the solution of \( (10) \) satisfying the low-rank constraint \( \text{rank}(A) \leq k \) with \( k \leq m \) is then obtained by a truncation of the SVD or the EVD of \( A^*_m \) using \( k \) terms.

3.1.2 Approximation by low-rank projected DMD

The so-called “projected DMD” proposed by Schmid in \( [29] \) is a low-dimensional approximation of \( A^*_m \). This approximation is also used by Jovanovic et al. in order to approximate \( A^*_k \) for \( k \leq m \) \( [17] \). Similar approximations are used to compute the so-called “optimized DMD” in \( [3] \) or “optimal mode decomposition” in \( [33] \). These approximations assume that columns of matrix \( AX \) are in the span of \( X \). This assumption is formalised in \( [29] \) as the existence of \( A^c \in \mathbb{R}^{m \times m} \), the so-called “companion matrix” of some matrix \( A \) parametrised by \( m \) coefficients\(^3\) such that

\[
AX = XA^c. \tag{13}
\]

Under this assumption, we obtain from \( (13) \) a low-dimensional representation of \( A \) in the span of \( U_X \),

\[
U_X A U_X = \hat{A}^c, \tag{14}
\]

\(^3\) The exact definition of the “companion matrix” \( A^c \) considered by Schmid is as follows:

\[
A^c = \begin{pmatrix}
0 & \alpha_1 & & 1 \\
1 & 0 & \alpha_2 & \\
& \ddots & \ddots & \ddots \\
& & 1 & 0 & \alpha_{m-1} \\
& & & 1 & \alpha_m
\end{pmatrix} \in \mathbb{R}^{m \times m}. \tag{12}
\]

It depends on the \( m \) coefficients \( \{\alpha_i\}^m_{i=1} \), see details in \( [29] \).
where $\tilde{A}^c = \Sigma_X V_X^T A^c V_X \Sigma_X^T \in \mathbb{R}^{m \times m}$. Jovanovic et al. then obtain an approximation of $A^*_k$ by plugging (13) in problem (9) and minimising the resulting cost with respect to $A^c$ [17]. Using the invariance of the Frobenius norm to unitary transforms, this approximation of $A^*_k$ can be rewritten as the solution of

$$\arg\min_{\tilde{A}^c : \text{rank}(\tilde{A}^c \Sigma_X) \leq k} \|U_X^T YV_X - \tilde{A}^c \Sigma_X\|_F^2. \quad (15)$$

Assuming $X$ is full-rank, the solution is given by the Eckart-Young theorem [7]:

the solution is the SVD representation of matrix $B = U_X^T YV_X$ truncated to $k$ terms multiplied by matrix $\Sigma_X^T$. Denoting by $\tilde{B}$ this truncated decomposition, we finally obtain the following approximation of $A^*_k$:

$$A^*_k \approx U_X \tilde{B} \Sigma_X^T U_X^T. \quad (16)$$

3.1.3 Approximation by Sparse DMD

Jovanovic et al. also propose in [17] a two-stage approach they call “sparse DMD”. It consists in solving two independent problems. The first stage computes the EVD of the approximated solution (16) for $k = m$. This first stage yields eigen-vectors $\zeta_i$, for $i = 1, \ldots, m$. In a second stage, the authors assume that a linear combination of $k$ out of the $m$ eigen-vectors approximates accurately the data. This assumption serves to design a relaxed convex optimisation problem using an $\ell_1$-norm penalisation. Solving this problem, they obtain $k$ eigen-vectors and their associated coefficients. Note that the sparse DMD approximation has an error norm always greater or equal than the one induced by an approximation by low-rank projected DMD.

This method relies on the resolution of an $\ell_1$-norm minimisation of a cost function built using the EVD of approximation (16) for $k = m$, which is easily deduced from the EVD of $B \Sigma_X^T \in \mathbb{R}^{m \times m}$. The overall complexity is $O(m^2(m+n))$.

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4 The penalisation parameter must be adjusted to induce $m - k$ coefficients nearly equal to zero.

5 By decomposing the error in two orthogonal components and by using the invariance of the Frobenius norm to unitary transforms, for any $A$ satisfying (13), we have $\|Y - AX\|_F^2 = \|Y - XA^c\|_F^2 = \|U_X^T YV_X - A^c \Sigma_X\|_F^2 + \|(U_X^T)^T Y\|_F^2$, where the columns of $(U_X^T)^T$ contain the $n - m$ vectors orthogonal to $U_X$. Taking the minimum over the set of low-rank companion matrices, we construct a lower bound on the error norm

$$\min_{\tilde{A}^c : \text{rank}(\tilde{A}^c \Sigma_X) \leq k} \|U_X^T YV_X - \tilde{A}^c \Sigma_X\|_F^2 + \|(U_X^T)^T Y\|_F^2 \leq \|Y - AX\|_F^2,$$

for any $A$ satisfying assumption (13). The lower bound is reached by definition if $A$ is the approximated solution (16). The sparse DMD approximation is built upon assumption (13) and thus has an error norm above or equal this bound.
3.1.4 Approximation by Total-Least-Square DMD

To ease the presentation, we reformulate the total-least-square (TLS) DMD problem studied by Hemati et al. [14]. Let us define the projector $V_K^k(V_K^k)\top$ where columns of $V_K^k \in \mathbb{R}^{m \times k}$ are the right singular vectors associated to the $k$ largest singular values of matrix $K = \begin{bmatrix} X \\ Y \end{bmatrix} \in \mathbb{R}^{2n \times m}$. The approximation introduced in Hemati et al. can be formulated as the solution of the following unconstrained convex optimization problem

$$\arg \min_{A \in \mathbb{R}^{n \times n}} \|Y' - AX'\|_F^2,$$  \hspace{1cm} (17)

where $X' = XV_K^k(V_K^k)\top$ and $Y' = YV_K^k(V_K^k)\top$. The solution of the least square problem \[17\] may constitute an approximation of the solution of the problem of interest, although the unconstrained problem \[17\] is intrinsically different from the low-rank approximation problem \[9\]. An analytical example provided in Appendix A highlights how the solutions of these two different problems differ. This method relies on the SVD of $K \in \mathbb{R}^{2n \times m}$ and $X \in \mathbb{R}^{n \times m}$ and thus involves a complexity of $O(m^2(m + n))$.

3.1.5 Approximation by Solving Regularised Problems

Some works propose to approximate \[9\] by a regularized version of the unconstrained problem \[10\], using Tikhonov penalization \[22\] or penalization enforcing structured sparsity \[34\]. However, these choices of regularizers do not guarantee in general that the solution is low-rank. In contrast, the solution of \[10\] may under certain theoretical conditions \[21,16\] be recovered by the following quadratic program

$$A_k^* \approx \arg \min_{A \in \mathbb{R}^{n \times n}} \|Y - AX\|_F^2 + \alpha_k \|A\|_*,$$  \hspace{1cm} \text{s.t.} \hspace{1cm} \begin{align*}
\|Y - AX\|_F^2 + \alpha_k \|B\|_* & = \min_{B \in \mathbb{R}^{n \times n}} \|Y - AX\|_F^2 + \alpha_k \|B\|_* \\
A = B & \end{align*} \hspace{1cm} (19)

where $\| \cdot \|_*$ refers to the nuclear norm (or trace norm) of the matrix, i.e., the sum of its singular values. In optimization problem \[19\], $\alpha_k \in \mathbb{R}_+$ represents an appropriate regularization parameter determining the rank $k$ of the solution. Program \[19\] is a convex optimization problem \[24\] which can be efficiently solved using modern optimization techniques, such as the alternate directions of multipliers method (ADMM) \[11\]. The algorithms solving \[19\] typically involve per iteration a complexity of $O(m(m^2 + n^2))$. 


3.2 Factorization of Approximations of $A_k^*$

In this section, we provide an overview of some state-of-the-art methods to compute factorizations of the form of (4) or (5) for the approximations of $A_k^*$ presented above.

We first note that a brute-force computation of the SVD or EVD of a matrix in $\mathbb{R}^{n \times n}$ leads in general to a prohibitive computational cost since it requires a complexity of $O(n^3)$. Hopefully, the factorizations (4) or (5) are computable with a complexity of $O(m^2(m + n))$, in most cases mentioned above.

In particular, in the case of low-rank projected DMD, a straightforward factorization of the form of (4) is $P = U_X$ and $Q^\top = \tilde{B}\Sigma^{\dagger}U_X^\top$. In the case of sparse DMD, the latter factorization holds by substituting $\tilde{B}$ by the “sparse” approximation of $B$. Another straightforward factorization of the form of (4) is intrinsic to the ADMM procedure, which uses an SVD to compute the regularized solution.

Concerning EVD factorization, in the case of the truncated approach, Tu et al. propose an algorithm scaling in $O(m^2(m + n))$ [30]. In the context of low-rank projected DMD or sparse DMD, Jovanovic et al. propose a procedure of analogous complexity, which approximates the first $m$ eigenvectors, and then estimate the related eigenvalues by solving a convex optimization problem [17]. In the case of TLS DMD, the diagonalization of a certain matrix in $\mathbb{R}^{m \times m}$ suffices to obtain the sought EVD factorization.

4 Optimal Solution in Polynomial Time

In this section, we provide the closed-form solution to problem (9) proposed in [12]. Algorithms are then proposed to compute and factorize this solution in the form of (4) or (5).

4.1 Closed-Form Solution to (9)

Let the columns of matrix $U_{Z,k} = (u_1 \cdots u_k) \in \mathbb{R}^{n \times k}$ be the left singular vectors $\{u_i\}_{i=1}^k$ associated to the $k$ largest singular values of matrix

$$Z = Y_P X^\tau \in \mathbb{R}^{n \times m},$$

where we recall that $P_X = V_X V_X^\top$ and consider the projector

$$P_{Z,k} = U_{Z,k} U_{Z,k}^\top. \tag{21}$$

Matrix (21) appears in the closed-form solution of (9), as shown in the following theorem. The proof is given in [12].
Theorem 1 Problem (9) admits the following solution

$$A_k^* = \mathbb{P}_Z Y X^\dagger.$$  \hspace{1cm} (22)

Moreover, the optimal approximation error can be expressed as

$$\|Y - A_k^* X\|^2_F = \sum_{i=k+1}^m \sigma_{Z,i}^2 + \|Y(I_m - \mathbb{P}_X X^\top)\|^2_F.$$  \hspace{1cm} (23)

In words, Theorem 1 shows that problem (9) is simply solved by computing the orthogonal projection of the solution of the unconstrained problem (10), onto the subspace spanned by the first $k$ left singular vectors of $Z$. The $\ell_2$-norm of the error is simply expressed in terms of the singular values of $Z$, and the square norm of the projection of the rows of $Y$ onto the orthogonal of the image of $X^\top$. If $X$ is full row-rank, we then obtain the simplifications $\mathbb{P}_X X^\top = I_m$ and $Z = Y$. In this case, the second term in the right-hand side of (23) vanishes and the approximation error reduces to $\|Y - A_k^* X\|^2_F = \sum_{i=k+1}^m \sigma_{Z,i}^2$. The latter error is independent of matrix $X$ and is simply the sum of the square of the $m - k$ smallest singular values of $Y$. This error also corresponds to the optimal error for the approximation $Y$ by a matrix of rank at most $k$ in the Frobenius norm [7].

Besides, note that $r = \text{rank}(A_k^*)$ can be smaller than $k$. Indeed, by the Sylvester’s theorem [15] we have that

$$r \leq \min(\text{rank}(\mathbb{P}_Z), \text{rank}(Y X^\dagger)) \leq \text{rank}(Y X^\dagger) \leq \min(\text{rank}(Y), \text{rank}(X^\dagger)) = \min(\text{rank}(Y), \text{rank}(X)),$$

which shows that $r < k$ if $\text{rank}(X)$ or $\text{rank}(Y)$ is smaller than $k$, but also if $\text{rank}(Y X^\dagger) < k$.

It is worth mentioning that a generalization of Theorem 1 to separable infinite-dimensional Hilbert spaces is proposed in [11]. This generalization characterizes the solution of low-rank approximations in reproducing kernel Hilbert spaces (where $n = \infty$) at the core of kernel-based DMD [13,32], and characterizes the solution of the DMD counterpart (where $m = \infty$) to the continuous POD problem presented in [27, Theorem 6.2].

4.2 Algorithm Evaluating $A_k^*$

The design of an algorithm computing the solution (22) is straightforward: evaluating $A_k^*$ consists in making a product of easily-computable matrices. The proposed procedure is summarized in Algorithm 1.

Steps 1) to 3) of Algorithm 1 implies the computation of the SVD of matrices $X, Z \in \mathbb{R}^{n \times m}$, and matrix multiplications involving $m^2$ vector products in $\mathbb{R}^n$ or $\mathbb{R}^m$. The complexity of these first three steps is therefore $O(m^2 (m + n))$. Computing explicitly each entry of $A_k^* \in \mathbb{R}^{n \times n}$ in step 4) of Algorithm 1 then requires a complexity of $O(n^2 k)$, which is prohibitive for large $n$. However, as detailed in the next section, this last step is not necessary to factorize the optimal solution $A_k^*$ in the form of (4) or (5).
**Algorithm 1** Computation of $A^*_k$, a solution of (9)

**inputs**: $(X, Y)$.

1) Compute the SVD of $X = V_X \Sigma_X U_X^T$.
2) Compute $Z = Y V_X \Sigma_X U_X^T$.
3) Compute the SVD of $Z$ to obtain the projector $P_{Z,k}$.
4) Compute $A^*_k = P_{Z,k} Y V_X \Sigma_X U_X^T$.

**output**: $A^*_k$.

**Algorithm 2** EVD of $A^*_k$ or low-rank DMD

**inputs**: $(X, Y)$.

1) Compute step 1 to 3 of Algorithm 1 and use (24) to obtain $W$.
2) Let $r = \text{rank}(A^*_k)$ and solve for $i = 1, \ldots, r$ the eigen-equations

\[
(W^T U_{Z,k}) w^e_i = \lambda_i w^r_i \quad \text{and} \quad (U_{Z,k} W) w^r_i = \lambda_i w^e_i,
\]

where $w^e_i, w^r_i \in \mathbb{C}^k$ and $\lambda_i \in \mathbb{C}$ such that $|\lambda_{i+1}| \geq |\lambda_i|$.
3) Compute for $i = 1, \ldots, r$ the right and left eigenvectors

\[
\xi_i = U_{Z,k} w^r_i \quad \text{and} \quad \zeta_i = W w^e_i.
\]

4) Rescale the $\xi_i$’s so that $\xi_i^T \zeta_i = 1$.

**outputs**: $L = (\xi_1 \cdots \xi_r)$, $R = (\zeta_1 \cdots \zeta_r)$, $S = \text{diag}(\lambda_1, \ldots, \lambda_r)$. (25)

### 4.3 Algorithms Factorizing $A^*_k$

Given the closed-form solution (22), we present in what follows how to compute from $X$ and $Y$ a factorization of the optimal solution $A^*_k$ in the form of (4) or (5). We will need matrix $W = (U_{Z,k} Y X^\dagger)^\dagger \in \mathbb{R}^{n \times k}$. (24)

**Factorization of the form of (4)**. By performing the first three steps of Algorithm 1 and then making the identifications $P = U_{Z,k}$ and $Q = W$, we obtain a factorization of $A^*_k$ of the form of (4). As mentioned in the introduction, trajectories of (2) can then be computed with system (3) setting $R = U_{Z,k}$, $L = W$ and $S = W^T U_{Z,k}$. The method relies on the first three steps of Algorithm 1 and on the computation of matrix $W$. The three steps in Algorithm 1 imply a complexity of $O(m^2(m + n))$ while the computation of $W$ requires a complexity of $O(nk^2)$. Since $k \leq m$, the off-line complexity to build the factorization (4) from $X$ and $Y$ scales as $O(m^2(m + n))$, which is the same order of complexity as the procedures described in Section 3.

**Factorization of the form of (5)**. According to the previous factorization of the form of (4), $A^*_k$ is the product of matrix $U_{Z,k}$ in $\mathbb{R}^{n \times k}$ with matrix
W^T in R^{k \times n}. Therefore, using standard matrix analysis, we expect the eigenvectors of A^\star k to belong to a k-dimensional subspace \[9\]. As shown in the next proposition, the non-zero eigenvalues of A^\star k are obtained by EVD of certain matrices in R^{k \times k}. The proof of this proposition is given in \[12\].

**Proposition 1** Assume A^\star k is diagonalizable. The elements of \((\zeta_i, \xi_i, \lambda_i)_{i=1}^{\text{rank}(A^\star k)}\) generated by Algorithm 2 are the right eigenvectors, the left eigenvectors and the eigenvalues of the economy size EVD of A^\star k.

In words, Proposition 1 shows that Algorithm 2 computes the EVD of A^\star k by diagonalizing two matrices in R^{k \times k}. The complexity to build this EVD from snapshots X and Y is O(m^2(m + n)). More precisely, as mentioned previously, performing the first three steps of Algorithm 1 (i.e., step 1) of Algorithm 2 requires a number of operations scaling as O(m^2(m + n)); the complexity of step 2) is O(k^3) since it performs the EVDs of k \times k matrices; step 3) involves r \times n vector products in R^n while step 4) involves r vector products in R^n, with r \leq k \leq m. Overall, the complexity of Algorithm 2 is dominated by step 1) and the EVD of A^\star k can be evaluated with a computational cost of the order of O(m^2(m + n)).

5 Conclusion

This work reviews the state-of-the-art algorithms proposed to compute low-rank DMD. In particular, it details an exact solution to this problem computable with a complexity of the same order as state-of-the-art sub-optimal methods.

A Analytical Comparison between Low-Rank DMD and TLS DMD

This simple example demonstrates that the solution given by TLS-DMD can be biased on the contrary to the one given by the optimal algorithm for low-rank DMD. It also shows that in the case (favorable to TLS-DMD) where the solution given by TLS-DMD is unbiased, the noise robustness of the two approaches are comparable.

**Example 1** Consider the case where \(k = 1\), the data X is set either to

\[
X_1 = \begin{pmatrix} 1 & 0 \\ 0 & 10 \\ 1 & 10 \end{pmatrix} \quad \text{or} \quad X_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 1 \end{pmatrix},
\]

and

\[
Y = \begin{pmatrix} 5 & 0 \\ \epsilon & 2 \\ 10 & 0 \end{pmatrix},
\]

where \(\epsilon\) is a scalar representing a small perturbation of the matrix entry.

- **Low-rank DMD solution.** Since in both cases X is full rank, we have Z = Y. Straightforward analytical calculations yield the vector \(U_{Z,1} = \frac{(\sigma_2 - 4)}{(\sigma_2(\sigma_2 - 4)^{1/2} + 4\epsilon^2)^{1/2}} \begin{pmatrix} 5 \\ \epsilon \\ 10 \end{pmatrix}.
\]
with the singular value $\sigma_2 = \frac{129 + \sqrt{14641 + 240 + 17}}{2}$, This leads to an optimal rank-1 solution (given by our algorithm)

$$A_1^* = P \mathbb{Z}_1 YX^\dagger = \frac{125(\sigma_2 - 4)^2}{\sigma_2 (\sigma_2 - 4)^2 + 4}\left(\begin{array}{c}5 + 0.04 \epsilon^2 & 0.08 \epsilon \\epsilon + 0.008 \epsilon^3 & 0.16 \epsilon \end{array}\right) X^\dagger.$$

The non-zero eigen value $\lambda(A_1^*)$ of matrix $A_1^*$ corresponds to the solution of a linear equation. It takes the form of

$$\lambda(A_1^*) = \frac{125(\sigma_2 - 4)^2}{\sigma_2 (\sigma_2 - 4)^2 + 4}\left(\begin{array}{c}20 \\epsilon + b \epsilon^2 - 0.008 \epsilon^3 \\epsilon \end{array}\right),$$

with $a = 0.992$ (resp. $a = 0.920$), $b = 0.0544$ (resp. $b = 0.0540$) for $X = X_1$ (resp. $X = X_2$). For a small perturbation $\epsilon$, we obtain for $X = X_1$ the approximation

$$\lambda(A_1^*) \approx \frac{20}{3} - 0.3416 \epsilon,$$

(resp. $\lambda(A_1^*) \approx \frac{20}{3} - 0.3168 \epsilon$ for $X = X_2$). For $\epsilon = 0$, the optimal error norm is

$$\|Y - A_1^* X\|_F = 2.00,$$

equally for $X = X_1$ and $X = X_2$.

- TLS-DMD solution. We remark that $K^*K = \left(\begin{array}{cc}127 + \epsilon^2 & 10 + 2 \epsilon \\ 10 + 2 \epsilon & 204 \end{array}\right)$ for $X = X_1$ (resp. $K^*K = \left(\begin{array}{cc}127 + \epsilon^2 & 10 + 2 \epsilon \\ 10 + 2 \epsilon & 204 \end{array}\right)$ for $X = X_2$) and simple algebra yields the singular vector

$$V_{K,1} = \frac{1}{\|10 + 2 \epsilon\|_2} \left(\begin{array}{c}10 + 2 \epsilon \\ \sigma_1 - 127 \end{array}\right),$$

with $\sigma_1 = \frac{331 + \sqrt{13663 + 16 \epsilon - 138 \epsilon^2}}{2} + O(\epsilon^2)$.

The TLS-DMD solution provided by Hemati et al. is

$$\hat{A}_1 = YV_{K,1}V_{K,1}^\dagger X^\dagger,$$

and the non-zero eigen value $\lambda(\hat{A}_1)$ of matrix $\hat{A}_1$ is the solution of a linear equation, more explicitly for $X = X_1$ (resp. $X = X_2$)

$$\lambda(\hat{A}_1) = \frac{20 + (\sigma_1 - 127)(a(\sigma_1 - 127) - b)}{3 + 0.03(\sigma_1 - 127)^2} + O(\epsilon),$$

with the constants $a = 0.004$ (resp. $a = 0.04$) and $b = 0.15$ (resp. $b = 0.30$). We obtain for $X = X_1$ the approximation

$$\lambda(\hat{A}_1) \approx 0.1754 + 0.0312 \epsilon,$$

(resp. $\lambda(\hat{A}_1) \approx 6.6746 - 0.3127 \epsilon$ for $X = X_2$). For $\epsilon = 0$, the Frobenius error norm related to Hemati et al.'s solution is

$$\|Y - \hat{A}_1 X\|_F \approx 11.09$$

for $X = X_1$ (resp. $\|Y - \hat{A}_1 X\|_F \approx 2.0021$ for $X = X_2$).

We note that in the case where $X = X_2$, the eigenvalue estimated with the approach of Hemati et al. is almost equal to the proposed eigenvalue estimate, whereas it is strongly biased for $X = X_1$. Moreover, in the favourable case where $X = X_2$, a small perturbation on the matrix input induces similar biases for the TLS-DMD and the low-rank DMD.
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