A Kernel-Based Approach to Data-Driven Koopman Spectral Analysis

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A data driven, kernel-based method for approximating the leading Koopman eigenvalues, eigenfunctions, and modes in problems with high dimensional state spaces is presented. This approach approximates the Koopman operator using a set of scalar observables, which are functions defined on state space, that is determined implicitly by the choice of a kernel. This circumvents the computational issues that arise due to the number of basis functions required to span a “sufficiently rich” subspace of the space of scalar observables in these problems. We illustrate this method on the FitzHugh-Nagumo PDE, a prototypical example of a one-dimensional reaction diffusion system, and compare our results with related methods such as Dynamic Mode Decomposition (DMD) that have the same computational cost as our approach. In this example, the resulting approximations of the leading Koopman eigenvalues, eigenfunctions, and modes are both more accurate and less sensitive to the distribution of the data used in the computation than those produced by DMD.

In many applications, the evolution of complex spatio-temporal phenomena can be replicated using models based on the interactions between a relatively low-dimensional set of modes. Due to the availability of data and computational power, algorithmic techniques for identifying these modes have become increasingly common [1–14]. Perhaps the best known of these methods is the Proper Orthogonal Decomposition (POD) [1, 2, 15], which is also known as Principal Component Analysis (PCA) [14, 15]. However, other algorithms that generate different modes exist. In recent years, (approximations of) the modes of the Koopman operator [16, 17] have become popular in fluid applications [5–8, 10, 18–20]. The Koopman modes of the full state observable, which are vectors for systems of ODEs or spatial profiles for PDEs, are intrinsic to a particular evolution law, and have temporal dynamics that are determined by their corresponding Koopman eigenvalue [21]; in effect, the Koopman modes look and act like the eigenvectors of a linear system even when the underlying evolution law is nonlinear.

This representation is possible because the Koopman operator, which defines these quantities, is a linear operator and therefore can have eigenfunctions and eigenvalues (which are later used to define the modes). However, it acts on scalar observables, which are functions defined on state space, and is therefore infinite dimensional even for finite dimensional dynamical systems. As a result, methods that approximate the Koopman operator (often implicitly) select a finite dimensional subspace of the space of scalar observables to use during the computation. Currently, the most widely used method is Dynamic Mode Decomposition (DMD) [3–6, 21] (along with its related modifications [8, 10, 20]), which implicitly selects linear functions of the state as the basis functions. This restrictive choice of basis allows DMD to be applied to large systems of ODEs or PDEs, but in many applications, this subspace is simply not “rich” enough to effectively approximate the Koopman operator [7, 11].

Other methods, such as Extended DMD [7], use an expanded set of observables, which can produce a more accurate approximation of the Koopman eigenvalues, eigenfunctions, and modes. For small systems of ODEs, a “sufficiently rich” subspace can often be spanned using a few hundred or thousand basis functions, which is computationally tractable even on a laptop. However, the size of the needed basis grows rapidly as the dimension of the state space increases, so the necessary computations quickly become infeasible as the state dimension grows. This explosion in the computational cost is common in machine learning applications, and one facet of the “curse of dimensionality” [15].

In this manuscript, we introduce a data driven, kernel-based method to approximate the Koopman operator in systems with large state dimension. This approach circumvents the dimensionality issues encountered by Extended DMD by defining a kernel function that implicitly computes inner products in the high-dimensional space of observables. Because we do not use this space explicitly, the computational cost of the method is determined by the number of snapshots and the dimension of state space rather than the number of basis functions used to represent the scalar observables; therefore, the cost of this approach is identical to that of DMD, and is applicable anywhere DMD also is. Using the FitzHugh-Nagumo PDE as an example, we will demonstrate that a general subspace of observables result in more accurate and (more reliably) reproducible approximations of the lead-
ing Koopman modes, eigenvalues, and eigenfunctions.

The Koopman Operator. Although our approach is data driven, the Koopman operator (along with its eigenvalues, eigenfunctions, and modes) is defined by a dynamical system and not a set of data. Given the discrete time dynamical system \((n, M, F)\), where \(n \in \mathbb{Z}\) is discrete time, \(M \subseteq \mathbb{R}^N\) is the state space, and \(x \mapsto F(x)\) defines the dynamics, the action of the Koopman operator, \(K\), on a scalar observable, \(\phi : M \rightarrow \mathbb{C}\), is

\[
(K\phi)(x) = (\phi \circ F)(x) = \phi(F(x)).
\]

Intuitively, \(K\phi\) is a new function that predicts the value of \(\phi\) “one step in the future”. Note that the Koopman operator acts on functions of state, and not the states themselves. Since \(\phi \in \mathcal{F}\), where \(\mathcal{F}\) is an appropriate space of scalar observables, the Koopman operator is infinite dimensional. However, it is also linear \([16, 17]\), and thus, it can have eigenvalues and eigenfunctions, which we refer to as Koopman eigenvalues and eigenfunctions. Accompanying the eigenvalues and eigenfunctions are the Koopman modes for a given vector valued observable, \(g : M \rightarrow \mathbb{R}^{N_o}\), where \(N_o \in \mathbb{N}\). These modes are vectors in a system of ODEs (or spatial profiles in a PDE) that contain the coefficients required to construct \(g\) using a Koopman eigenfunction basis \([5, 7]\). One particularly useful set of modes is that of the full state observable, \(g(x) = x\), which we refer to as simply the Koopman modes in all that follows.

In many systems \([5, 18, 22]\), tuples consisting of an eigenvalue, an eigenfunction, and a mode enable a simple yet powerful means of representing the system state and making predictions of future values. In particular,

\[
x = \sum_{k=1}^{K} \xi_k \varphi_k(x), \quad F(x) = \sum_{k=1}^{K} \mu_k \xi_k \varphi_k(x)
\]

where \(\xi_k\) is the \(k\)-th Koopman mode corresponding to the eigenfunction \(\varphi_k\), and the eigenvalue \(\mu_k\), and \(K\) is the number of tuples required for the reconstruction, which could be infinite. Once again, the eigenfunction \(\varphi_k : M \rightarrow \mathbb{C}\) is a function, but the mode \(\xi_k \in \mathbb{C}^N\) is a vector. From (2), the coefficient associated with the \(k\)-th mode, \(\xi_k\), is obtained by evaluating the \(k\)-th eigenfunction, \(\varphi_k\), and the temporal evolution is dictated by \(\mu_k\).

One benefit of the Koopman approach is that the eigenvalues, eigenfunctions, and modes are intrinsic to the dynamical system, and do not depend on data at all.

The Numerical Approach. Although the data do not define these Koopman tuples, they allow them to be approximated. The connection between the kernel approach and the Koopman operator is made through Extended DMD \([7]\), and is shown explicitly in the supplementary materials. Both our kernel method and Extended DMD define a \(K\)-dimensional subspace of the space of scalar observables, \(\mathcal{F}_K \subset \mathcal{F}\), using a set of (at least) \(K\) scalar observables that we refer to as dictionary elements. For simplicity, we assume this dictionary contains a basis for \(\mathcal{F}_K\), but the analysis still holds even if some of the elements are linearly dependent.

We denote the \(k\)-th element as \(\psi_k : M \rightarrow \mathbb{C}\), and define a vector-valued function \(\psi : M \rightarrow \mathbb{C}^K\) where \(\psi(x) = [\psi_1(x), \psi_2(x), \ldots, \psi_K(x)]^T\). Then, any function \(\phi \in \mathcal{F}_K\) can be written as \(\phi = \psi^T a\), for some appropriate vector of coefficients \(a \in \mathbb{C}^K\). Borrowing terminology from the machine learning community, we refer to \(\psi\) as the mapping from state space to feature space.

As shown in the supplement, the Extended DMD procedure can be written entirely in terms of inner products in feature space. Previously, these inner products were computed directly (e.g., \(\psi(z)^* \psi(x)\)), which becomes computationally intractable in problems where \(K\) is large. This is common in problems with high-dimensional state spaces; for example, if \(\mathcal{F}_K\) is the space of all polynomials up to 10-th order defined in \(\mathbb{R}^{400}\), then \(K \sim 10^{19}\), which is far too large for practical computations \([15]\).

The kernel trick is a common technique for implicitly computing inner products in such spaces \([23-26]\), which overcomes this difficulty. Instead of defining \(\psi\), we define a kernel function \(f : M \times M \rightarrow \mathbb{C}\) that computes inner products in feature space given pairs of data points; that is, \(f(x_i, x_j) = \langle x_i, x_j \rangle = \psi(x_i)^* \psi(x_j)\) \([23]\). In effect, the choice of \(f\) defines \(\psi\), which is equivalent to choosing the dictionary in Extended DMD. It is, however, crucial to note that \(f\) does not compute these inner products directly. The simplest example is the polynomial kernel

\[
f(x, z) = (1 + z^2 x)^2
\]

with \(x, z \in \mathbb{R}^2\), which, when expanded, is

\[
f(x, z) = (1 + x_1 z_1 + x_2 z_2)^2
\]

\[
= (1 + 2 x_1 z_1 + 2 x_2 z_2 + 2 x_1 z_2 + 2 x_2 z_1 + x_1^2 z_1^2 + x_2^2 z_2^2)
\]

\[
= \psi(z)^* \psi(x)
\]

if \(\psi(x) = [1, \sqrt{2} x_1, \sqrt{2} x_2, \sqrt{2} x_1 x_2, x_1^2, x_2^2]\). In general, a kernel of the form \(f(x, z) = (1 + z^2 x)^n\) is equivalent to a dictionary that includes all monomials up to and including terms of order \(n\), but computes inner products in feature space in \(O(N)\) rather than \(O(K)\) time.

In the example that follows, we use a polynomial kernel with \(\alpha = 10\). We selected this kernel because the Koopman eigenfunctions are often analytic in a disk about a fixed point \([27]\), and polynomial kernels mimic an \(\alpha\) order power-series expansion. The choice of \(\alpha = 10\) is more ad hoc. In general, large values of \(\alpha\) use a “richer” set of basis functions, but also deleteriously impact the condition numbers of the matrices used in the computation. We chose the largest value of \(\alpha\) that did not result in an ill-conditioned matrices, which appears to be \(\alpha = 10\) here.

Other choices of kernels, such as Gaussian kernels (i.e., \(f(x, y) = \exp(-\|x - y\|^2/\sigma^2)\)), are also used in machine learning applications \([15, 25, 28]\), and may result in bet-
Kernel Method

where + denotes the pseudo-inverse.

To extract the Koopman eigenvalues, eigenfunctions, and modes, we compute the eigenvectors and eigenvalues of $\hat{K}$. This yields the matrices of eigenvectors, $\hat{V}$, and eigenvalues, $\mu$ (i.e., $\hat{K}\hat{V} = \hat{V}\mu$). The eigenvalues contained in $\mu$ are an approximation of the Koopman eigenvalues. The values of the eigenfunctions of the Koopman operator evaluated at $x_i$ and $y_i$ are contained in the $i$-th row of the matrices

$\Phi_x \triangleq \hat{G}\hat{V}^{-1}$, and $\Phi_y \triangleq \hat{A}\hat{V}$,

respectively. To approximate the Koopman modes, we compute

$\Xi \triangleq \Phi_x^T X$

where $X = [x_1, x_2, \ldots, x_M]^T$. The $k$-th row of $\Xi$ is the $k$-th Koopman mode $\xi_k$. When the underlying system is sampled using the fixed interval $\Delta t$, we also define $\lambda_k \triangleq \log(\mu_k)/\Delta t$, which is an approximation of the continuous time eigenvalue.

The total cost of this approach is $O(M^2 \max(M,N))$ where $N$ is the dimension of the state space and $M$ the number of snapshots. This cost is either due to forming ($O(M^2N)$) or decomposing ($O(M^3)$) $G$ and $A$, and is equivalent to the cost of DMD as it is typically implemented [11, 21]. As a result, this technique will be numerically feasible anywhere that DMD also is.

An Illustrative Example. To demonstrate the effectiveness of our method, we apply it and (as a benchmark) DMD to data from the FitzHugh-Nagumo PDE [30] in one spatial dimension:

\begin{align*}
\partial_t v &= \partial_{xx} v + v - w - v^3, \\
\partial_t w &= \delta \partial_{xx} w + \epsilon (v - c_1 w - c_0),
\end{align*}

where $v$ is the activation field, $w$ is the inhibition field, $c_0 = -0.03$, $c_1 = 2.0$, $\delta = 4.0$, $\epsilon = 0.03$, for $x \in [0,20]$ with Neumann boundary conditions. Both $v$ and $w$ are discretized using 200 interior points, and second order finite difference methods are used to approximate spatial derivatives. With these parameter values, (7) has a stable fixed point that resembles a wave-front in both the activation and inhibition fields.

The data are generated by applying 10 different, “large” perturbations to the stable fixed point, evolving that initial point for 200 units in time to allow fast transients to dissipate, and observing the subsequent evolution with a sampling interval of $\Delta t = 1$. Thus, the master data set contains 10 separate trajectories consisting of 401 snapshots each. This set is subdivided into five sets indicated by the various colors and markers in Fig. 1, which consist of 500, 1000, 2000, 3000, and 4000 snapshot pairs. As the number of snapshots grows, data further from the fixed point (and, hence, more impacted by the
nonlinearity in the evolution law) appear; the purpose of sampling in this way is to characterize the response of our method to additional “nonlinearities” in the data. Note that each data set was normalized so that the mean value of \(|\|x\|| = 1\), which is equivalent to introducing a scaling parameter in the kernel \(f\).

Figure 2 shows the approximation of the continuous time eigenvalues obtained for the five different data sets using the kernel method in (a) and DMD in (b). Although both methods produce eigenvalues not contained in the windows shown, those obtained by the kernel method are all in the left half plane, which predicts that the fixed point is stable [27]. On the other hand, the spectrum obtained by DMD has eigenvalues in the right half plane, which incorrectly implies the stable spiral is unstable. For the first two data sets, which are indicated by blue and green markers, only the leading three eigenvalues (i.e., those with \(\Re(\lambda) > -0.015\)) obtained by the kernel method have converged, and there is visible variability in the remaining eigenvalues. However, when larger data sets are used, three additional eigenvalues appear. This agrees with results from Koopman spectral analysis that imply nonlinearities are represented through the inclusion of additional tuples [31, 32]. Indeed, the spectrum of the Koopman operator should include a “pyramid” of eigenvalues [32], though we recover only the first three layers here. Although the numerically computed eigenvalues are data dependent, the leading eigenvalues are far more consistently approximated using our approach than they are by the DMD benchmark.

The modes corresponding to the three leading eigenvalues are shown in Fig. 3. The first mode, which has \(\lambda \approx 0\), is a scaled version of the solution at the fixed point where the appropriate scaling factor is determined by evaluating the corresponding Koopman eigenfunction. In Fig. 3a, the “true” profile is indicated by the dashed line, and the numerically computed mode by the solid lines. The next pair of modes, which have \(\lambda = -6.5 \times 10^{-2} \pm 0.52i\), can be shown to be the “slowest” pair of eigenvectors of the system linearization, and provide a useful description of the evolution near the fixed point. The real part of this eigenvector, which is obtained via the direct linearization of (7), is indicated by the dashed line in Fig. 3b. Once again, this Koopman mode is obtained consistently despite the differences in the data used to compute it.

The first mode associated with nonlinear effects, which has the eigenvalue \(\lambda = -0.013\), is pictured in Fig. 3c. Unlike the other three, this mode is not identified by the kernel method using the smallest (i.e., most linear) set of data, so no mode is plotted for that data set. Intuitively, this is because nonlinear effects are not required to describe the data in that regime. Even the second smallest data set produces a mode, shown in green, with a large amount of error. While no analytical solution is known for this mode, the differences between this mode and those obtained from the three largest data sets, where the neither the mode nor the associated eigenvalue change significantly, make the error clear. Although not shown, the modes associated with the eigenvalues \(\lambda = -0.013 \pm 0.1i\) also have little variance for these three data sets, so this entire “layer” of the pyramid of eigenvalues is captured using the kernel approach when a sufficiently large amount of data is available.

Conclusions. We presented a data driven method for approximating the Koopman operator in problems with large state spaces, a common setting in physical applications such as fluid dynamics. The kernel method we have developed defines a subspace of scalar observables implicitly through a kernel function: this enables us to approximate the Koopman operator with the same asymptotic cost as DMD, but with a far larger set of observables. As shown by the FitzHugh-Nagumo example, this difference is critical if the Koopman modes and eigenvalues are to be computed accurately and consistently in nonlinear problems. In the end, the Koopman operator is an appealing mathematical framework for defining a set of spatial modes because these modes are intrinsic to the dynamics rather than associated with a set of data, and although obtaining an effective approximation is non-trivial, approaches like the one presented here
have the potential to produce useful approximations of this operator in practical applications.

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Supplementary Material

In this supplement, we present a reformulation of the Extended Dynamic Mode Decomposition (Extended DMD) method that (partially) circumvents the “curse of dimensionality,” and enables the leading tuples of Koopman eigenvalues, eigenfunctions, and modes to be computed in systems with high-dimensional state spaces like those that appear in fluid dynamics. The crux of this approach is the so-called “kernel trick,” which is a conceptually simple but useful method that computes inner products in high-dimensional Hilbert spaces, which we refer to as “feature space,” implicitly through a user-defined kernel function. The kernel trick has been used in machine learning and classification algorithms, such as support vector machines [23, 28], but is more broadly applicable. Indeed, any algorithm where operations in feature space can be written entirely in terms of inner products has the potential to be re-expressed as a kernel method.

In what follows, we will introduce a few, relevant properties of the Koopman operator, and briefly demonstrate how the Extended DMD algorithm produces a data-driven approximation of it. Next, we will show that the formulæ used to numerically approximate the Koopman tuples can be written entirely in terms of inner products in an appropriate feature space, which we will define shortly, and proves that Extended DMD could be formulated as a kernel method. Finally, we will present the kernel version of the algorithm by replacing these inner products with a user-defined kernel.

The Koopman Operator and Extended DMD: The purpose of the Extended DMD procedure is to generate a finite-dimensional approximation of the Koopman operator, which is defined for the autonomous, discrete time dynamical system \((n, M, F)\), where \(n \in \mathbb{Z}\) is (discrete) time, \(M \subset \mathbb{R}^N\) is state space, and \(F : M \to M\) is the evolution operator. The Koopman operator \(K\) acts on scalar observables, which are functions that map from state space to complex scalars (i.e., \(\psi : M \to \mathbb{C}\)), in some appropriate function space that we denote as \(\mathcal{F}\).

The action of this operator \(K : \mathcal{F} \to \mathcal{F}\) is given by

\[
(K \psi)(x) = (\psi \circ F)(x) = \psi(F(x)),
\]

which is simply the composition of the observable with the map defining the dynamics. Because it acts on functions, the Koopman operator is infinite dimensional, but it is also linear even if \(F\) is nonlinear. As a result, it can have eigenfunction and eigenvalue pairs, which we denote as \(\varphi_k \in \mathcal{F}\) and \(\mu_k \in \mathbb{C}\) respectively.

Accompanying the eigenvalues and eigenfunctions are the Koopman modes, which for the full state observable \(g(x) = x\), we denote as \(\xi_k \in \mathbb{C}^N\) [5, 6, 18]. The modes allow the state at the current time to be written as

\[
x = \sum_{k=1}^{K} \xi_k \varphi_k(x), \quad (9a)
\]

and future values to be predicted via

\[
F(x) = \sum_{k=1}^{K} \mu_k \xi_k \varphi_k(x). \quad (9b)
\]

Here \(K\) is the number of non-zero Koopman modes (i.e., \(|\xi_k| \neq 0\)), and could be infinite; furthermore, we have assumed that the continuous spectrum of the Koopman operator [17] can be neglected. Motivated by (9), we define a Koopman tuple as \((\mu_k, \varphi_k, \xi_k)\), which is a triplet of a Koopman eigenvalue, eigenfunction, and mode. Note that this procedure can be repeated for different vector-valued observables, and will result in a different set of Koopman modes. For simplicity however, we consider only the case of the full state observable in what follows.

To obtain a finite-dimensional approximation of the Koopman operator, we define a dictionary that consists of \(K\) scalar observables, which we denote as \(\psi_k\) for \(k = 1, \ldots, K\), that span \(\mathcal{F}_K \subset \mathcal{F}\). We also define the vector valued observable, \(\psi : M \to \mathbb{C}^K\), where

\[
\psi(x) = \begin{bmatrix} \psi_1(x) \\ \psi_2(x) \\ \vdots \\ \psi_K(x) \end{bmatrix}. \quad (10)
\]

In this application, \(\psi\) is the mapping from physical space to feature space. Any \(\phi, \hat{\phi} \in \mathcal{F}_K\) can be written as

\[
\phi = \sum_{k=1}^{K} a_k \psi_k = \psi^T a, \quad \hat{\phi} = \sum_{k=1}^{K} \hat{a}_k \psi_k = \psi^T \hat{a}, \quad (11)
\]

for some \(a, \hat{a} \in \mathbb{C}^K\). Although \(F\) is unknown, we assume access to a data set of snapshot pairs, \(\{(x_m, y_m)\}_{m=1}^{M}\) where \(x_m, y_m \in M\) and \(y_m = F(x_m)\). One important special case of such a data set is a single time-series of data, which can be written in the above form by “grouping” sequential pairs of snapshots.

Let \(\phi = K \phi + r\), where \(r \in \mathcal{F}\) is a residual function that appears because \(\mathcal{F}_K\) is not necessarily invariant to the action of the Koopman operator. Using the notation in (11), the objective of the Extended DMD procedure [7] is to define a mapping from some given \(a\) to a new vector \(\hat{a}\) that minimizes this residual. Because the Koopman operator is linear, this mapping is represented by the matrix \(K \in \mathbb{C}^{K \times K}\). To determine the entries of \(K\), the Extended DMD approach takes ideas from collocation methods typically used to solve PDEs, but uses \(x_m\) as the collocation points rather than a pre-determined grid [23, 28]. As a result, the finite dimensional approximation is

\[
K \triangleq \Psi_x^T \Psi_y, \quad (12a)
\]

\[
\Psi_x \triangleq \left[ \psi(x_1), \psi(x_2), ..., \psi(x_M) \right] \in \mathbb{C}^{MK \times K},
\]

\[
\Psi_y \triangleq \left[ \psi(y_1), \psi(y_2), ..., \psi(y_M) \right] \in \mathbb{C}^{MK \times K},
\]

\[
\Psi \triangleq \left[ \psi(x_1), \psi(x_2), ..., \psi(x_M), \psi(y_1), \psi(y_2), ..., \psi(y_M) \right] \in \mathbb{C}^{2MK \times K}.
\]
where

\[
\Psi_x \triangleq \begin{bmatrix}
\psi(x_1)^T \\
\psi(x_2)^T \\
\vdots \\
\psi(x_M)^T
\end{bmatrix}, \quad \Psi_y \triangleq \begin{bmatrix}
\psi(y_1)^T \\
\psi(y_2)^T \\
\vdots \\
\psi(y_M)^T
\end{bmatrix}, \quad (12b)
\]

are in \(\mathbb{C}^{M \times K}\), and \(\dagger\) denotes the pseudoinverse. For details on the convergence of this method, see Ref. [7]. The properties that are important for what follows are: (i) the \(k\)-th eigenvalue of \(K\), \(\mu_k\), is an approximation of an eigenvalue of \(K\), and (ii) the corresponding eigenvector, \(v_k\), approximates an eigenfunction of the Koopman operator via \(\varphi_k = \psi^T v_k\).

A Reformulation of Extended DMD. Now, we show that the eigenvectors and eigenvalues of (12) can be written entirely in terms of inner products in feature space, rather than requiring \(\Psi_x\) and \(\Psi_y\) explicitly. To begin, \(\mathcal{R}(K) \subseteq \mathcal{R}(\Psi_x)\), i.e., the range of \(\Psi_x\) contains the range of \(K\). Therefore, an eigenvector of \(K\) with \(\mu_k \neq 0\), which is by definition an element of the range, can be written (though not necessarily uniquely) as \(v = \Psi_x^* \hat{\psi}\), for some \(\hat{\psi} \in \mathbb{C}^M\). Then using the identity \(\Psi_x^* = \Psi_x^*(\Psi_y \Psi_x)^{\dagger}\), we have

\[
\mu v = K v \\
\iff \mu \Psi_x \hat{\psi} = \Psi_x^* (\Psi_y \Psi_x)^{\dagger} \hat{\psi} \\
= \Psi_x^* (\Psi_y \Psi_x)^{\dagger} (\Psi_y \Psi_x^*) \\
= \Psi_x^* G^+ A \hat{\psi}
\]

where \(G = \Psi_x \Psi_x^*\) and \(A = \Psi_y \Psi_y^*\). Therefore, an alternative method for computing the eigenvectors of \(K\) is to form the matrix

\[
\hat{K} \triangleq G^+ A, \quad (13)
\]

compute an eigenvector, \(\hat{\psi}\), and multiply by \(\Psi_x^*\) to obtain \(v\) (and therefore an approximation of a Koopman eigenfunction). Here \(\hat{K} \in \mathbb{C}^{M \times M}\); therefore, the computational cost of the decomposition is determined by the number of snapshots rather than the dimension of the system state or “feature” space. The benefit of the expression in \(\hat{K}\) is that, despite appearing “flipped,” the elements of both \(G\) and \(A\) are inner products in feature space. In particular, \(G_{ij} = \psi(x_i)^* \psi(y_j)\), and \(A_{ij} = \psi(x_j)^* \psi(y_i)\).

Let \(\hat{V}\) be the matrix whose columns are the eigenvectors of \(\hat{K}\), then using (11) we define

\[
\Phi_x \triangleq G \hat{V}, \quad \Phi_y \triangleq A \hat{V}, \quad (14)
\]

whose \(i\)-th row contain the numerically computed eigenfunctions evaluated at \(x_i\) or \(y_j\), respectively, and \(\mu\) is the diagonal matrix whose entries are the eigenvalues of \(K\).

To compute the Koopman modes, we use (9), which when evaluated at each of the data points, results in the matrix equation

\[
X = \Phi_x \Xi, \quad (15)
\]

where

\[
X \triangleq \begin{bmatrix}
\psi(x_1)^T \\
\psi(x_2)^T \\
\vdots \\
\psi(x_M)^T
\end{bmatrix}, \quad \Xi \triangleq \begin{bmatrix}
\xi_1^T \\
\xi_2^T \\
\vdots \\
\xi_M^T
\end{bmatrix} = \Phi_x^* X = \hat{V}^{-1} G^{-1} X,
\]

provided that \(G\) is invertible and \(\hat{K}\) has a full set of eigenvectors. In this case,

\[
\hat{V}^{-1} = \begin{bmatrix}
\hat{w}_1^* \\
\hat{w}_2^* \\
\vdots \\
\hat{w}_M^*
\end{bmatrix},
\]

where \(\hat{w}^*\) is a left eigenvector of \(\hat{K}\) scaled so that \(\hat{w}^* \hat{\psi}_j = \delta_{ij}\). This implies that the \(k\)-th Koopman mode, \(\xi_k\), is

\[
\xi_k = (\hat{w}_k^* G^{-1} X)^T,
\]

and therefore approximate Koopman tuples can be obtained via the left and right eigenvectors of \(\hat{K}\), and do not require \(\hat{K}\) to be computed in its entirety. For the problems considered here, the complete decomposition of \(\hat{K}\) is computed, but for problems with larger numbers of snapshots, Krylov methods could be used to compute a (leading) subset of the eigenvalues and vectors [?].

Extended DMD as a Kernel Method. The crux of the kernel approach is (13), which involves two matrices \(G\) and \(A\). As noted previously, the elements of these matrices are inner products taken in feature space, which in many practical problems, can be extremely large. Instead, we define a kernel function, \(f : \mathcal{M} \times \mathcal{M} \to \mathbb{C}\) that implicitly defines the feature space (i.e., the subspace of scalar observables used in the Extended DMD computation) and evaluates these inner products implicitly. In the manuscript, we gave an example of a polynomial kernel of the form \(f(x, y) = (1 + y^T x)^\alpha\), and demonstrated how this kernel implicitly chooses the dictionary elements to be all monomials up to and including those of degree \(\alpha\).

Therefore, converting Extended DMD to a kernel method is simple: we generate the matrices \(G\) and \(A\) entry-wise using the kernel \(f\), rather than by evaluating \(\Psi_x \Psi_x^*\) and \(\Psi_y \Psi_y^*\). Then, the numerical procedure for approximating the Koopman tuples is:

1. Define the kernel function, \(f\), which implicitly defines the dictionary used in Extended DMD.
2. Given the data set of snapshot pairs, compute the elements of the matrices \(G\) and \(A\) using the kernel function. \(G_{ij} = f(x_i, x_j)\) and \(A_{ij} = f(y_i, x_j)\).
3. Form \(\hat{K}\) using (13), and compute its (leading) eigenvalues and left and right eigenvectors.
4. Compute the approximate Koopman modes using (18).
Assuming that evaluating $f$ is an $O(N)$ operation, the asymptotic cost of this procedure is $O(M^2 \max(M,N))$. If $M > N$, the “most expensive step” is the eigendecomposition of $\hat{K}$. Although $G^+$ must be computed, because $G$ is Hermitian and $\hat{K}$ is not, the constant is smaller. If $N > M$, then forming $A$ and $G$ will determine the asymptotic cost of the method. In practice, however, this task is embarrassingly parallel, and so it is the eigendecomposition that truly dominates the “wall clock” computational time. Ultimately, the kernel approach consists of a similar sequence of steps and has a nearly identical cost as the DMD algorithms proposed in Refs. [11, 21]; the primary difference is that a (more general) higher-dimensional feature space is used, but since this space only appears implicitly, it does not significantly impact the total cost of the method (provided, again, that the kernel requires only $O(N)$ time to evaluate; in most of the “commonly used” kernels, this is the case).

**Conclusions.** In this supplement, we have outlined a kernel-based approach and its connection to Extended Dynamic Mode Decomposition and the Koopman operator. The differences between the algorithms used in our kernel approach and DMD [11, 21] are small, but as shown in the manuscript, the impact on the resulting spectrum and modes can be profound. Rewriting Extended DMD as a kernel only partially overcomes the “curse of dimensionality,” since data collection in high-dimensional spaces is still a challenge. Indeed in problems with high-dimensional state spaces, both our approach and DMD will have difficulties if the data do not lie on some low dimensional manifold embedded. In the end, however, the Koopman operator acts on observables of state space rather than state space itself, and methods like our kernel approach have the promise to generate effective (if not fully converged) approximations of the leading Koopman eigenvalues, eigenfunctions, and modes for the same computation cost as more commonly used approaches such as Dynamic Mode Decomposition that also claim to be based on approximate decompositions of the Koopman operator.