NON-LINEAR REDUCED MODELING OF DYNAMICAL SYSTEMS USING KERNEL METHODS AND LOW-RANK APPROXIMATION

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Abstract. Reduced modeling of a computationally demanding dynamical system aims at approximating its trajectories, while optimizing the trade-off between accuracy and computational complexity. In this work, we propose to achieve such an approximation by first embedding the trajectories in a reproducing kernel Hilbert space (RKHS), which has interesting approximation and calculation capabilities, and then solving the associated reduced model problem. More specifically, we propose a new efficient algorithm for data-driven reduced modeling of non-linear dynamics based on linear approximations in a RKHS. This algorithm takes advantage of the closed-form solution of a low-rank constraint optimization problem while exploiting advantageously kernel-based computations. Reduced modeling with this algorithm reveals a gain in approximation accuracy, as shown by numerical simulations, and in complexity with respect to existing approaches.

Key words. Reduced modeling, kernel methods, low-rank approximations, non-linear dynamics

1. Introduction. Consider a high-dimensional system of the form:

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

where the \(x_t\)'s and \(\theta\) in \(\mathbb{R}^p\), constitute respectively a state trajectory and an initial condition, and where \(f_t : \mathbb{R}^p \to \mathbb{R}^p\) is an arbitrary function whose direct evaluation is considered to be time consuming when \(p\) is large. Reduced modeling of the dynamical systems aims to lighten the computation load for the evaluation of a trajectory. The idea common to all model reduction methods is the projection of the high-dimensional system (1.1) onto a low-dimensional manifold, which enables a rapid and reliable approximation of a trajectory for any initial condition. Projections onto well-chosen linear subspaces have been extensively studied in the reduced modeling literature, leading in particular to the well-established reduced basis methods [35]. Data-driven approaches have emerged for the case where the function \(f_t\) is unknown and we only have access to a set of representative solutions of (1.1). Dynamic mode decomposition (DMD) [36] is a popular framework for this purpose. It consists in the data-driven linear approximation of the function \(f_t\): a matrix substituting \(f_t\) is learned from representative trajectories, so-called snapshots, by minimizing the norm of the residual of linear approximations subject to specific constraints [10, 14, 16, 22].

In recent decades, the community’s interest has shifted to nonlinear reduced modeling, in particular, projections onto time-dependent subspaces [5, 8, 25, 33] or approaches based on nonlinear embeddings of the solution manifold in a space with better approximation capabilities [21, 39]. Among the latter approaches, the data-driven DMD has been extended [1] to a method often referred to as extended DMD (EDMD) [7, 12, 30, 42, 43, 45]. Basically, DMD and EDMD are identical, except that
EDMD first immerses the trajectory through a non-linear mapping $\Psi$ in a space exhibiting better low-rank approximation capabilities. More explicitly, let $\Psi : \mathbb{R}^p \rightarrow \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space endowed with the inner product $\langle \cdot, \cdot \rangle_\mathcal{H}$ and the induced norm $\| \cdot \|_\mathcal{H}$. EDMD approximates system (1.1) through a system taking the form of

$$
\begin{aligned}
\eta_t(\theta) &= \hat{A}_k \eta_{t-1}(\theta), \quad t = 2, \ldots, T, \\
\eta_1(\theta) &= \Psi(\theta),
\end{aligned}
$$

(1.2)

where $\hat{A}_k : \mathcal{H} \rightarrow \mathcal{H}$ is a linear operator of rank at most $k$ (satisfying some optimality criterion which will be specified later), yielding an approximation of the state $x_T(\theta)$ by an inverse mapping

$$
\tilde{x}_T(\theta) = \Psi^{-1}(\eta_T(\theta)).
$$

(1.3)

A proper definition of the inverse map $\Psi^{-1}$ will be given in the next section.

This paper focuses on reduced models of the form (1.2)-(1.3), where $\dim(\mathcal{H}) \gg p$ (including $\dim(\mathcal{H}) = \infty$). Such embeddings are appealing due to the ability of high-dimensional Hilbert spaces to linearize differential equations [26, 28, 31]. Nevertheless, computing a reduced model using these high-dimensional embeddings is difficult since neither the inference of operator $\hat{A}_k$ nor the recursion (1.2) or the inversion (1.3) is tractable in a general setting. To obtain a “good” trade-off between accuracy and complexity of the reduced model, one needs to accomplish two challenging tasks: \(i\) learn a tractable representation of a low-rank operator $\hat{A}_k$ yielding an accurate approximation of the form (1.2)-(1.3), \(ii\) build a low-complexity algorithm able to compute $\tilde{x}_T(\theta)$ satisfying (1.2)-(1.3) for a given $\theta$ and $T$.

State-of-the-art methods such as [10, 16, 19, 22, 41] involve a complexity in $\dim(\mathcal{H})$, thus are non-efficient in high-dimensional settings. Alternatively, authors in [33] have introduced an efficient algorithm to compute (1.2) - (1.3) for any map $\Psi$ related to a reproducing kernel Hilbert space (RKHS) [38]. This algorithm known as kernel-based DMD (K-DMD) enjoys an advantageous complexity linear in $p$ and independent of $\dim(\mathcal{H})$ and of the trajectory length $T$. Unfortunately, it relies on a set of restrictive assumptions. The regularized kernel regression technique [37] known as kernel analog forecasting [1, 12] can be seen as the K-DMD algorithm, in the particular case where the reduced model is trained to compute only (1.3) for some specific and predefined path length $T$. In the article [7], the authors propose a kernel method similar to K-DMD [2] but alleviating some of its restrictive assumptions. However, it should be noted that the method involves additional approximation steps using regularized kernel regression techniques. In addition, the method produces a reduced model whose complexity is no longer independent of $T$.

The contribution of this work is to propose a new algorithm dubbed “generalized kernel-based DMD (GK-DMD)” that generalizes K-DMD to less restrictive assumptions, while being characterized by a gain in computational complexity and approximation accuracy, as evidenced by our numerical simulations. To put this work into context, it is important to make the following two points: \(i\) although DMD-type approximations in RKHS have recently attracted the interest of several research
groups \[11\] \[23\] \[24\] \[27\] , a theoretical characterization of the convergence of the proposed approximation is out of the scope of our paper; this paper is limited to providing a methodology and empirical evidence of its performances through relevant numerical simulations; ii) in contrast to most of the recent studies concerned with the Koopman operator approximation, the paper focuses instead on the approximation the trajectories of (1.1) in the ambient space, by means of learning a low-rank operator in a RKHS, in the line of the kernel method proposed in \[7\] and of previous results obtained in \[15\] \[16\].

The paper is organized as follows. Section 2 specifies the reduced modeling problem of interest and reviews existing solutions. Our generalized kernel-based algorithm is presented in Section 3. The proposed algorithm is evaluated numerically in Section 4. Proofs of theoretical results and technical details are provided in the appendices.

2. Problem and Existing Solutions.

2.1. The reduced modeling problem. In this work, we are interested in the design of an algorithm evaluating for any \( \theta \in \mathbb{R}^p \) the approximation \( \hat{x}_T(\theta) \) given by (1.2), with a complexity constant with respect to the dimension \( \dim(\mathcal{H}) \) and the trajectory length \( T \). Moreover, we are interested in a data-driven approach: the algorithm should rely on a reduced model learned from a set of representative trajectories \( \{ x_i(\theta_{i, \text{learn}}) \}_{i=1}^{N_{\text{learn}}} \) of the high-dimensional system (1.1) corresponding to \( N_{\text{learn}} \) initial conditions \( \{ \theta_{i, \text{learn}} \}_{i=1}^{N_{\text{learn}}} \) and where \( T_{\text{learn}} \) is possibly different from \( T \). We thus consider a particular instance of the family of data-driven reduced model given by (1.2), where the low-rank operator \( \hat{A}_k \) and the inverse map \( \Psi^{-1} \) have specific definitions.

In order to introduce these definitions, we need some notations. The function space \( \mathcal{B}(\mathcal{V}, \mathcal{U}) \) will be the set of linear bounded operators from \( \mathcal{V} \) to \( \mathcal{U} \). The subset of low-rank operators will be denoted

\[ \mathcal{B}_k(\mathcal{V}, \mathcal{U}) = \{ M \in \mathcal{B}(\mathcal{V}, \mathcal{U}) : \text{rank}(M) \leq k \}. \]

The adjoint of an operator \( M \in \mathcal{B}(\mathcal{V}, \mathcal{U}) \) will be denoted \( M^* \in \mathcal{B}(\mathcal{U}, \mathcal{V}) \). The Hilbert-Schmidt norm \( \| \cdot \|_{HS} \) of \( M \in \mathcal{B}(\mathcal{V}, \mathcal{U}) \) is defined as \( \| M \|_{HS}^2 = \sum_{i=1}^{\dim(\mathcal{V})} \| Me_i \|_{\mathcal{U}}^2 \), where \( \{ e_i \}_{i=1}^{\dim(\mathcal{V})} \) is an orthonormal basis of \( \mathcal{V} \). The \( \ell_2 \)-norm of a vector \( v \in \mathcal{V} \), with \( \dim(\mathcal{V}) < \infty \), will be denoted \( \| v \|_2 \). For a vector \( v \in \mathcal{V} \), the subscript notation \( v_i \) will denote its \( i \)-th component. The distinction from the subscript notation \( \theta_{i, \text{learn}} \) denoting the \( i \)-th element of a set \( \{ \theta_{i, \text{learn}} \}_{i>0} \) will be clear from the context.

Low-rank operator. The first definition concerns the low-rank operator learned from the training data set \( \{ x_i(\theta_{i, \text{learn}}) \}_{i=1}^{N_{\text{learn}}} \) to \( \mathbb{R}^m \) as the linear combinations

\[ \Psi_{\mathcal{X}} w = \sum_{i,t=1}^{N_{\text{learn}},T_{\text{learn}}-1} \Psi(x_t(\theta_{i, \text{learn}})) w_{\ell(i,t)} \quad \text{and} \quad \Psi_{\mathcal{Y}} w = \sum_{i,t=1}^{N_{\text{learn}},T_{\text{learn}}-1} \Psi(x_t+1(\theta_{i, \text{learn}})) w_{\ell(i,t)}, \]

where \( \ell(i,t) = (T_{\text{learn}} - 1)(i-1) + t \). Using these operators, we consider the constrained optimization problem

\[ A_k^* \in \arg \min_{A \in \mathcal{B}_k(\mathcal{H}, \mathcal{H})} \| \Psi_{\mathcal{Y}} - A \Psi_{\mathcal{X}} \|_{HS}. \]
We remark that the square of the Hilbert-Schmidt norm in (2.1) can be rewritten as a sum of square norms of the form $\|\Psi(x_{t+1}(\theta_{i}^{\text{learn}})) - A\Psi(x_{t}(\theta_{i}^{\text{learn}}))\|_{H}^{2}$ over $t = 1, \ldots, T_{\text{learn}} - 1$ and $i = 1, \ldots, N_{\text{learn}}$. Hence, the objective function in (2.1) measures the overall discrepancy between the true states and their prediction by operator $A$ from the previous states, mapped into the Hilbert space.

**Definition 2.1.** The low-rank operator $\hat{A}_{k}$ in (1.2) is defined as the solution of (2.1).

This first definition stipulates that the learned low-rank linear operator for reduced modeling in $\mathcal{H}$ is optimal in the Hilbert-Schmidt norm. Note that (2.1) is a generalization of the solution of the minimization problem in [12, 13], subject to a low-rank constraint as in [10, 22]. Indeed, let $\hat{A}_{k}^{ls}$ be defined as a $k$-term truncation of the eigendecomposition of the solution of the unconstrained problem $\Psi_{Y}\Psi_{X}^{\dagger} = \arg \min_{A \in B(\mathcal{H}, \mathcal{H})} \| \Psi_{Y} - A\Psi_{X} \|_{\text{HS}}$ [11]. Then $\hat{A}_{k}^{ls}$ differs from the optimal solution $A_{k}^{\ast}$ for $k < m$, while for $k \geq m$, both operators are equivalent.

**Minimum distance estimation.** The second definition concerns the inverse map.

**Definition 2.2.** The inverse map $\Psi^{-1}$ from $\mathcal{H}$ to $\mathbb{R}^{p}$ in (1.3) is defined as

$$\Psi^{-1}(\eta) \in \arg \min_{z \in \mathbb{R}^{p}} \| \eta - \Psi(z) \|_{H}. \quad (2.2)$$

This second definition stipulates that the inverse mapping is optimal in a minimum distance sense. This definition is further discussed in Appendix C.1.

**Low complexity.** In addition, we require the algorithm evaluating the approximation $\tilde{x}_{T}(\theta)$ to be a low-complexity one in the following sense.

**Constraint 1.** The complexity for evaluating $\tilde{x}_{T}(\theta)$ given by (1.2) - (1.3) is constant with respect to $\dim(\mathcal{H})$ and $T$.

In order to enable a complexity constant in $T$, we will assume all along this work that $\mathcal{H}$ is separable and that $A_{k}^{\ast}$ is diagonalizable. These assumptions enable to evaluate recursion (1.2) independently of the trajectory length $T$. Explicitly, let $\{\xi_{i}\}_{i \in \mathbb{N}}$ and $\{\zeta_{i}\}_{i \in \math{N}}$ be bases of $\mathcal{H}$ associated to the left and right eigen-vectors of $A_{k}^{\ast}$, i.e., $A_{k}^{\ast}\xi_{i} = \lambda_{i}\xi_{i}$ and $(A_{k}^{\ast})^{\dagger}\zeta_{i} = \lambda_{i}\zeta_{i}$ for $i = 1, \ldots, \dim(\mathcal{H})$, where $\{\lambda_{i}\}$ is the related sequence of eigen-values sorted by decreasing magnitude. The finite rank of operator $A_{k}^{\ast}$ (which has at most rank($A_{k}^{\ast}$) $\leq k$ non-zero eigen-values) and the bi-orthogonality of the left and right eigen-vectors yield $A_{k}^{\ast}\Psi = \sum_{i=1}^{k} \lambda_{i} \langle \xi_{i}, \Psi \rangle_{H}\zeta_{i}$. Defining $\varphi_{i}(\theta) = \langle \xi_{i}, \Psi(\theta) \rangle_{H}$, (1.3) then becomes

$$\tilde{x}_{T}(\theta) = \Psi^{-1}(\sum_{i=1}^{k} \nu_{i,T}\zeta_{i}), \quad \nu_{i,T} = \lambda_{i}^{-1}\varphi_{i}(\theta). \quad (2.3)$$

Note that in the case where $\Psi^{-1}$ is linear, then (2.3) simplifies to

$$\tilde{x}_{T}(\theta) = \sum_{i=1}^{k} \nu_{i,T}\mu_{i}, \quad \text{with} \quad \mu_{i} = \Psi^{-1}\zeta_{i} \in \mathbb{C}^{p}. \quad (2.4)$$

\(^{3}\)This assumption holds in particular if the linear bounded operator $A_{k}^{\ast}$ is compact self-adjoint or normal [10], or in the case where $\dim(\mathcal{H}) < \infty$ and all non-zero eigen-values are distinct [20].
We mention that, under specific assumptions, \( \varphi_i \)'s, \( \mu_i \)'s and \( \lambda_i \)'s may be convergent approximations of the \( i \)th Koopman’s eigen-function, eigen-mode and eigen-value \([11, 27]\). However, this issue is beyond the scope of this paper.

In summary, the problem is to design an algorithm computing for any \( \theta \in \mathbb{R}^p \) the approximation \( \hat{x}_T(\theta) \) given by (1.2)-(1.3) using Definitions 2.1 and 2.2 with a complexity satisfying Constraint 1.

### 2.2. Existing solutions.

In this section, we discuss existing methods that can be used to partially solve the problem described in Section 2.1. They will serve as ingredients for our GK-DMD algorithm. To introduce these state-of-the-art methods, we need to introduce the notations used for SVDs, pseudo-inverses and orthogonal projectors.

First, the SVD of \( M \in \mathcal{B}(\mathcal{V}, \mathcal{U}) \) will be denoted \( M = \sum_{i=1}^{k} \sigma_i^{M} u_i^{M} (v_i^{M}, \cdot)_{\mathcal{U}} \), where \( \{u_i^{M}\}_{i=1}^{k} \) are respectively the left and right singular vectors associated to the sequence of decreasing singular values \( \{\sigma_i^{M}\}_{i=1}^{k} \) of \( M \). We will use the short-hand SVD notations:

\[
M = U_M \Sigma_M V_M^*,
\]

where \( U_M \in \mathcal{B}(\mathbb{C}^k, \mathcal{U}) \), \( \Sigma_M \in \mathcal{B}(\mathbb{C}^k, \mathbb{C}^k) \) and \( V_M^* \in \mathcal{B}(\mathcal{V}, \mathbb{C}^k) \) are defined for any vector \( w \in \mathcal{V}, s \in \mathbb{C}^k \) as \( U_M w = \sum_{j=1}^{m} u_j^{M} s_j \), \( (V_M w)_i = (v_i^{M}, w)_{\mathcal{U}} \) and \( (\Sigma_M s)_i = \sigma_i^{M} s_i \).

Then, the pseudo-inverse of \( M \) denoted \( M^\dagger \in \mathcal{B}(\mathcal{U}, \mathcal{V}) \) is defined as

\[
M^\dagger = \sum_{i=1}^{m} (\sigma_i^{M})^\dagger u_i^{M} (v_i^{M}, \cdot)_{\mathcal{U}}, \quad \text{where} \quad (\sigma_i^{M})^\dagger = \begin{cases} (\sigma_i^{M})^{-1} & \text{if} \quad \sigma_i^{M} > 0 \\ 0 & \text{else} \end{cases}.
\]

Its SVD will be written in short-hand notations as \( M^\dagger = V_M \Sigma_M^* U_M^* \). Finally, the orthogonal projector onto the image of \( M \) (resp. of \( M^* \)) will be denoted by \([13]\)

\[
\mathcal{P}_M = M M^\dagger \quad \text{(resp.} \quad \mathcal{P}_{M^*} = M^\dagger M)\).

We are now in a position to present the two main classes of approaches that exist.

#### Optimal but intractable

Reduced model \([2.3]\) where \( A_k^* \) is replaced by \( \hat{A}_k^{\ell_k} \), \( i.e. \), by a truncation to \( k \) terms of the eigendecomposition of \( A_m^* = \Psi_X \Psi_X^\dagger \), is called EDMD. The reduced model \([2.3]\) with \( A_k^* \) given by \([2.1]\) is called low-rank EDMD. As in general for \( k < m \), \( A_k^* \neq \hat{A}_k^{\ell_k} \), the two reduced models differ, while for \( k \geq m \) \( A_k^* = \hat{A}_k^{\ell_k} = A_m^* \). As we wish to be in agreement with Definition \([2.1]\) in any setting, and typically for \( k < m \), we focus on low-rank EDMD and the characterization of operator \( A_k^* \).

A closed-form expression for operator \( A_k^* \) is available using the generalization of our result in \([16]\) Theorem 4.1 to separable infinite-dimensional Hilbert spaces \([15]\) Theorem 2.1. The latter theorem yields a solution\(^4\) of problem \([2.1]\) for arbitrary value of \( k \)

\[
A_k^* = \mathcal{P}_{Z_k} \Psi_X \Psi_X^\dagger, \tag{2.5}
\]

\(^4\)Note that the solution \( A_k^* \) is not unique when \( \Psi_X \) is not full rank. Indeed, there exist an infinity of solutions of \([2.1]\) of the form \( A_k^* + M \), where the columns of \( V_M \) are orthogonal to those of \( U \Psi_X \).
with the orthogonal projector $\mathbb{P}_{Z_k^*} = \hat{P}_k \hat{P}_k^*$ and

$$\hat{P}_k \in \mathcal{B}(\mathbb{R}^k, \mathcal{H}) : w \rightarrow \sum_{i=1}^k u_i^* w_i,$$  \hspace{1cm} (2.6)

where singular vectors $u_i^*$'s are issued from the SVD (see notations above) of

$$Z = \Psi_Y \mathbb{P}_X \in \mathcal{B}(\mathbb{R}^m, \mathcal{H}).$$ \hspace{1cm} (2.7)

However, to meet Definition 2.2 and achieve Constraint 1, it remains to propose a low-complexity algorithm able to build and evaluate reduced model (2.3) from the closed-form, but potentially infinite-dimensional, solution $A_k^*$. Interestingly, the projector $\mathbb{P}_{Z_k^*}$ in the closed-form solution (2.5) implies that $A_k^* \eta$, for any $\eta \in \mathcal{H}$, belongs to the span of operator $\Psi_Y$. Therefore, an algorithm able to compute (2.3) by evaluation of scalar products of the form $\langle \Psi(y_1), \Psi(z) \rangle_{\mathcal{H}}$, where $z \in \mathbb{R}^p$, will have a complexity linear in the cost of the evaluation of a scalar product of the form $\langle \Psi(y_1), \Psi(z) \rangle_{\mathcal{H}}$, where the elements in the set $\{x_{t+1}|(\theta_{\text{learn}})\}_{t=1,i=1}^{N_{\text{learn}}}$ define the columns $\{y_i\}_{i=1}^m$ of matrix $Y \in \mathbb{R}^{p \times m}$. This idea constitutes the grounds of our algorithm presented in Section 3.2.

**Tractable but restrictive.** To tackle the high-dimensional setting $\dim(\mathcal{H}) \gg p$ related to an EDMD reduced model, authors of the seminal work [43] consider a specific class of mapping suited for the case where $\dim(\mathcal{H}) \gg m$: the mapping $\Psi$ is such that a scalar product in $\mathcal{H}$ of the form $\langle \Psi(y_1), \Psi(z) \rangle_{\mathcal{H}}$ with $z, y \in \mathbb{R}^p$ is given by the evaluation of a symmetric positive definite kernel

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

According to the Moore-Aronszajn theorem, there is a unique Hilbert space of functions on $\mathbb{R}^p$, called a reproducing kernel Hilbert space (RKHS) [38], for which $h$ is a symmetric positive definite kernel, also known as a reproducing kernel. The advantage of such a construction is that the kernel trick\(^5\) can be used to compute inner products in the RKHS $\mathcal{H}$ with a complexity equal to that required to evaluate the kernel $h$, which is in general independent of $\dim(\mathcal{H})$ [6]. The key idea of their method called K-DMD is to use the kernel trick to evaluate inner products with eigen-vectors of $A_k^*$. Assuming that the complexity for the evaluation of the kernel is $\mathcal{O}(p)$, the overall complexity of the K-DMD algorithm is independent of $\dim(\mathcal{H})$ and $T$, i.e., guaranteeing Constraint 1.

However, as proposed in [43], K-DMD computes an approximation of reduced model (2.3) under restrictive assumptions. In particular the following assumptions are needed: i) the low-rank constraint in (2.4) is ignored, i.e., $A_k^* = A_k^\epsilon$; ii) the operator $\Psi_X$ is full-rank; iii) $\Psi^{-1}$ is linear; iv) the $\Psi^{-1} \xi_i$'s belong to the span of $Y$. The reduced model computed by K-DMD therefore does not meet Definition 2.1 because assumptions i) and ii) do not hold in general, nor Definition 2.2 because assumptions iii) and iv) do not hold either. A description of the algorithm can be found in Appendix A.

\(^5\)Let us illustrate the kernel trick with the polynomial kernel $h(y, z) = (1 + y^2 z^2)^2$ and $p = 2$. The kernel maps $\mathbb{R}^2$ onto the RKHS $\mathcal{H} = \mathbb{R}^6$. Expanding the kernel, we obtain $h(y, z) = (1 + y^2 z^2)^2 = 1 + 2y_1 z_1 + 2y_2 z_2 + 2y_1 y_2 z_1 z_2 + y_1^2 z_1^2 + y_1^2 z_2^2$, where $y = (y_1 \ y_2)^T$ and $z = (z_1 \ z_2)^T$ in $\mathbb{R}^2$ so that we have $h(y, z) = \Psi(y)^* \Psi(z)$, with $\Psi(y) = (1 \ \sqrt{2} y_1 \ \sqrt{2} y_2 \ \sqrt{2} y_1 y_2 \ y_1^2 \ y_2^2)^T \in \mathbb{R}^6$. Therefore, we can evaluate an inner product of vectors in $\mathcal{H}$ by computing a function of an inner product in $\mathbb{R}^2$. 


On the other hand, while the kernel method [7] is not in agreement either with Definition 2.1, it relaxes the assumptions iii) and iv) made by the K-DMD algorithm and to some extent satisfies Definition 2.2. Indeed, the inverse map \( \Psi^{-1} \) is learned by additional kernel regression steps in the sense of (regularized) minimum distance estimation, similar to (2.2) to some extent. The resulting reduced model is of the form (1.2)-(1.3), but still does not provide a diagonalised form like the targeted reduced system (2.3). This implies that the kernel method [7] is characterized by linear complexity in \( T \), and therefore does not fulfill Constraint 1.

3. A Generalized Kernel-Based Algorithm. We present in this section our algorithm called GK-DMD. The proposed method enables to compute the low-rank reduced model (2.3) for \( \mathcal{H} \) being a RKHS, with a complexity independent of \( \dim(\mathcal{H}) \) and \( T \) and is relieved from the assumptions made in K-DMD. As for K-DMD, the GK-DMD exploits the kernel-trick and resorts to an analogous computation of eigen-functions. Its main innovation in comparison to the latter state-of-the-art algorithm is that GK-DMD computes reduced model (2.3) based on the exact solution (2.5) of problem (2.1) and on the inverse definition (2.2). The GK-DMD algorithm, given in Algorithm 1 thus fulfills the definitions and constraint exposed in Section 2.1. It will be presented in detail in Section 3.2. In short, it consists of an off-line part, which computes a low-dimensional representation of \( A_k^* \), and an on-line part, which uses the latter to evaluate an approximate trajectory for a given initial condition.

3.1. Main results. The proposed algorithm is based on the following two original results:

- the right and left eigen-vectors of the optimal operator \( A_k^* \) belong to a low-dimensional sub-space of \( \mathcal{H} \), their low-dimensional representations are tractable and computed using the kernel function; this result is detailed in Section 3.1.1
- taking advantage of the fact that, in the reduced model (2.3), the inverse argument belongs to a low-dimensional subspace of \( \mathcal{H} \), the high-dimensional minimization problem reduces to a tractable \( p \)-dimensional optimization problem; this result is detailed in the section 3.1.2

3.1.1. Low-dimensional spectral representation of \( A_k^* \). Our algorithm relies on the following proposition. Its proof is detailed in Appendix [3]. This result extends the closed-form eigen-decomposition of operator \( A_{\text{edmd}}^m \) classically studied for EDMD (see e.g., [11, 23, 24, 27, 43]), to the spectral characterization of the low-rank operator \( A_k^* \) at the heart of the low-rank version of EDMD of interest to us, which has not been studied in the literature. Let \( \{\xi_i\}_{i=1}^k \) and \( \{\zeta_i\}_{i=1}^k \) denote the left and right eigen-vectors of \( A_k^* \) associated to its at most \( k \) non-zero eigen-values \( \{\lambda_i\}_{i=1}^k \).

**Proposition 3.1.** For \( i = 1, \ldots, k \), the left and right eigen-vectors of \( A_k^* \) and its eigen-values satisfy \( \xi_i = U_\Psi \xi_i \), \( \zeta_i = \hat{P}_k \hat{\zeta}_i \) and \( \lambda_i = \hat{\lambda}_i \), where \( \{\xi_i, \lambda_i\}_{i=1}^k \) and \( \{\zeta_i, \hat{\lambda}_i\}_{i=1}^k \) denote respectively the first \( k \) right eigen-vectors and eigen-values of the matrices in \( \mathbb{R}^{m \times m} \)

\[
R \Psi Y S_k^* R^* \quad \text{and} \quad S_k \Psi Y R^* R \Psi Y S_k^*,
\]

with \( R = \Sigma_\Psi V_\Psi \) and \( S_k = \text{diag}(a_1^2, \ldots, a_k^2, 0, \ldots, 0) V_Z^* \).

This proposition gives a closed-form decomposition for the \( \xi_i \)'s and the \( \zeta_i \)'s, the left and right eigen-vectors of the optimal solution \( A_k^* \) given in (2.5) and supplies the related eigen-values \( \lambda_i \)'s. The decompositions involve operator \( \hat{P}_k \) defined in (2.6) and
operator $U_{\Psi X}$ appearing in the short-hand notation of the SVD of $\Psi_X$. A consequence of this proposition is that parameters $\{\{\xi_i, \zeta_i, \lambda_i\}\}_{i=1}^k$ of reduced model (2.3) can be written in terms of their low-dimensional counterpart $\{(\bar{\xi}_i, \bar{\zeta}_i, \bar{\lambda}_i)\}_{i=1}^k$. We notice that the first $k$ left and right eigen-vectors of $A_k^*$ are normalized, i.e., that for $i = 1, \ldots, k$ the condition $\bar{\zeta}_i^* \bar{\xi}_i = 1$ stands, if $\bar{\zeta}_i^* E \bar{\xi}_i = 1$ with $E = S_k^* \Psi_Y \Psi_X R^*$. This normalization condition can be verified using some algebraic calculus. We ensure condition $\bar{\zeta}_i^* E \bar{\xi}_i = 1$ for $i = 1, \ldots, k$ by first computing the complex number $\gamma_i = \bar{\zeta}_i^* E \bar{\xi}_i$ and then rescaling the eigen-vector $\bar{\zeta}_i$ by $\gamma_i^{-1}$.

3.1.2. Kernel-based inversion for reduced modeling. The low-dimensional representation of eigen-vectors of $A_k^*$ provided in Proposition 3.1 constitutes an essential ingredient of the GK-DMD algorithm. However, to achieve the design of this algorithm, it remains to provide a feasible manner to evaluate the inverse map $\Psi^{-1}$ in (2.3), with the inverse map definition in (2.2). Once more, the idea consists in relying on the kernel trick in order to evaluate the inverse with a complexity independent of $\text{dim}(\mathcal{H})$. The following result shows that the sought reduced model boils down to solving a $p$-dimensional minimization problem involving scalar product in $\mathcal{H}$ evaluated thanks to the kernel-trick.

**Proposition 3.2.** For a symmetric positive definite kernel $h$, using the low-rank operator Definition 2.3 and the inverse map Definition 2.3, the reduced model (2.3) of the high-dimensional dynamics (1.1) solves at any point $\theta \in \mathbb{R}^p$

$$\tilde{x}_T(\theta) \in \arg \min_{x \in \mathbb{R}^p} \left( h(z, z) - 2 \sum_{i=1}^m g_i^T h(y_i, z) \right), \quad (3.2)$$

where $g_i^T = S_k^* (\bar{\zeta}_1 \cdots \bar{\zeta}_k) \left( \lambda_{T,1}^{T-1} \varphi_1(\theta) \cdots \lambda_{T,k}^{T-1} \varphi_k(\theta) \right)^\ast \in \mathbb{R}^m$ and where for $i = 1, \ldots, k$ the $i$th eigen-function is given by

$$\varphi_i(\theta) = \bar{\zeta}_i R \Psi_X \Psi(\theta). \quad (3.3)$$

The proof is provided in Appendix C.2. Sufficient conditions for the existence of minimizer (3.2) are provided and discussed for various kernel choices in Appendix C.3. A minimizer (3.2) can be computed (up to some accuracy) using standard optimization methods with a complexity independent of $\text{dim}(\mathcal{H})$ and of $T$, thus satisfying Constraint 1. Moreover, the gradient of the objective is in general closed-form, which enables the use of efficient large-scale optimization techniques such as limited memory quasi-Newton methods [32]. In this case, the complexity to compute the inverse is linear in $p$.

3.2. The GK-DMD algorithm. We begin by detailing the off-line computation. According to Proposition 3.1, the low-dimensional representation of the right and left eigen-vectors, and the associated eigen-values of the optimal operator $A_k^*$ are obtained by eigen-decomposition of matrices given in (3.1). As detailed hereafter, the first five steps of the algorithm precisely compute this low-dimensional representation. Relying on the kernel function, step 1 first computes the inner products in $\mathcal{H}$ needed to build matrices $\Psi_X \Psi_X, \Psi_Y \Psi_Y, \Psi_Y \Psi_X$ in $\mathbb{R}^{m \times m}$. In steps 2 and 3, the matrices $R$ and $S_k$ in $\mathbb{R}^{m \times m}$ are obtained by eigen-decomposition of $\Psi_X \Psi_X$ and $Z^\ast Z$ belonging also to $\mathbb{R}^{m \times m}$. These three first steps enable to obtain matrices given in (3.1) by simple matrix products. Step 4 of the algorithm computes the right and left
Algorithm 1: GK-DMD

**Off-line.**

*Inputs:* \( x_{\text{learn}} \)’s

1) Compute matrices \( \Psi^*X \Psi, \Psi_Y \Psi_Y, \Psi^*Y \Psi_X \) in \( \mathbb{R}^{m \times m} \) with the kernel trick.
2) Compute \( (V \Psi_X, \Sigma \Psi_X) \) by eigen-decomposition of \( \Psi^*X \Psi \).
3) Compute \( (V \Psi_Z, \Sigma \Psi_Z) \) by eigen-decomposition of \( Z^*Z \) with \( Z \) given by (2.7).
4) Compute the two matrices given in Proposition 3.1 and compute their eigen-vector/eigen-value couples \( \{ (\tilde{\xi}_i, \tilde{\lambda}_i) \}_{i=1}^k \) and \( \{ (\tilde{\zeta}_i, \tilde{\lambda}_i) \}_{i=1}^k \).
5) Rescale each right eigenvector \( \tilde{\zeta}_i \) by factor \( \frac{\tilde{\zeta}_i^*E \tilde{\xi}_i}{\tilde{\zeta}_i^*E \tilde{\xi}_i - 1} \) with \( E = \sum_k \Psi_Y \Psi_X R^* \).

*Outputs:* \( R, S_k, \tilde{\xi}_i \)’s, \( \tilde{\zeta}_i \)’s and \( \tilde{\lambda}_i \)’s

**On-line.**

*Inputs:* off-line outputs and \( \theta \)

6) Compute \( \Psi^*X \Psi(\theta) \) in \( \mathbb{R}^m \) with the kernel trick.
7) Compute eigen-functions \( \{ \phi_i(\theta) \}_{i=1}^k \) defined in (3.3).
8) Compute \( \tilde{x}_T(\theta) \) solving (3.2);

*Output:* \( \tilde{x}_T(\theta) \).

eigen-vectors and the associated eigen-values of matrices given in (3.1). Step 5 finally normalizes the latter eigen-vectors, as detailed in Section 3.1.1.

In the on-line part of the algorithm, the low-dimensional representation given by the outputs of the off-line part is exploited to compute the reduced model output \( \tilde{x}_T(\theta) \), for a given initial condition \( \theta \). As discussed in Section 3.1.2 the computation of \( \tilde{x}_T(\theta) \) is obtained by solving the \( p \)-dimensional optimization problem (3.2). The objective function of this problem depends on kernel functions weighted by the \( m \)-dimensional coefficient vector \( g_{\theta,T} \) defined in Proposition 3.2. This vector depends itself on the low-dimensional representation of operator \( A^a_k \) computed in the off-line part and on the eigen-functions \( \{ \phi_i(\theta) \}_{i=1}^k \). These eigen-functions are obtained in steps 6 and 7 of the algorithm: step 6 uses the kernel trick to compute the \( m \)-dimensional vector \( \Psi^*_X \Psi(\theta) \) while step 7 deduces the eigen-functions (3.3) using the low-dimensional representation. With these eigen-functions, we then compute the vector component \( g^\theta_T \) weighting the kernel function \( h(y_i, z) \) in the objective function of (3.2). Step 8 finally solves this optimization problem and provides the reduced model \( \tilde{x}_T(\theta) \).

3.3. Performance analysis. In this section, we begin by analyzing the advantage of the GK-DMD algorithm in terms of computational complexity and then show that the approximation error is optimal in some sense in the RKHS. Moreover, we show that the norm of the learning approximation error is tractable without any increase of the algorithm complexity.

3.3.1. Complexity. Assuming a complexity \( O(p) \) for the evaluation of the kernel function\(^6\) and the overall complexity of the proposed algorithm scales in \( O(m^3 + m^2p) \), just as for K-DMD, as detailed in Appendix A. More precisely, in the off-line part, eigen-decompositions (involving step 2, 3 and 4) are computed\(^7\) in \( O(m^3) \), while the kernel evaluations (step 1) and the rescaling (step 5) are respectively done in \( O(m^2p) \).

---

\(^6\)This property is true for most standard kernels, e.g., polynomial or Gaussian kernels \([4]\).

\(^7\)In the case of large \( m \), randomized algorithms for low-rank matrix approximation can significantly reduce the cubic complexity of the proposed kernel method \([2, 40, 44]\).
and $O(m^2 k)$, with $k \leq m \leq p$. We remark that those off-line complexities are independent of $T$ thanks to the diagonalization of $A^*_t$, and independent of $\dim(H)$ due to the use of the kernel-trick in the first and last steps of the algorithm.

Reduced modeling is very concerned by the on-line computational cost, i.e., complexity of computation steps depending on the input $\theta$. As typically $k \ll p$, GK-DMD is attractive by its on-line complexity in $O(m^2 k + mp)$, thus it scales linearly with respect to the dimension of the reduced model $k$ or the ambient dimension $p$, in comparison to $O(m^2 p)$ operations for K-DMD. Indeed, the matrix-vector product $\Psi_X^* \Psi(\theta)$ (step 6) and the inversion (step 8) are both computed in $O(pm)$ operations using standard optimization tools, while eigen-functions (step 7) require $O(m^2 k)$ operations.

Note that, as well as being constant in $T$ and $\dim(H)$, the complexity characterizing the reduced dynamics in GK-DMD is of complexity $O(m^2 k)$. It is thus also constant with respect to the dimension of the ambient space $p$, which is a standard desired feature for reduced models. Note that the initialization or the final reconstruction step of any reduced model will involve at least $p$ operations. In the case of GK-DMD, the mapping from the initial state (living in the ambient space of dimension $p$) to the reduced space (in step 6) or the inverse mapping from the reduced space to the ambient space (in step 8) are computed in $O(mp)$.

3.3.2. Learning accuracy. The learning error of our GK-DMD algorithm is optimal in the sense it is equal to the minimal Hilbert-Schmidt norm of the error achievable in the RKHS for the minimization problem \cite{16}. The norm of this optimal error, given by a generalization of \cite[Theorem 4.1]{16} to separable infinite-dimensional Hilbert spaces, is closed-form

$$\|\Psi_Y - A^*_t \Psi_X\|_{HS}^2 = \sum_{i=1}^{m} (\sigma^2 Z)_i^2 + \sum_{i=1}^{i^*} \sum_{j=1}^{m} (\sigma^2 Y)_j^2 \left((v^*_Y)^* u^*_X\right)^2,$$  \hspace{1cm} (3.4)

with $i^* = \text{rank}(\Psi_X) + 1$ \cite{15}.

Moreover, it is worth noticing that the optimal error norm \cite{3.4} is tractable. It possibly involves a little extra computation which does not increase the complexity of Algorithm \cite{1}. More precisely, we notice that the left singular vectors $\{v^*_X\}_{i=1}^m$ and $\{v^*_Z\}_{i=1}^m$ respectively of $\Psi_X$ and $Z$ and their associated singular values $\{\sigma^2 Y\}_{i=1}^m$ and $\{\sigma^2 Z\}_{i=1}^m$ have been precomputed in step 2) and 3) of the algorithm. We distinguish the two following cases depending on the value of $i^*$, which equals to the number of non-zero singular values in the set $\{\sigma^2 Y\}_{i=1}^m$ plus one.

- If $i^* = m + 1$, i.e., $\Psi_X$ is full rank, the second term on the right-hand side vanishes, and the error norm is directly computable.
- Otherwise, in order to evaluate the error norm, we need to make the extra computation of the left singular vectors $\{v^*_Y\}_{i=1}^m$ and singular values $\{\sigma^2 Y\}_{i=1}^m$ of $\Psi_Y$. They are obtained by eigen-decomposition of matrix $\Psi_Y^* \Psi_Y \in R^{m \times m}$, precomputed using the kernel trick in step 1) of the algorithm. This additional eigen-decomposition will involve a complexity in $O(m^3)$, i.e., preserves the global algorithm complexity in $O(m^3(m + p))$.

4. Numerical Simulations. In this section, we assess four data-driven reduced modeling methods for the approximation of two high-dimensional systems.

4.1. Experimental setup. Our benchmark consists of the four following algorithms:
• low-rank DMD (LR-DMD) \[16\], Algorithm 3,
• total-least-square DMD (TLS-DMD) \[19\],
• kernel-based DMD (K-DMD) \[43\],
• the proposed generalized kernel DMD (GK-DMD), i.e., Algorithm 1.

For the K-DMD and GK-DMD algorithms, we use a quadratic polynomial kernel or a Gaussian kernel with a standard deviation of 10 \[6\]. Details on these kernels are provided in Appendix C.4. The table below summarizes the off-line and on-line complexities of the different algorithms.

|                | LR-DMD                  | TLS-DMD                  | K-DMD                  | GK-DMD                  |
|----------------|-------------------------|--------------------------|------------------------|-------------------------|
| off-line       | \(\mathcal{O}(m^2(m+p))\) | \(\mathcal{O}(m^2(m+p))\) | \(\mathcal{O}(m^2(m+p))\) | \(\mathcal{O}(m^2(m+p))\) |
| on-line        | \(\mathcal{O}(pk)\)     | \(\mathcal{O}(Tpm)\)    | \(\mathcal{O}(pm^2)\)  | \(\mathcal{O}(pm + m^2k)\) |

**Table 4.1**

Off-line and on-line complexities of reduced modeling algorithms. We recall that \(p\) is the ambient state dimension, \(k\) is the reduced model dimension, \(T\) is the predicted trajectory length and \(m\) is the size of the training data set.

These algorithms are used to approximate two high-dimensional systems.

• A Rayleigh-Bénard convection \[9\] model, which is a standard benchmark in meteorology for the evolution of vorticity and temperature fields. Convection is driven by two coupled non-linear partial differential equations.

• A divergence-free fractional Brownian motion (fBm) evolution model, which is inspired by the turbulence phenomenology. The aim is to assess the ability of reduced modeling methods to capture the non-linear dynamics and the precise fractal structure of eddies.

A precise description of these high-dimensional systems, together with details on the experimental setting used in our numerical simulations, are provided below.

**Rayleigh-Bénard convection.** Rayleigh-Bénard convection \[9\] is a standard benchmark model in meteorology. Convection is driven by two coupled partial differential equations. Let \(\nabla = (\partial_{s_1}, \partial_{s_2})^*\), \(\nabla^\perp = (\partial_{s_2}, -\partial_{s_1})^*\) and \(\Delta = \partial^2_{s_1} + \partial^2_{s_2}\) denote the gradient, the curl and the Laplacian with respect to the two spatial dimensions \((s_1, s_2)\). Boundary conditions are 1-periodic along \(s_1\) and of Dirichlet type\[9\] on \(s_2\). At any point of the unit cell \(s = (s_1, s_2) \in [0, 1]^2\) and for any time \(t \geq 1\), the temperature \(\tau(s, t) \in \mathbb{R}\), the vorticity \(b(s, t) \in \mathbb{R}\) and the velocity \(v(s, t) \in \mathbb{R}^2\) in the cell satisfy

\[
\begin{align*}
\partial_t b(s, t) + v(s, t)^* \nabla b(s, t) - Pr \Delta b(s, t) - Pr Ra \partial_{s_1} \tau(s, t) = 0, \\
\partial_t \tau(s, t) + v(s, t)^* \nabla \tau(s, t) - \Delta \tau(s, t) - \partial_{s_1} \Delta^{-1} b(s, t) = 0,
\end{align*}
\]

where velocity is related to vorticity according to \(v(s, t) = \nabla^\perp \Delta^{-1} b(s, t)\), and where \(\Delta^{-1}\) represents the inverse of \(\Delta\) defined in the Fourier domain. We set the Rayleigh number to \(Ra = 1.5e5\) and the Prandtl number to \(Pr = 1.0e1\). We use a Runge-Kutta fourth-order time discretization. For spatial discretization, we use a Fourier-based implementation of spatial derivatives except for the advection term for which we use a second-order finite difference scheme. For time-integration of the dynamic model, we use a time step of \(1e-4\). We obtain a discrete system of the form of \([1, 1]\) with \(x_t = (b_t, \tau_t)^* \in \mathbb{R}^p\), and \(p = 4096\), where \(b_t\’s\) and \(\tau_t\’s\) are spatial discretizations on a grid of size \(64 \times 32\) of vorticity and temperature fields at time \(t\). In our experiments, we assume that the initial condition belongs to the Lorenz attractor \([22]\). The initial state is of the form \(b(s, 1) = \kappa b \sin(a_s s_1) \sin(\pi s_2), \tau(s, 1) = \kappa \tau_0 \cos(a_s s_1) \sin(\pi s_2) - \kappa \tau_0 \sin(2\pi s_2),\)

\[\text{In order to simplify the Fourier-based numerical implementation of the model, we will assume periodicity for the discretised system in the two spatial directions.}\]
with the parameter vector \((a_b, a_\tau, \kappa_b, \kappa_{\tau_1}, \kappa_{\tau_2})\) \(\in \mathbb{R}^5\). In our experiments, we sample parameters to generate the training and test data sets using a uniform distribution on the hyper-cube \((a_b, a_\tau, \kappa_b, \kappa_{\tau_1}, \kappa_{\tau_2}) \in [0, 0.1]^5\).

**Divergence-free fractional Brownian motion evolution.** A simple model inspired by the turbulence phenomenology is proposed to evaluate the capability of reduced modeling methods. The states are discrete motion fields defined on a square grid satisfying \((1.1)\) with the quadratic model

\[
f(x_t) = (x_{t-1} + 1)^2 + \alpha L x_{t-1} - 1,
\]

where the square power is taken component-wise, the diffusion coefficient is \(\alpha = 0.5\) and \(L \in \mathbb{R}^{p \times p}\) is a second-order finite difference approximation of the (bi-variate) two-dimensional Laplacian operator. Initial states used to generate the training and test data sets are samples from a bi-dimensional divergence-free fractional Brownian motion (fBm) field of Hurst exponent \(1/3\). The ambient dimension is set to \(p = 512\) and the size of the square grid is set \(16 \times 16\). The fBm vector fields are parametrized according to the fractional wavelet representation proposed in [18, Proposition 3.1], using 18 random coefficients drawn according to a normal law.

Note that the complexity of evaluating a trajectory using these high-dimensional systems is generally of the order of \(O(p T (\delta t)^{-1})\), where \(\delta t\) represents the unit time discretization step. To obtain a stable simulation, \(\delta t\) often has to be very small, which makes trajectory evaluation very demanding. The on-line complexity \(O(pm + m^2 k)\) offered by GK-DMD for approximating a trajectory is very attractive in this context. For example, in our Rayleigh-Bénard convection framework \((p=4096, m=90, T=10, \delta t = 1e-4)\), the complexity gain provided by GK-DMD is for any \(k \leq m\) of more than two orders of magnitude.

### 4.2. Evaluation criteria

We study the evolution with respect to the rank \(k\) of the

- **reconstruction error**
  
  \[
  \epsilon_{\text{rec}} = \left( \sum_{j=1}^{N} \sum_{t=1}^{T-1} \frac{\| \hat{x}_2(x_t(\theta_j)) - x_{t+1}(\theta_j) \|_2^2}{\| x_{t+1}(\theta_j) \|_2^2} \right)^{1/2},
  \]

  for a set of initial conditions \(\{\theta_j\}_{j=1}^{N}\) where \(N\) is given (which differ from the set of initial conditions \(\{\theta_j^{\text{learn}}\}_{j=1}^{N_{\text{learn}}}\) used for training); it measures the overall discrepancy between the true state \(x_{t+1}(\theta_j)\) at time \(t + 1\) and the approximated state \(\hat{x}_2(x_t(\theta_j))\) predicted with the reduced model from the true state at time \(t\) for \(t = 1, \ldots, T - 1\);

- **learning error**
  
  \[
  \epsilon_{\text{learn}} = \left( \sum_{j=1}^{N_{\text{learn}}} \sum_{t=1}^{T_{\text{learn}}-1} \frac{\| \hat{x}_2(x_t(\theta_j^{\text{learn}})) - x_{t+1}(\theta_j^{\text{learn}}) \|_2^2}{\| x_{t+1}(\theta_j^{\text{learn}}) \|_2^2} \right)^{1/2};
  \]

  it measures the overall discrepancy between the state \(x_{t+1}(\theta_j^{\text{learn}})\) and the prediction \(\hat{x}_2(x_t(\theta_j^{\text{learn}}))\) at time \(t\) for \(t = 1, \ldots, T_{\text{learn}} - 1\); it reveals the capability of the reduced model to approximate the training data used during the learning stage.
Rayleigh-Bénard convection

We mention that a small learning error $\epsilon_{\text{learn}}$ will not necessarily yield a small reconstruction error $\epsilon_{\text{rec}}$. A small $\epsilon_{\text{learn}}$ may be related to model overfitting. The learning error will nonetheless help to understand the behavior of the different methods.

The size of the training data is set to $m = 90$ for the two high-dimensional systems. The experimental setup is as follows.

- For the Rayleigh-Bénard convection model, $10$ initial conditions $\theta_{\text{learn}}^j$ are sampled from a uniform distribution on a hyper-cube in $\mathbb{R}^5$ parametrizing solutions of the Lorenz attractor [29]. Then using $\theta_{\text{learn}}^j$ to initialize the dynamic model, we compute trajectories for $t = 1, \ldots, 10$ (resulting in 100 states $x_t(\theta_{\text{learn}}^j)$). Examples of $x_t(\theta_{\text{learn}}^j)'s$ are displayed in Figure 4.1. We design the test data in order to evaluate the capability of the reduced models to perform predictions for the Rayleigh-Bénard convection model, which is known to be chaotic [9, 29]. Therefore, we set the test data as the prolongation of the training data trajectories: the 10 initial conditions are $\theta_j = x_{10}(\theta_{\text{learn}}^j)$ and trajectories $x_t(\theta_j)$ for $t = 1, \ldots, 10$ are computed in the same way as for the training data set.

- For the divergence-free fBm evolution model, $100$ noisy fBms vector fields $\theta_{\text{learn}}^j$ are used as initial conditions. More precisely, fBms vector fields are drawn using the wavelet representation proposed in [18, Proposition 3.1] with 18 fractional wavelet coefficients and then corrupt by a weak additional Gaus-
4.3. Results.

4.3.1. Analysis of accuracy vs. rank of approximation. The reconstruction error $\epsilon_{\text{rec}}$ is evaluated as a function of the reduced model dimension for the approximation of the two high-dimensional systems. Plots comparing the four algorithms are presented in Figure 4.2 and Figure 4.3 respectively for the Rayleigh-Bénard convection and for the divergence-free fBm evolution. Overall, we observe that GK-DMD outperforms almost everywhere the other methods.

Rayleigh-Bénard convection. We first discuss the results shown in Figure 4.2 for the Gaussian kernel. While K-DMD and GK-DMD perform similarly for $k \geq 18$, GK-DMD exhibits for $k < 18$ a clear gain in accuracy compared to the other methods reaching almost an order of magnitude. The gain in accuracy between GK-DMD and K-DMD may be due to the fact that GK-DMD computes exactly the reduced model (2.3), and in particular considers the low-rank solution $A_k^*$ instead of the truncated least square solution $\hat{A}_k$. Besides, as $\text{rank}(\Psi_x^T \Psi_x) = m$, i.e.,
operator $\Psi_X$ is full-rank, similar performances of the two kernel-based methods in the case where $k \geq 18$ can be explained by the fact that the low-rank constraint becomes inactive (implying that $\hat{A}_k^{(s)} = A_k^{(s)}$), $\Psi^{-1}$ is well approximated by a linear mapping and furthermore the $\Psi^{-1}\zeta_j$’s are well represented in the span of $Y$. A lower value on the accuracy is reached around $k$ slightly greater than 5, suggesting that the reduced model can explain up to 5 components in $\mathcal{H}$. This lower bound on the error shows that the snapshots used for training have redundant information in $\mathcal{H}$ about the Rayleigh-Bénard convection system and are insufficient to represent the wide variety of trajectories belonging to the solution manifold. Similar results are obtained with a polynomial kernel. Nevertheless, for K-DMD and GK-DMD, the reconstruction error is higher with polynomials than for Gaussian kernels, revealing that their performance is kernel-dependent. The problem of the kernel choice, and more generally the inference of a relevant mapping $\Psi$, is an open question out of the scope of this paper. We refer the interested reader to recent works on this issue [30, 45].

Additionally, the reconstruction errors of GK-DMD, LR-DMD and TLS-DMD are comparable for $k < 4$. However, for larger values of $k$, the performance of non-linear methods is much better: the error gain brought about by the use of kernels reaches around 93% for the Gaussian kernel and 73% for the polynomial kernel. More precisely, the accuracy of LR-DMD and TLS-DMD reaches a lower bound around $k \simeq 4$ and then deteriorates as $k$ increases or reaches an asymptote, suggesting data overfitting. This undesirable effect will be discussed in the numerical experiences of Section 4.3.3.

Divergence-free fBm evolution. We now turn to the reduction of our simplified turbulence model. Results shown in Figure 4.3 are in agreement with observations made in the case of the Rayleigh-Bénard convection. In particular the gain in accuracy in comparison to state-of-the-art methods reaches a peak of more than an order of magnitude at $k = 89$. However, we can point out two important differences with the previous results shown in Figure 4.2. First, while the GK-DMD error is a monotonic strictly decreasing function with respect to the dimension $k$, K-DMD has a plateau up to $k \sim 20$ and then is chaotic before reaching the GK-DMD performance near the point $k = m$. The conclusion that can be drawn is that GK-DMD provides a preferable reduced model, in the sense that approximation becomes increasingly accurate as $k$ grows. Second, LR-DMD and TLS-DMD operate in a very similar way as GK-DMD up to $k \sim 40$, but the accuracy of these methods deteriorates considerably as $k$ increases. As already observed for the Rayleigh-Bénard model, overfitting at the learning stage is likely to be the explanation to this performance loss of these state-of-the-art algorithms. This issue is further discussed in Section 4.3.3. Finally, we can also note the continuous decrease of the error with $k$, even if it is slow, which suggests that the snapshots used for training better represent the solution manifold than for the Rayleigh-Bénard system.

4.3.2. Analysis of error maps. To complement the quantitative evaluation performed in Section 4.3.1, we proceed to the visual inspection of the spatial distribution of the error. Error maps are shown in Figure 4.4 and Figure 4.5. Figure 4.4 displays the absolute vorticity of the bi-variate error field $\tilde{x}_2(\theta) - x_2(\theta)$ defined over the bi-dimensional grid, where $\tilde{x}_2(\theta)$ denotes the approximation provided by the algorithms for a given initial condition $\theta$. Error maps are displayed for increasing value of the dimension $k$. The distribution of the error produced by K-DMD in Figure 4.4 reveals that its chaotic behavior for $k < 15$ is caused by the occurrence of errors at large scales. Error maps obtained with the LR-DMD and TLS-DMD algorithms
Fig. 4.4. Reconstruction error maps of the different reduced models for increasing value of \( k \). The image above represents the absolute vorticity field \( x_2(\theta) \), while each image in the table below represents the absolute vorticity of the bi-variate field \( \tilde{x}_2(\theta) - x_2(\theta) \), for a typical initial condition \( \theta \).

| \( k = 5 \) | \( k = 10 \) | \( k = 15 \) | \( k = 20 \) |
|-------------|-------------|-------------|-------------|
| LR-DMD      |             |             |             |
| TLS-DMD     |             |             |             |
| K-DMD       |             |             |             |
| GK-DMD      |             |             |             |

Fig. 4.5. Reconstruction errors maps of the different ROM approximations for \( k = 70 \). The vector field at upper left corner is related to the snapshot \( x_2(\theta) \) for a typical initial condition \( \theta \), while other vector fields enlarged at scale 20:1 are related to the reconstruction error \( \tilde{x}_2(\theta) - x_2(\theta) \) superimposed on the maps of the absolute error \( |\tilde{x}_2(\theta) - x_2(\theta)| \).

are very similar. Moreover they seem not to evolve significantly as \( k \) increases, except for high frequency appearing at \( k \geq 10 \). The error maps for GK-DMD show that the decrease in error with respect to \( k \) is related to refinements occurring at increasingly finer scales. Interestingly, the simplified turbulence model confirms this scale analysis.
of errors. In Figure 4.5 we observe that the large vortices of the flow are correctly approximated by GK-DMD for $k = 70$. By contrast, GK-DMD does not reconstruct accurately less energetic small vortices of the divergence-free fBm. Although TLS-DMD produces a reasonable error, we remark that TLS-DMD and LR-DMD clearly fail at identifying some of the large structures of the flow. The inspection of error maps produced by K-DMD reveal large errors at all scales, and its inaccuracy for reduced modeling of the fractal structure of turbulence.

4.3.3. Robustness to overfitting. We pointed out in the previous analysis that LR-DMD and TLS-DMD might be prone to overfitting, while kernel methods seem to be more robust. We now discuss this point by evaluating the learning error $\epsilon_{\text{learn}}$ as a function of the reduced model dimension $k$ for the approximation of Rayleigh-Bénard convection. Curves illustrating the learning error attained by the four algorithms are presented in Figure 4.6.

The plot of Figure 4.6 shows that LR-DMD, TLS-DMD or GK-DMD perform good and similarly in terms of learning error up to $k \sim 7$ (while K-DMD fails completely). From then, the learning error is continuously reduced as $k$ grows by LR-DMD and TLS-DMD, while GK-DMD reaches an asymptote (the same as K-DMD from $k = 17$). We point out that the gain of LR-DMD and TLS-DMD compared to GK-DMD reaches more than five orders of magnitude at $k = 50$. Noticing that, on the contrary to this continuous decrease of the learning error, the reconstruction error of LR-DMD and TLS-DMD in Figure 4.2 stagnates for $k \geq 7$, we conclude that these methods overfit the training samples. The observed robustness of GK-DMD and K-DMD in our experiments is in accordance with empirical results obtained for K-DMD in [43]: in their numerical simulations the authors showed that immersing the dynamics in the high-dimensional space $\mathcal{H}$ enhanced the eigen-values estimates by lowering their variance and discarding neglectible ones.

4.3.4. Robustness to noise. We assess the robustness of the reduced models by evaluating the learning error $\epsilon_{\text{learn}}$ in the noiseless case or in the case of an additive Gaussian noise of increasing variance. We consider the approximation of Rayleigh-Bénard convection. Figure 4.7 presents the learning error as a function of the reduced model dimension. We observe that performances of kernel-based methods, and par-
particularly GK-DMD, seem to be weakly sensitive to the power of the additive noise. On the contrary, we remark a significant increase of the learning error for LR-DMD or TLS-DMD in the presence of noise. This deterioration is accentuated by the noise power. However, comparing the curves in Figure 4.2 and Figure 4.7 we notice that the reconstruction error $\epsilon_{\text{rec}}$ of LR-DMD and TLS-DMD is lower in the presence of noise, and thus that an additive noise in the learning phase increases the prediction capabilities of these two reduced models. This behavior is likely to be the consequence of overfitting. On the contrary, in the case of a noisy setting, the analysis of the reconstruction error confirms that the reduced model learned by GK-DMD is relevant for prediction. In particular, results in Figure 4.7 are consistent with those obtained in a noiseless setting in Figure 4.2. In particular, GK-DMD outperforms in terms of accuracy the other methods for $k \leq 16$.

5. Conclusions. This work presents a data-driven algorithm for the tractable approximation of a linear low-rank operator characterizing dynamics embedded in a RKHS. Taking advantage of the reproducing kernel property, the algorithm computes off-line a low-dimensional spectral representation of the solution of a low-rank constrained optimization problem, and then solves on-line a minimum distance problem which yields the sought approximation. By contrast to existing algorithms, the proposed reduced model exhibits a low computational complexity and requires mild
identifies the underlying assumption that $\Psi^{-1}$ is linear (assumption iii). In steps 7), K-DMD identifies the $\mu_j$’s as the minimizers in $C^p$ of the square of the $\ell_2$-norm of the reduced model error $\|x_{t+1}(\theta^{\text{learn}}) - \sum_{j=1}^{m} \mu_j \langle \xi_j, \Psi(x_t(\theta^{\text{learn}})) \rangle \|_2^2$ for any data pair $(x_t(\theta^{\text{learn}}), x_{t+1}(\theta^{\text{learn}}))$ satisfying (1.13). The authors thus implicitly assume that the eigen-modes belong to a sub-space in the span of $\Psi^{-1}$ (assumption iv). We notice that by using (3.3), where $\Psi(\theta)$ is substituted by $\Psi(x_t(\theta^{\text{learn}}))$ for $i \in 1, \ldots, N_{\text{learn}}$ and $j \in 1, \ldots, T_{\text{learn}} - 1$, we have for $i = 1, \ldots, m$ that

$\langle (\xi_i, \Psi(x_1(\theta^{\text{learn}}))), \ldots, (\xi_i, \Psi(x_{T_{\text{learn}}-1}(\theta^{\text{learn}}))) \rangle_{\mathcal{H}} = \xi_i^* \sum_{j=1}^{m} \mu_j \lambda_j \xi_j^* \Psi(x_{T_{\text{learn}}-1}(\theta^{\text{learn}})) \|_{\mathcal{H}}^2$.

The estimated $\hat{\mu}_j$’s are thus rewritten as the solution of

$$\arg \min_{\mu_1, \ldots, \mu_m} \| Y - (\mu_1 \cdots \mu_m) \text{diag}(\hat{\lambda}_1 \cdots \hat{\lambda}_m) (\hat{\xi}_1 \cdots \hat{\xi}_m)^* \sum_{j=1}^{m} \mu_j \lambda_j \xi_j^* \Psi(x_t(\theta^{\text{learn}})) \|_{\mathcal{H}}^2, $$
where we remark that the Hilbert-Schmidt norm \( \| \cdot \|_{HS} \) boils down here to the Frobenius norm of a matrix in \( \mathbb{R}^{p \times m} \). A minimizer of this least-square optimization problem is

\[
(\hat{\mu}_1, \ldots, \hat{\mu}_m) = \mathbf{Y} R^* ((\hat{\xi}_1, \ldots, \hat{\xi}_m)^*)^\dagger \text{diag}(\hat{\lambda}_1^\dagger, \ldots, \hat{\lambda}_m^\dagger).
\]  

Finally, using the identification \( \{\lambda_i = \hat{\lambda}_i\}_{i=1}^k \), the \( k \) first eigen-modes estimates \( \{\hat{\mu}_i\}_{i=1}^k \) in \( \mathbf{A} \) with the \( \varphi_i(\theta) \)'s given by \( \{3.3\} \) fully parametrize \( \{2.4\} \), yielding the approximation \( \hat{x}_T(\theta) = \sum_{i=1}^k \hat{\lambda}_i^{-1} \varphi_i(\theta) \hat{\mu}_i \).

The suitability of K-DMD for reduced modeling is weak in the case \( k < m \) and \( p \gg 1 \). Indeed, we can show that the computation burden to compute the approximation is independent of the reduced model dimension \( k \), but requires \( m^2 \) vector operations in \( \mathbb{R}^p \). More precisely, the overall complexity of the K-DMD algorithm may be divided in an on-line and off-line part, defined as the complexity of the steps respectively independent or not of the initial condition \( \theta \) we want to evaluate. We observe that the off-line part requires \( O(m^2(m + p)) \) operations to compute the matrix products in step 1, the eigen-decompositions in steps 2) and 3) and the pseudo-inversion in step 4), while the on-line part requires \( O(pm^2) \) operations to compute the least-square solution in step 7). Thus the on-line computation is lighter than the off-line one but the complexity is in \( O(pm^2) \) whatever the reduced model dimension. A consequence is that the lower \( k \), the higher the ratio complexity/accuracy, which is obviously not a desirable property for reduced modeling.

Appendix B. Proof of Proposition 3.1

Let

\[
\hat{A}_{t,k} = (R \Psi^* \Psi \quad \mathbf{S}_k^* \mathbf{S}_k \quad \Psi^* \Psi \mathbf{R}^* \quad R \Psi^* \Psi \quad \mathbf{S}_k^*), \quad \hat{A}_{r,k} = \mathbf{S}_k \Psi^* \Psi \mathbf{R}^* \quad R \Psi^* \Psi \quad \mathbf{S}_k^*.
\]

We begin by proving that the \( \mathbf{U}_k \xi_i \)’s are right eigen-vectors of \( \hat{A}_k^* \). We verify after some algebraic manipulations that \( \mathbf{U}_k \xi_i \hat{A}_k = \hat{A}_{t,k} \xi_i \). Then, as \( \mathbf{U}_k \xi_i \) is unitary we have \( (\hat{A}_k)^* \mathbf{U}_k \xi_i = \mathbf{U}_k \xi_i \hat{A}_k^* \), and in particular \( (\hat{A}_k)^* \mathbf{U}_k \xi_i = \mathbf{U}_k \xi_i \hat{A}_k^* \xi_i \). Exploiting the fact that \( (\hat{\xi}_i, \hat{\lambda}_i) \) are eigen-vectors and eigen-values of \( \hat{A}_{t,k} \), we obtain for \( i = 1, \ldots, k \) the sought result: \( (\hat{A}_k)^* \mathbf{U}_k \xi_i = \hat{\lambda}_i \mathbf{U}_k \xi_i \).

We continue by showing that the \( \hat{P}_k \xi_i \)’s are right eigen-vectors of \( \hat{A}_k \). From the definition of \( \hat{A}_k \) and \( \hat{A}_{r,k} \) we obtain \( \mathbf{P}_k^* \hat{A}_k^* \hat{P}_k = \hat{A}_{r,k} \). Then, \( \hat{P}_k \xi_i \) is a right eigen-vector of \( \hat{A}_{r,k} \), which can be rewritten as \( \hat{A}_k^* \hat{P}_k = \hat{P}_k \hat{A}_{r,k} \), since matrix \( \hat{P}_k \hat{P}_k^* \) is idempotent and \( \hat{P}_k \hat{P}_k^* \hat{A}_k = \hat{P}_k \hat{P}_k^* \hat{P}_k \Psi \Psi \mathbf{X} = \hat{A}_k \). Because \( \xi_i \) are eigen-vectors of \( \hat{A}_{r,k} \), we deduce for \( i = 1, \ldots, k \) the sought result: \( \hat{A}_k^* \hat{P}_k \xi_i = \hat{\lambda}_i \hat{P}_k \xi_i \). \( \square \)

Appendix C. Inverse mapping.

C.1. Extended definition. In this section, we first show that their exists an implicit definition of the inverse mapping for any element of the subset \( \mathcal{S} = \{ x \in \mathcal{H} : x = \Psi(y), y \in \mathbb{R}^p \} \subseteq \mathcal{H} \), where we recall that \( \mathcal{H} \) is a RKHS characterized by the reproducing kernel

\[
\forall (y, z) \in \mathbb{R}^p \times \mathbb{R}^p, \quad b(y, z) = \langle \Psi(y), \Psi(z) \rangle_\mathcal{H}.
\]

We then propose an extension of this definition for any element of \( \mathcal{H} \).

First, let us show that the inverse of any \( \eta \in \mathcal{S} \), \( \Psi^{-1}(\eta) \) is implicitly defined as the unique element of \( \mathbb{R}^p \) given by

\[
(\hat{\mu}_1, \ldots, \hat{\mu}_m) = \mathbf{Y} R^* ((\hat{\xi}_1, \ldots, \hat{\xi}_m)^*)^\dagger \text{diag}(\hat{\lambda}_1^\dagger, \ldots, \hat{\lambda}_m^\dagger).
\]
\[ \Psi^{-1}(\eta) = \arg \max_{z \in \mathbb{R}^p} \frac{\langle \eta, \Psi(z) \rangle_H}{\|\Psi(z)\|_H}. \quad (C.2) \]

Indeed, the positive-definiteness of the kernel \( h \) implies that we have for any \( y, z \in \mathbb{R}^p \)

\[
\det \begin{pmatrix} h(y, y) & h(y, z) \\ h(z, y) & h(z, z) \end{pmatrix} \geq 0,
\]

and the lower bound is reached if and only if \( y = z \). Using the kernel symmetry, this is equivalent to

\[
\frac{h(y, z)^2}{h(y, y)h(z, z)} \leq 1,
\]

and, according to \( (C.1) \), it follows that

\[
\frac{\langle \Psi(y), \Psi(z) \rangle_H^2}{\|\Psi(y)\|_H^2 \|\Psi(z)\|_H^2} \leq 1,
\]

for any \( y, z \in \mathbb{R}^p \) where the upper bound is reached if and only if \( y = z \). \( (C.3) \) then implies definition \( (C.2) \).

Then, as proposed in \( (2.2) \), we extend definition \( (C.2) \) holding for elements of \( S \) to any \( \eta \) in \( H \) (i.e., including elements outside \( S \)), as an element \( \Psi^{-1}(\eta) \) of \( \mathbb{R}^p \) satisfying

\[
\Psi^{-1}(\eta) \in \arg \min_{z \in \mathbb{R}^p} \|\eta - \Psi(z)\|_H.
\]

The definition \( (C.2) \) coincides with definition \( (C.4) \) for normalized kernels (or more generally if \( \|\Psi(z)\|_H = \text{cte} \)).

**C.2. Proof of Proposition 3.2.** We first deduce from Proposition 3.1 the closed-form \( i \)th eigen-function approximation \( \varphi_i(\theta) \) for \( i = 1, \ldots, k \) at any point \( \theta \in \mathbb{R}^p \)

\[
\varphi_i(\theta) = \langle \xi_i, \Psi(\theta) \rangle_H = \langle U_{\mathbf{X}} \xi_i, \Psi(\theta) \rangle_H = \hat{\xi}_i^* \mathbf{Y} \Psi(\theta).
\]

Then, noticing that

\[
\hat{P}_k = \mathbf{Y} \Psi \mathbf{X} \hat{S}_k^* = \Psi \mathbf{X} S_k^*,
\]

as by construction \( \text{span}(S_k^*) \subseteq \text{span}(V_Z) \subseteq \text{span}(\Psi \mathbf{X}) \), relying again on Proposition 3.1, we can rewrite the reduced model \( (2.3) \) in terms of \( \hat{\xi}_i \)'s, \( \varphi_i(\theta) \)'s and \( \hat{\lambda}_j \)'s as

\[
\tilde{x}_T(\theta) = \Psi^{-1} \left( \sum_{j=1}^k \hat{P}_k \hat{\xi}_j \hat{\lambda}_j^{-1} \varphi_j(\theta) \right) = \Psi^{-1}(\Psi \mathbf{Y} g^{0,T}),
\]

with \( g^{0,T} \) defined in Proposition 3.2. Equation \( (C.5) \) implies the inverse of a linear combination of the \( \Psi(y_i) \)'s, where \( y_i = x_{i+1}(\theta_{\text{learn}}^j) \) with \( i = (T_{\text{learn}} - 1)j + t \) for \( j = 1, \ldots, N_{\text{learn}} \) and \( t = 1, \ldots, T_{\text{learn}} - 1 \). From \( (2.2) \), we rewrite the inverse of the linear combination appearing in \( (C.5) \) in terms of scalar products in \( H \)

\[
\tilde{x}_T(\theta) \in \arg \min_{z \in \mathbb{R}^p} \|\mathbf{Y} g^{0,T} - \Psi(z)\|_H = \arg \min_{z \in \mathbb{R}^p} \|\mathbf{Y} g^{0,T} - \Psi(z)\|_H^2
\]

\[
= \arg \min_{z \in \mathbb{R}^p} \|\Psi(z)\|_H^2 - 2\langle \mathbf{Y} g^{0,T}, \Psi(z) \rangle_H.
\]

The sought minimization problem is obtained by evaluating scalar products in \( H \) with the kernel trick \(<>\).
C.3. Sufficient conditions for existence. In this section, we provide a set of mild sufficient conditions so that the inverse \( \Psi^{-1}(\sum_{i=1}^{m} g_i \theta_i^T \Psi(y_i)) \) exists, \( \Psi^{-1} \) being defined in (C.4). This inverse is involved in (3.2) and was reformulated as the problem of the existence of a vector \( z^* \in \mathbb{R}^p \) satisfying \( f(z^*) = \inf_{z \in \mathbb{R}^p} f(z) \), where the objective function is \( f(z) = h(z, z) - 2 \sum_{i=1}^{m} \theta_i^T h(y_i, z) \).

**Proposition C.1.** A vector \( \arg \inf_{z \in \mathbb{R}^p} f(z) \) exists if one of the two following conditions holds.

1. \( f(z) \) is coercive and lower semicontinuous.
2. \( i) h(x, x) \) is constant for any \( x \in \mathbb{R}^p \),
   ii) \( \lim_{\|z\| \to \infty} h(x, z) = 0 \) for any \( x \in \mathbb{R}^p \),
   iii) \( \int_{\mathbb{R}^p} h(x, z)dz = c \) with \( c \geq 0 \) constant for any \( x \in \mathbb{R}^p \),
   iv) \( f(z) \) is lower semicontinuous,
   v) \( \sum_{i=1}^{m} \theta_i^T > 0 \).

**Proof of condition (1).** As \( \mathbb{R}^p \) is closed, the Weierstrass’ Theorem [4, Proposition A.8] states that a minimizer exists under condition (1). □

**Proof of condition (2).** Under condition (2-i), we have

\[
\arg \inf_{z \in \mathbb{R}^p} f(z) = \arg \inf_{z \in \mathbb{R}^p} \left( -\sum_{i=1}^{m} g_i \theta_i^T h(y_i, z) \right),
\]

(C.6)

and condition (2-ii) implies that for \( i = 1 \ldots, m \) we have

\[
\lim_{\|z\| \to \infty} -\sum_{i=1}^{m} g_i \theta_i^T h(y_i, z) = 0.
\]

(C.7)

Moreover, under conditions (2-iii) and (2-v),

\[
\exists z^* \in \mathbb{R}^p \text{ such that } -\sum_{i=1}^{m} g_i \theta_i^T h(y_i, z^*) < 0.
\]

(C.8)

Indeed, by contraposition, assume that \( -\sum_{i=1}^{m} g_i \theta_i^T h(y_i, z) \geq 0 \) for all \( z \in \mathbb{R}^p \). By integrating with respect to \( z \), as each term in the sum is independent of the point \( y_i \) under condition (2-iii), we obtain that \( -c \sum_{i=1}^{m} \theta_i^T \leq 0 \) and as \( c \geq 0 \), that \( \sum_{i=1}^{m} \theta_i^T \leq 0 \), which contradicts (2-v).

The existence of a minimizer then follows from (C.6), (C.7), (C.8) and assumption (2-iv). Indeed, assume a sequence \( \{x_k\} \subset \mathbb{R}^p \) such that \( \lim_{k \to \infty} f(x_k) = \inf_{z \in \mathbb{R}^p} f(z) \). \( \{x_k\} \) must be bounded since (C.6) and (C.7) show, that on the one hand the objective function \( f(z) \) tends to 0 as the norm of \( z \) grows to infinity, and on the other hand (C.8) guarantees that there exists at least one point for which the objective function is negative. Using the lower semicontinuity of \( f \), the proof then proceeds like the proof of the Weierstrass’ Theorem [4, Proposition A.8]. □

C.4. Examples. The sufficient conditions for existence of the inverse hold for several class of kernels. In particular, condition (1) holds for the polynomial kernels of the form \( h(y_i, z) = (1 + y_i^T z)^\gamma \), \( \gamma \in \mathbb{N}^* \). Indeed, the objective function \( f(z) = (1 + \|z\|_2^2)^\gamma - 2 \sum_{i=1}^{m} g_i \theta_i^T (1 + y_i^T z)^\gamma \) is in this case continuous and coercive since \( \lim_{\|z\| \to \infty} f(z) = \lim_{\|z\| \to \infty} \|z\|_2^{2\gamma} = +\infty \). Conditions (2-i), (2-ii), (2-iii) and (2-iv)
are in particular verified for Gaussian kernels of the form \( h(y_i, z) = \exp^{-\frac{1}{2\sigma^2}\|y_i - z\|^2} \) with \( \sigma > 0 \), or Laplacian kernels of the form \( h(y_i, z) = \exp^{-\frac{1}{\beta}\|y_i - z\|^2} \) with \( \beta > 0 \).

The existence of the inverse is therefore guaranteed for these kernels as long as we check that condition \( (2-v) \) holds. This positivity condition was always observed in our numerical simulations.

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