

Group-Convolutional Extended Dynamic Mode Decomposition

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Abstract

This paper explores the integration of symmetries into the Koopman-operator framework for the analysis and efficient learning of equivariant dynamical systems using a group-convolutional approach. Approximating the Koopman operator by finite-dimensional surrogates, e.g., via extended dynamic mode decomposition (EDMD), is challenging for high-dimensional systems due to computational constraints. To tackle this problem with a particular focus on EDMD, we demonstrate—under suitable equivariance assumptions on the system and the observables—that the optimal EDMD matrix is equivariant. That is, its action on states can be described by group convolutions and the generalized Fourier transform. We show that this structural property has many advantages for equivariant systems, in particular, that it allows for data-efficient learning, fast predictions and fast eigenfunction approximations. We conduct numerical experiments on the Kuramoto–Sivashinsky equation, a nonlinear and chaotic partial differential equation, providing evidence of the effectiveness of this approach, and highlighting its potential for broader applications in dynamical systems analysis.

1. Introduction

Dynamical systems are fundamental to the modeling of various natural phenomena and engineering systems. These systems are often modeled by differential equations which may describe mechanical systems, the diffusion of heat in a material, the propagation of sound waves in air, or the flow of fluids in pipes and oceans. These equations are indispensable in fields ranging from physics and engineering to finance and biology, making them critical tools for solving practical problems in both theoretical and applied contexts.

Linear systems are particularly appealing due to their well-understood properties and the powerful mathematical techniques available for their analysis. For example, one can characterize the behavior of these systems by analyzing their eigenvalues and eigenvectors. In case of nonlinear dynamics, the Koopman operator, see [Koopman \(1931\)](#); [Rowley et al. \(2009\)](#), provides a transformation into a linear framework by focusing on the evolution of observables—functions of the system state—rather than the state itself. This linearization can reveal underlying structures and long-term behavior. Still, the Koopman operator is

likely to be infinite-dimensional, and hence intractable, which requires an approximation by means of extended dynamic mode decomposition (EDMD).

EDMD constructs a matrix that can contain prohibitively many entries. This can happen when the state dimension is already very large, as is usually the case for discretizations of partial differential equations (PDEs). To address this issue, one can often exploit system-inherent symmetries. Accordingly, symmetry-exploiting methods have become more popular in recent years, even beyond the scope of dynamical systems: For example, convolutional neural networks and more generally geometric deep-learning methods Bronstein et al. (2021) are designed to respect task-inherent equivariances. Constructing learning algorithms that respect these equivariances can increase performance and reduce the necessary training data, see Masci et al. (2015); Cohen and Welling (2016); Bronstein et al. (2017); Atz et al. (2021); Bronstein et al. (2021); Harder et al. (2024).

The presence of symmetry can lead to a decomposition of the EDMD matrix into simpler, more tractable components. It appears that hitherto proposed symmetry-based methods can be split into two categories: Some methods enforce block-wise diagonal structures in the EDMD matrix, see Sinha et al. (2020); Peitz et al. (2024), and some methods enforce diagonal structures in Fourier space. Our contribution falls into the latter category and is related to the works of Salova et al. (2019); Baddoo et al. (2023); Hochrainer and Kar (2024). Here, the work of Salova et al. (2019) provides a more general group-theoretic treatment and, among other things, discusses the importance of choosing appropriate symmetry-respecting observables. Another focus is on efficient methods for translation-equivariant dynamical systems, see Baddoo et al. (2023); Hochrainer and Kar (2024) (the work of Baddoo et al. (2023) also considers different aspects, but their proposed method for translational equivariance is most relevant for our purposes). In particular, both Baddoo et al. (2023) and Hochrainer and Kar (2024) discuss how the EDMD matrix can be forced to be (block-)diagonal in Fourier space for PDEs.

Contributions and organization. Our approach extends and generalizes these developments into multiple directions: Firstly, we assume a more general group-theoretic setting. In this regard, we show how one can enforce an equivariant structure in the EDMD matrix and demonstrate that this approach is optimal under suitable assumptions on the system dynamics, the observables and the sampling distribution. Finally, we make use of the generalized Fourier transform to effectively learn the corresponding EDMD matrix (representing it only implicitly by means of a convolution kernel), and show how this may be leveraged to efficiently approximate eigenfunctions of the Koopman operator.

To this end, we provide an introduction to the Koopman operator and its approximation via EDMD (Section 2), followed by a discussion of basic group-theoretic aspects (Sections 2.1 and 2.3). Section 3 contains the main contributions of this work: On the one hand, assuming an appropriate choice of the sampling distribution and the observables, we show that equivariance is inherited by the EDMD matrix and that it can be represented by a group convolution (Theorem 3.1). On the other hand, we show how one can conveniently learn the corresponding convolution kernel in Fourier space using the generalized Fourier transform. And finally, we conduct experiments by means of the two-dimensional Kuramoto–Sivashinsky equation to demonstrate the advantages of our proposed group-convolutional approach in the

low-data regime (see Section 3.1).

Notation. We will frequently require sets of the form \mathbb{C}^I , $\mathbb{C}^{I \times J}$, $\mathbb{C}^{I \times J \times K}$, etc., where I , J and K are finite sets. The intention is to think of the elements in \mathbb{C}^I as vectors instead of functions, similarly we think of elements in $\mathbb{C}^{I \times J}$ as matrices. The individual entries of $A \in \mathbb{C}^{I \times J}$ are denoted by $A_{i,j}$ for $(i,j) \in I \times J$. Vector-vector or matrix-vector products are defined accordingly. The main advantage is that this simplifies indexing: For example, if $J = J_1 \times J_2$, we can easily define the matrix-vector product of $A \in \mathbb{C}^{I \times J}$ with $x \in \mathbb{C}^J$ by $Ax \in \mathbb{C}^I$, $(Ax)_i = \sum_{(j_1, j_2) \in J} A_{i, (j_1, j_2)} x_{j_1, j_2}$.

Code and resources. The code for our experiments in Section 3.1 and some supplementary material for Example 2.7 can be found on GitHub,

<https://github.com/graps1/convolutional-edmd>.

For the case of Example 2.7, our codebase contains an implementation that models the system dynamics using a group-convolutional approach. For the experiments on the Kuramoto-Sivashinsky equation in Section 3.1, we provide a readable implementation that mimics the mathematical descriptions used in this paper.

2. Preliminaries: The Koopman operator, EDMD, and symmetries

The Koopman operator evolves functions (called observables) forward in time by composing them with a given dynamical system. For such a system $\Phi : Y \rightarrow Y$ on some state space Y , one defines the Koopman operator \mathcal{K} on observables of the form $f : Y \rightarrow \mathbb{C}$ via the composition

$$\mathcal{K}f := f \circ \Phi.$$

If f is a vector-valued function $f : Y \rightarrow \mathbb{C}^m$, then $\mathcal{K}f$ is defined analogously. The Koopman operator is linear by definition, even though the underlying system dynamics may be nonlinear, but it is infinite-dimensional in general. By studying properties of the Koopman operator, such as its eigenvalues and eigenfunctions, one can obtain insights into the underlying system dynamics. However, due to the infinite number of dimensions, one has to resort to finite-dimensional approximations using extended dynamic mode decomposition (EDMD), see, e.g., Williams et al. (2015). In EDMD, one projects \mathcal{K} onto a set of *base observables*, whose evolution is described by a finite linear system. This system is found by drawing states from some distribution and solving a certain least-squares problem. We need the following additional assumptions:

- In order to draw samples from Y , we assume that it is part of a probability space (Y, Σ, P) , where $\Sigma \subseteq 2^Y$ is a set of events and $P : \Sigma \rightarrow [0, 1]$ a probability function.
- Additionally, if the Koopman operator is applied to square-integrable observables, it must again produce square-integrable observables. In other words, $f \in L_P^2(Y)$ implies $\mathcal{K}f \in L_P^2(Y)$. (So that the EDMD loss in (1) has a well-defined expectation.)
- The dictionary of base observables is given by a set of predefined $\psi_1, \dots, \psi_m \in L_P^2(Y)$, or, more simply, $\psi \in L_P^2(Y)^m$.

The EDMD matrix K is now any matrix solving the optimization problem

$$\min_{K \in \mathbb{C}^{m \times m}} \mathbb{E}_{\mathbf{y} \sim P} [\|K\psi(\mathbf{y}) - \mathcal{K}\psi(\mathbf{y})\|^2]. \quad (1)$$

Intuitively, K defines a linear map in \mathbb{C}^m that mimics the Koopman operator’s action on the observables ψ_1, \dots, ψ_m . The corresponding EDMD *operator* is defined on the span of the base observables, $f = c^T \psi \in \text{span} \{\psi_1, \dots, \psi_m\}$, with $c \in \mathbb{C}^m$, via the mapping

$$(\mathcal{K}_{\text{EDMD}} f)(y) := c^T K \psi(y).$$

Under some additional assumptions, it can be shown that $\mathcal{K}_{\text{EDMD}}$ converges to the true Koopman operator when $m \rightarrow \infty$, see [Korda and Mezić \(2018\)](#). Besides the projection error, one may deviate from the true EDMD matrix if the expectation in (1) is approximated using finitely many samples. The resulting finite-data error term is well studied and can be bounded, see, e.g., [Mezić \(2022\)](#); [Zhang and Zuazua \(2023\)](#); [Nüske et al. \(2023\)](#) and [Philipp et al. \(2024\)](#) for kernel EDMD, in case of either i.i.d. or ergodic sampling. Moreover, uniform error bounds on the approximation error were recently derived in [Köhne et al. \(2024\)](#).

Most Koopman-theoretic investigations have hitherto considered ordinary or stochastic differential equations. More general settings can be found in [Baddoo et al. \(2023\)](#); [Hochrainer and Kar \(2024\)](#); [Philipp et al. \(2024\)](#), which cover PDEs as well. Due to the usually very high state dimension in the PDE case stemming from spatial discretization, it is prohibitive to learn a full-scale EDMD matrix and advantageous to apply more efficient approaches. Previous works such as [Baddoo et al. \(2023\)](#); [Hochrainer and Kar \(2024\)](#) already indicated that one may exploit the Fourier transform using translational symmetries. In general, symmetries occur in a large number of PDE systems implying that the dynamics are equivariant under certain group actions, which depend on the system dynamics as well as on the domain and the boundary conditions. One example is the Kuramoto–Sivashinsky equation, which can be written in coordinate-free form as

$$y_t = \mathcal{N}(y) = -\Delta y - \Delta^2 y - \frac{1}{2} \|\nabla y\|^2, \quad (2)$$

where y is an underlying time-dependent scalar field, Δ the Laplace operator, Δ^2 the biharmonic operator and $\|\nabla y\|^2$ the squared length of y ’s time-dependent gradient field. The resulting flow Φ can be obtained by solving the PDE for a fixed time step, say $\Phi(y(t)) = y(t+\delta)$ for some $\delta > 0$. This particular PDE is equivariant under any transformation of the Euclidean group. This means that shifting, rotating or reflecting the solution y and then applying \mathcal{N} yields the same result as shifting, rotating or reflecting $\mathcal{N}(y)$, see, e.g., [Harder et al. \(2024\)](#). Here, we utilize this group-theoretic perspective to leverage the generalized Fourier transform for efficient learning.

2.1. Groups and group actions

The following discussion of group-theoretic aspects takes orientation from [Åhlander and Munthe-Kaas \(2005\)](#); [Åhlander and Munthe-Kaas \(2006\)](#) and [Terras \(1999\)](#). A *group* is a set G along with an associative composition operation $G \times G \rightarrow G$, $(g, h) \mapsto gh$ that contains an identity e and inverses. It is said to be *abelian* if the composition operation is commutative. Throughout this text, G is assumed to be finite.

Example 2.1. *The symmetry group of the square describes rotations and reflections of a square across its center. It consists of an identity element, rotations of 90, 180 and 270 degrees, and reflections across the diagonal as well as horizontal and vertical axes. The group operation chains these elements, in the sense that two 90 degree rotations amount to one 180 degree rotation.*

A left group action of G on a set Y is defined as a mapping $G \times Y \rightarrow Y, (g, y) \mapsto g \cdot y$, associating a group element $g \in G$ and a point $y \in Y$ with some other point in Y in a way that is compatible with the group operation, i.e., $e \cdot y = y$ and $(gh) \cdot y = g \cdot (h \cdot y)$ for all $g, h \in G$ and $y \in Y$. An analogous definition holds for right group actions, but in the sense that $(g, y) \mapsto y \cdot g$ with $y \cdot e = y$ and $y \cdot (gh) = (y \cdot g) \cdot h$. We say that a left resp. right group action is *free* if $g \cdot y = y$ resp. $y \cdot g = y$ already implies $g = e$ (that is, only the identity element can map elements in Y to themselves). Finally, we call a set $G \cdot y = \{g \cdot y : g \in G\}$ resp. $y \cdot G = \{y \cdot g : g \in G\}$ an *orbit* of a left resp. right group action. Notably, the set of orbits forms a partition of Y . Intuitively, an orbit collects a (maximal) subset of elements in Y that can be transformed into each other by application of group operations.

Example 2.2 (Orbits). *Suppose \mathbb{Z}_2 is the cyclic group of order two, that is, $\mathbb{Z}_2 = \{0, 1\}$ together with addition modulo 2 as the group operation. Defining $Y = \mathbb{Z}_2 \times \mathbb{Z}_2$ and $G = \mathbb{Z}_2$, the mapping $(y_1, y_2) \cdot g = (y_1 + g, y_2 + g)$ is a free right group action. This results in the orbits $\{(0, 0), (1, 1)\} = (0, 0) \cdot G$ and $\{(1, 0), (0, 1)\} = (0, 1) \cdot G$. An analogous left action can be defined.*

If G acts from the left on two sets X and Y , we say that a function $f : X \rightarrow Y$ is *left invariant* if $f(x) = f(g \cdot x)$, and we say that it is *left equivariant* if $g \cdot f(x) = f(g \cdot x)$ holds for all $g \in G$ and $x \in X$. (Note that the spaces X and Y might be unrelated, and that the group action might behave differently in both spaces.) If G acts on X and Y from the right, the definition is analogous.

Example 2.3 (Actions on PDEs). *Consider the group $(\{+1, -1\}, \cdot)$, which acts on \mathbb{R} via multiplication. We can define a group action on the set of twice-differentiable functions $y \in C^2(\mathbb{R})$ by setting $(g \cdot y)(x) = y(-g \cdot x)$, and get $\partial_x(g \cdot y) = g \cdot (-\partial_x y)$. Hence, equivariance for $\mathcal{N}(y) = \partial_{xx}^2 y$ or $\mathcal{N}(y) = (\partial_x y)^2$ holds, but not for $\mathcal{N}(y) = \partial_x y$.*

Remark 1 (Orbits and free actions). *If G acts freely from the right on some finite set O , then the set of orbits defines an equivalence class on the elements in O . If $S \subseteq O$ is a complete collection of orbit representatives (that is, S contains exactly one element from every orbit and nothing else), then we have a one-to-one correspondence between O and $S \times G$ via the bijection $S \times G \rightarrow O, (s, g) \mapsto s \cdot g$. This fact allows us to switch back-and-forth between vectors $y \in \mathbb{C}^O$ and vector-valued functions on G , namely $y : G \rightarrow \mathbb{C}^S$, via the mapping $y_s(g) := y_{s \cdot g}$. We note that this also holds for left group actions.*

Example 2.4. *Consider $O := Y = \mathbb{Z}_2 \times \mathbb{Z}_2$ and $G = \mathbb{Z}_2$ from Example 2.2. A valid set of orbit representatives would be $S = \{(0, 0), (1, 0)\}$ and we indeed have a one-to-one correspondence between O and $S \times G$ via the identification:*

$$(0, 0) \mapsto ((0, 0), 0), \quad (1, 1) \mapsto ((0, 0), 1), \quad (1, 0) \mapsto ((1, 0), 0), \quad (0, 1) \mapsto ((1, 0), 1).$$

Intuitively, every $o \in O$ can be uniquely represented as $o = s \cdot g$ for an orbit representative $s \in S$ and a group element $g \in G$, and hence we can simply identify o with (s, g) .

Throughout this paper, we assume that G defines a free right-group action on a finite set O . By Remark 1, there is a set of orbit representatives $S \subseteq O$ such that $S \times G$ and O are in one-to-one correspondence, and that a bijection is defined by $(s, g) \mapsto s \cdot g$.

2.2. Equivariant matrices

We call a matrix $K \in \mathbb{C}^{O \times O}$ *equivariant* if it satisfies $K_{o,o'} = K_{o \cdot g, o' \cdot g}$ for all $g \in G$. Matrices of this type are used to model equivariant structures in dynamical systems. As an important property, matrix-vector multiplications involving equivariant matrices can be efficiently evaluated by *group convolutions*. Here, in view of symmetry-exploiting learning, we utilize the inherent connection of equivariant matrices with convolution kernels in two ways: First, we reduce the storage requirements, as the convolution kernel stores fewer elements than the corresponding matrix, and second, we achieve a significant speed-up in computations, as propagating the system or computing its eigenvalues may be performed by a generalized version of the Fourier transform.

To understand the connection between equivariant matrices and equivariant linear functions, Lemma 1 shows that both are equivalent for group actions that permute indices:

Lemma 1. *Suppose G acts on O from the right, $K \in \mathbb{C}^{O \times O}$ is a matrix, and a left group action on \mathbb{C}^O is defined via $(g \cdot y)_o := y_{o \cdot g^{-1}}$ for all $y \in \mathbb{C}^O$ and $o \in O$. Then the following statements are equivalent:*

- (i) K is an equivariant matrix.
- (ii) The function $f(y) = Ky$ is left equivariant.

Proof. For the direction (i) \Rightarrow (ii), pick an arbitrary $o \in O$. Then note that

$$\begin{aligned} (K(g \cdot y))_o &= \sum_{o' \in O} K_{o,o'} (g \cdot y)_{o'} = \sum_{o' \in O} K_{o \cdot g^{-1}, o' \cdot g^{-1}} y_{o' \cdot g^{-1}} \\ &= \sum_{o' \in O} K_{o \cdot g^{-1}, o'} y_{o'} = (Ky)_{o \cdot g^{-1}} = (g \cdot Ky)_o. \end{aligned}$$

It follows that $K(g \cdot y) = g \cdot Ky$, and hence f must be equivariant. For the direction (ii) \Rightarrow (i), pick $o, o' \in O$ and $g \in G$ arbitrarily. Suppose that $e_{o'} \in \mathbb{C}^O$ denotes the canonical unit vector for index o' , and note that $g \cdot e_{o'} = e_{o' \cdot g}$. Using equivariance of f ,

$$K_{o,o'} = (Ke_{o'})_o = (g^{-1} \cdot K(g \cdot e_{o'}))_o = (Ke_{o' \cdot g})_{o \cdot g} = K_{o \cdot g, o' \cdot g}.$$

It follows that K is an equivariant matrix. □

Example 2.5 (Circulant matrices; heat equation). *To give an instructive example, we consider the one-dimensional heat equation with periodic boundary conditions. After space dis-*

cretization via finite differences, we obtain a linear equation of the form

$$\dot{y} \propto \begin{bmatrix} 2 & -1 & 0 & 0 & \dots & 0 & -1 \\ -1 & 2 & -1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -1 & 0 & 0 & 0 & \dots & -1 & 2 \end{bmatrix} y.$$

This structure is typical for equivariant systems. Indeed, systems that are equivariant with respect to a cyclic group can be described by matrices whose rows are shifted versions of each other – in that case, they are called circulant matrices. More formally, one sets $O := G := \mathbb{Z}_n$ and defines a group action of G on O (that is, itself) simply by applying the group operation. One then may verify that the above-described matrix is indeed equivariant, or simply consider Example 2.6.

Example 2.6 (Block-circulant matrices). Suppose $K \in \mathbb{R}^{nm \times nm}$ is a block-circulant matrix,

$$K = \begin{bmatrix} C_0 & C_{n-1} & \dots & C_1 \\ C_1 & C_0 & \dots & C_2 \\ \vdots & \vdots & \ddots & \vdots \\ C_{n-1} & C_{n-2} & \dots & C_0 \end{bmatrix}$$

where $C_i \in \mathbb{R}^{m \times m}$, i.e., K consists of blocks of size $m \times m$. Intuitively, the number of orbits m corresponds to the size of each block, while the number of blocks n corresponds to the size of the group. To show equivariance of K with respect to $G = \mathbb{Z}_n$, we first identify $O = \{1, \dots, m\} \times G$ with $\{1, \dots, nm\}$ using the bijection $\iota : (i, j) \mapsto jm + i$. A free group action is defined on O by $(i, j) \cdot g = (i, j + g)$, and on $\{1, \dots, nm\}$ by $\iota(i, j) \cdot g = \iota((i, j) \cdot g)$. Indeed, one has for $(i, j), (i', j') \in O$,

$$K_{\iota(i,j), \iota(i',j')} = K_{jm+i, j'm+i'} = (C_{j-j'})_{i,i'} = (C_{(j+g)-(j'+g)})_{i,i'} = K_{\iota(i,j) \cdot g, \iota(i',j') \cdot g}.$$

For the orbit representatives, one can, for example, pick $S = \{(1, 0), \dots, (m, 0)\}$.

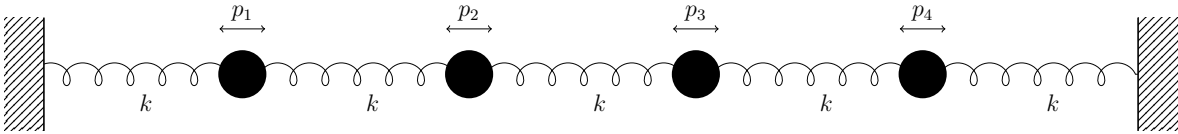


Figure 1: A spring system of four nodes connected in a row with equal stiffness coefficients. This system is equivariant with respect to reflections along the center.

Example 2.7 (Symmetric spring system¹). Consider the spring system from Figure 1, which consists of four nodes that deviate from their resting positions by $p_1(t), p_2(t), p_3(t), p_4(t) \in \mathbb{R}$,

¹Code available online, <https://github.com/graps1/convolutional-edmd>.

$p(t) = [p_1(t), p_2(t), p_3(t), p_4(t)] \in \mathbb{R}^4$. All springs have the same fixed stiffness coefficient k and the nodes have mass m . The force acting on the i -th node is given by $F_i(p)$, where

$$\begin{aligned} F_1(p) &= -2kp_1 + kp_2, & F_4(p) &= -2kp_4 + kp_3, \\ F_2(p) &= -2kp_2 + kp_1 + kp_3, & F_3(p) &= -2kp_3 + kp_2 + kp_4. \end{aligned}$$

From Newton's second law, we have $\ddot{p}(t) = F(p(t))/m$. By moving to position-velocity variables $y(t) = (p(t), \dot{p}(t)) \in \mathbb{R}^8$, we may consider the first-order differential equation $\dot{y} = Ky$, where

$$\begin{bmatrix} \dot{p}_1 \\ \dot{p}_2 \\ \dot{p}_3 \\ \dot{p}_4 \\ \ddot{p}_1 \\ \ddot{p}_2 \\ \ddot{p}_3 \\ \ddot{p}_4 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -2k/m & k/m & 0 & 0 & 0 & 0 & 0 & 0 \\ k/m & -2k/m & k/m & 0 & 0 & 0 & 0 & 0 \\ 0 & k/m & -2k/m & k/m & 0 & 0 & 0 & 0 \\ 0 & 0 & k/m & -2k/m & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \\ \dot{p}_1 \\ \dot{p}_2 \\ \dot{p}_3 \\ \dot{p}_4 \end{bmatrix}$$

This system is equivariant with respect to reflections along the center, that is, when swapping nodes 1 and 2 with nodes 4 and 3. More formally, the reflection group $G = \{e, a\}$, $aa = e$, acts on Y via

$$a \cdot [p_1 \ p_2 \ p_3 \ p_4 \ \dot{p}_1 \ \dot{p}_2 \ \dot{p}_3 \ \dot{p}_4]^T = [p_4 \ p_3 \ p_2 \ p_1 \ \dot{p}_4 \ \dot{p}_3 \ \dot{p}_2 \ \dot{p}_1]^T,$$

with e doing nothing. That is, a just reflects the p 's and \dot{p} 's along the center. One can then verify that the system satisfies $g \cdot Ky = K(g \cdot y)$ for all $g \in G$ and $y \in Y$ (this can be checked by simply computing $a \cdot Ky$ and $K(a \cdot y)$ separately). Additionally, mind that this action simply permutes vector indices, and hence K is also an equivariant matrix by means of Lemma 1. The corresponding action of G on $O = \{1, \dots, 8\}$ would then be given by e doing nothing and

$$\begin{aligned} 1 \cdot a &= 4, & 2 \cdot a &= 3, & 3 \cdot a &= 2, & 4 \cdot a &= 1, \\ 5 \cdot a &= 8, & 6 \cdot a &= 7, & 7 \cdot a &= 6, & 8 \cdot a &= 5. \end{aligned} \tag{3}$$

Convolution kernels. The convolution kernel $A : G \rightarrow \mathbb{C}^{S \times S}$ that corresponds to an equivariant matrix K is defined by

$$A_{s,s'}(g) := K_{s,s' \cdot g^{-1}}. \tag{4}$$

By assumption, G acts freely on O , and thus O and $S \times G$ are in one-to-one correspondence via the bijection $(s, g) \mapsto s \cdot g$. Therefore, vice versa, the equivariant matrix that corresponds to any kernel is (well-)defined by

$$K_{s \cdot g, s' \cdot h} := A_{s,s'}(gh^{-1}). \tag{5}$$

Equation (5) defines the inverse of (4) if one sees these equations as functions between the set of equivariant matrices and the set of convolution kernels.

The *convolution* of a kernel $A : G \rightarrow \mathbb{C}^{S \times S}$ with $u : G \rightarrow \mathbb{C}^S$ is defined by

$$A * u : G \rightarrow \mathbb{C}^S, \quad g \mapsto \sum_{h \in G} A(h)u(h^{-1}g). \quad (6)$$

By the identification of O with $S \times G$, we can define the convolution of A with a *vector* $u \in \mathbb{C}^O$ by viewing u as a function $u : G \rightarrow \mathbb{C}^S$ defined by $u_s(g) = u_{s,g}$ (see Remark 1). In the same sense, one can also view $A * u$ as a vector in \mathbb{C}^O . If K is A 's corresponding equivariant matrix, one always has

$$Ku = A * u. \quad (7)$$

Hence, if one makes use of the generalized Fourier transform, one may gain a computational advantage when it comes to computing matrix-vector products.

Example 2.8 (Symmetric spring system: Convolutions). *From Example 2.7, recall that the state can be viewed as an element of \mathbb{R}^O , where $O = \{1, \dots, 8\}$. We have defined a group action of $G = \{e, a\}$ on O via (3). The corresponding set of orbits is given by*

$$\{1, 4\}, \{2, 3\}, \{5, 8\}, \{6, 7\},$$

and we may pick the orbit representatives $S = \{1, 2, 5, 6\}$. The identification of $y \in \mathbb{R}^O$ with $y : G \rightarrow \mathbb{R}^S$ according to Remark 1 is given by

| | | | | | | | | |
|----------------------------------|----------|----------|----------|----------|-------------|-------------|-------------|-------------|
| | p_1 | p_2 | p_3 | p_4 | \dot{p}_1 | \dot{p}_2 | \dot{p}_3 | \dot{p}_4 |
| $y \in \mathbb{R}^O$ | y_1 | y_2 | y_3 | y_4 | y_5 | y_6 | y_7 | y_8 |
| $y : G \rightarrow \mathbb{R}^S$ | $y_1(e)$ | $y_2(e)$ | $y_2(a)$ | $y_1(a)$ | $y_5(e)$ | $y_6(e)$ | $y_6(a)$ | $y_5(a)$ |

Finally, let us consider the convolution kernel for the matrix K . To simplify notation, we sort S in ascending order, and view $y(e), y(a) \in \mathbb{R}^S$ as vectors in $\mathbb{R}^{|S|}$,

$$y(e) = [p_1 \ p_2 \ \dot{p}_1 \ \dot{p}_2]^T, \quad y(a) = [p_4 \ p_3 \ \dot{p}_4 \ \dot{p}_3]^T.$$

From eq. (7) together with (6), we can derive

$$\begin{bmatrix} \dot{y}(e) \\ \dot{y}(a) \end{bmatrix} = \begin{bmatrix} (A * y)(e) \\ (A * y)(a) \end{bmatrix} = \begin{bmatrix} A(e) & A(a) \\ A(a) & A(e) \end{bmatrix} \begin{bmatrix} y(e) \\ y(a) \end{bmatrix}. \quad (8)$$

Here, we view $A(e), A(a) \in \mathbb{R}^{S \times S}$ as matrices in $\mathbb{R}^{|S| \times |S|}$. From eq. (4) and the entries of K in Example 2.7, we can derive their values by inspection:

$$A(e) = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -2k/m & k/m & 0 & 0 \\ k/m & -2k/m & 0 & 0 \end{bmatrix}, \quad A(a) = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & k/m & 0 & 0 \end{bmatrix}.$$

Inserting these into (8), we obtain the following system of equations:

$$\begin{bmatrix} \dot{p}_1 \\ \dot{p}_2 \\ \ddot{p}_1 \\ \ddot{p}_2 \\ \dot{p}_4 \\ \dot{p}_3 \\ \ddot{p}_4 \\ \ddot{p}_3 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 & | & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & | & 0 & 0 & 0 & 0 \\ -2k/m & k/m & 0 & 0 & | & 0 & 0 & 0 & 0 \\ k/m & -2k/m & 0 & 0 & | & 0 & k/m & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & | & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & | & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & | & -2k/m & k/m & 0 & 0 \\ 0 & k/m & 0 & 0 & | & k/m & -2k/m & 0 & 0 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ \dot{p}_1 \\ \dot{p}_2 \\ p_4 \\ p_3 \\ \dot{p}_4 \\ \dot{p}_3 \end{bmatrix}$$

Notice that this yields the same solution as the original system. However, by re-ordering the variables, we have achieved a block-circulant format (compare eq. (8) with Example 2.6 for the case $n = 2$), which is due to the isomorphism of G with \mathbb{Z}_2 . Therefore, instead of solving the equation $\dot{y} = Ky$ by explicit construction of K , one can compute convolutions using A , if it is known. Notice also that we do not need to store the full 8×8 matrix K (ignoring its sparsity), but can rather store two 4×4 matrices, namely $A(e)$ and $A(a)$.

In the next section, we show how the Fourier transform of the convolution kernel can be used to speed up linear operations.

2.3. The generalized Fourier transform

Before introducing the generalized Fourier transform, we require the notion of a *group representation*. Essentially, a representation maps every group element to a matrix that describes the action of this element on points in space. In case of abelian groups, this notion simplifies significantly, but we are also interested in the more general case.

Group representations. A representation of a finite group G is a function $\rho : G \rightarrow \mathbb{C}^{d_\rho \times d_\rho}$, where $d_\rho \in \mathbb{N}$ is the *degree* of ρ , such that $\rho(g)$ is invertible for all $g \in G$ and compatibility with the underlying group is ensured: for $h, g \in G$, one has $\rho(h)\rho(g) = \rho(hg)$. Two representations ρ, σ with $d_\rho = d_\sigma = d$ are *equivalent* if there is an invertible $T \in \mathbb{C}^{d \times d}$ such that $\rho(g) = T^{-1}\sigma(g)T$ for all $g \in G$. A representation ρ is called *reducible* if there is an equivalent representation σ such that all $\{\sigma(g) : g \in G\}$ have the same block-diagonal structure. Finally, there exists a finite set of *irreducible* representations that are pairwise inequivalent. This set is denoted by \widehat{G} , and it satisfies $\sum_{\rho \in \widehat{G}} d_\rho^2 = |G|$.

Example 2.9 (Cyclic group). *The cyclic group \mathbb{Z}_3 has three irreducible representations: $\rho_0, \rho_1, \rho_2 : G \rightarrow \mathbb{C}$, defined by $\rho_k(g) = \exp(-2\pi i g k / 3)$ for $k = 0, 1, 2$.*

Example 2.10 (Permutation group). *The permutation group of three elements can be defined by the set of bijective functions from $\{1, 2, 3\}$ to itself together with function composition. A representation in \mathbb{R}^3 is given for $\sigma : \{1, 2, 3\} \rightarrow \{1, 2, 3\}$ by $\rho(\sigma) \in \mathbb{R}^{3 \times 3}$, with $\rho(\sigma)_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. That is, by the set of permutation matrices in \mathbb{R}^3 .*

The generalized Fourier transform. For a representation ρ , the generalized Fourier transform is defined on $u : G \rightarrow \mathbb{C}$ by

$$\widehat{u}(\rho) = \sum_{g \in G} u(g)\rho(g) \in \mathbb{C}^{d_\rho \times d_\rho}. \quad (9)$$

That is, \widehat{u} takes a representation ρ and maps it to a complex *matrix* of size $d_\rho \times d_\rho$. The inverse of the generalized Fourier transform is given by

$$u(g) = \frac{1}{|G|} \sum_{\rho \in \widehat{G}} d_\rho \text{Tr}(\rho(g^{-1})\widehat{u}(\rho)). \quad (10)$$

The *convolution theorem* connecting Fourier transformations and convolutions also holds in this case; for $u, v : G \rightarrow \mathbb{C}$, one has $\widehat{u * v}(\rho) = \widehat{u}(\rho)\widehat{v}(\rho)$ (see, for example, [Terras \(1999\)](#), Theorem 4, p. 261).² For the general case of matrices and vectors, let $A : G \rightarrow \mathbb{C}^{S \times S}$ and $u : G \rightarrow \mathbb{C}^S$ and introduce:

$$\begin{aligned} \widehat{A}(\rho) &\in \mathbb{C}^{(S \times D_\rho) \times (S \times D_\rho)}, & \widehat{A}_{(s,i),(s',j)}(\rho) &:= (\widehat{A}_{s,s'})_{i,j}(\rho), \\ \widehat{u}(\rho) &\in \mathbb{C}^{(S \times D_\rho) \times D_\rho}, & \widehat{u}_{(s',j),k}(\rho) &:= (\widehat{u}_{s'})_{j,k}(\rho), \end{aligned}$$

where $D_\rho = \{1, \dots, d_\rho\}$. Intuitively, this way we treat the $S \times S$ resp. S like batch dimensions by defining the Fourier transform individually for every $A_{s,s'}$ and u_s . Here, $\widehat{A}(\rho)$ and $\widehat{u}(\rho)$ can also be seen as matrices with shape $|S|d_\rho \times |S|d_\rho$ and $|S|d_\rho \times d_\rho$. This perspective is comfortable because it extends the convolution theorem to matrix multiplication:

$$\widehat{A * u}(\rho) = \widehat{A}(\rho)\widehat{u}(\rho). \quad (11)$$

Eigenvalues and eigenvectors. As discussed by [Åhlander and Munthe-Kaas \(2006\)](#), the Fourier transform closely connects the eigenvalues of group convolutions with the eigenvalues of $\widehat{A}(\rho)$, where ρ ranges over the irreducible representations:

Proposition 1 ([\(Åhlander and Munthe-Kaas, 2006, Proposition 2\)](#)). *Let $A : G \rightarrow \mathbb{C}^{S \times S}$ be a convolution kernel. Then,*

1. *If λ is an eigenvalue of $u \mapsto A * u$, then there is $\rho \in \widehat{G}$ s.t. λ is an eigenvalue of $\widehat{A}(\rho)$.*
2. *If λ is an eigenvalue of $\widehat{A}(\rho)$ for a $\rho \in \widehat{G}$, then λ is a d_ρ -fold eigenvalue of $u \mapsto A * u$.*

Besides eigenvalues, [Åhlander and Munthe-Kaas \(2006\)](#) also describe how one can obtain the corresponding eigenvectors, that is, those $v : G \rightarrow \mathbb{C}^S$ that satisfy $A * v = \lambda v$ for some eigenvalue λ . Since $v \mapsto A * v$ is a linear operation on vectors of size $|S||G|$, there are equally many eigenvectors, and one can index them by (σ, i, j) , where $\sigma \in \widehat{G}$, $i = 1, \dots, |S|d_\sigma$ and $j = 1, \dots, d_\sigma$ (this follows from $\sum_{\sigma \in \widehat{G}} d_\sigma^2 = |G|$). For (σ, i, j) fixed, let (λ, ξ) be the i -th eigenpair of the Fourier-transformed kernel at σ ,

$$\widehat{A}(\sigma)\xi = \lambda\xi.$$

²Here, the convolution of u with v is defined as in [\(6\)](#), resulting in a function $u * v : G \rightarrow \mathbb{C}$.

Define v in Fourier space by a zero-padded version of ξ , i.e., $\widehat{v}(\rho) \in \mathbb{C}^{|S|d_\rho \times d_\rho}$ with:

$$\widehat{v}_{\bullet,\ell}(\rho) = \begin{cases} \xi & \text{if } \ell = j \text{ and } \rho = \sigma, \\ 0 & \text{else} \end{cases}$$

for all $\rho \in \widehat{G}$ and $\ell = 1, \dots, d_\rho$. Note that $\widehat{A}(\rho)\widehat{v}(\rho) = \lambda\widehat{v}(\rho)$ holds for all $\rho \in \widehat{G}$. Using the convolution theorem (11) and the inverse Fourier transform, one can then see that (λ, v) is an eigenpair of $u \mapsto A * u$. By ranging over all (σ, i, j) , this procedure allows one to construct a full set of eigenvectors.

If K is A 's corresponding equivariant matrix, then every eigenpair of $u \mapsto A * u$ is a *right* eigenpair of K . *Left* eigenpairs of K correspond to right eigenpairs of K^T , and hence we can compute them by introducing a “transposed” kernel

$$A^T : G \rightarrow \mathbb{C}^{S \times S}, \quad (A^T)_{s,s'}(g) := A_{s',s}(g^{-1}),$$

that computes the matrix-vector product $K^T u = A^T * u$. Therefore, one can construct *left* eigenpairs of K by computing eigenpairs of $u \mapsto A^T * u$ in the above-described way. (This is in particular necessary when it comes to approximating eigenfunctions of the Koopman operator.)

Plancherel's identity. This result relates the norm of $u : G \rightarrow \mathbb{C}^S$ with a “weighted” norm of its Fourier transform. Recall that $\widehat{u}(\rho)$ can be seen as a $|S|d_\rho \times d_\rho$ matrix. From this perspective, the two norms considered here are

$$\|u\|^2 := \sum_{s \in S} \|u_s\|_2^2 \quad \text{and} \quad \|\widehat{u}\|^2 := \frac{1}{|G|} \sum_{\rho \in \widehat{G}} d_\rho \|\widehat{u}(\rho)\|_F^2,$$

where $\|\cdot\|_F$ is the Frobenius norm. In particular, if $u : G \rightarrow \mathbb{C}$, Plancherel's identity (see, for example, (Terras, 1999, Theorem 2, p. 258, exercise on p. 263)) states that $\|u\|^2 = \|\widehat{u}\|^2$. Even further, one can see that it also holds for the case $u : G \rightarrow \mathbb{C}^S$:

$$\|u\|^2 = \sum_{s \in S} \frac{1}{|G|} \sum_{\rho \in \widehat{G}} d_\rho \|\widehat{u}_s(\rho)\|_F^2 = \frac{1}{|G|} \sum_{\rho \in \widehat{G}} d_\rho \sum_{s \in S} \|\widehat{u}_s(\rho)\|_F^2 = \frac{1}{|G|} \sum_{\rho \in \widehat{G}} d_\rho \|\widehat{u}(\rho)\|_F^2 = \|\widehat{u}\|^2.$$

We state this result independently:

Lemma 2 (Plancherel's identity). *For $u : G \rightarrow \mathbb{C}^S$, one has $\|u\|^2 = \|\widehat{u}\|^2$.*

Abelian groups. If G is abelian, then the situation simplifies significantly. In this case, G can be expressed as the direct sum of cyclic groups, $G = \mathbb{Z}_{p_1} \oplus \dots \oplus \mathbb{Z}_{p_m}$. Assuming that we can decompose G this way, the order of every irreducible representation $\rho \in \widehat{G}$ is exactly $d_\rho = 1$, and moreover, we can write $\widehat{G} = \{\rho_g : g \in G\}$ with

$$\rho_g(h) = \exp(-2\pi i \sum_{n=1}^m g_n h_n / p_n) \in \mathbb{C}.$$

The Fourier transform simplifies to:

$$\widehat{u}(\rho_g) = \sum_{h \in G} u(h) \exp(-2\pi i \sum_{n=1}^m g_n h_n / p_n),$$

which is essentially the multi-dimensional discrete Fourier transform. For the multi-channel case, $\widehat{A}(\rho)$ is a matrix in $\mathbb{C}^{S \times S}$ and $\widehat{u}(\rho)$ a vector in \mathbb{C}^S . Note that Proposition 1 also simplifies in the sense that the multiplicity of the eigenvalues vanishes.

3. Group-convolutional EDMD: Theory and Application

In this section, we show how equivariant structures can be exploited in EDMD when the observables are appropriately defined. We build on the previously established results from Sections 2.1 to 2.3 to show a number of results: The first result concerns the “optimality” of convolutions (Theorem 3.1), that is, we show that there is indeed an optimal equivariant EDMD matrix under certain conditions. Next, we show how one can construct appropriate observables, how one can learn the convolution kernel, and how one can approximate eigenfunctions of the Koopman operator.

Recall from Section 2 that Φ defines a flow on a state space Y , stemming, for instance, from the discretization of an ODE or PDE in time. Additionally, Y comes with a probability measure P that allows us to draw samples from it. To define the EDMD loss, we additionally require that the observables are square-integrable and indexed by a finite set O , i.e., $\psi : Y \rightarrow \mathbb{C}^O$ with $\psi_o, \mathcal{K}\psi_o \in L_P^2(Y)$ for all $o \in O$. Finally, recall that G denotes a finite group.

Our assumptions are then:

- (A1) G acts on Y from the left, and it acts freely on O from the right.
- (A2) $\psi_o(g \cdot y) = \psi_{o \cdot g}(y)$ for $g \in G, o \in O$ and $y \in Y$.
- (A3) $\Phi(g \cdot y) = g \cdot \Phi(y)$ for $g \in G$ and $y \in Y$.
- (A4) If $\mathbf{y} \sim P$, then $g \cdot \mathbf{y} \sim P$.

Assumption (A1) is very basic; it ensures that the group can act on both the system state and the observables. Intuitively, we need a group action on the system state to even consider group-based methods, and we need a group action on the index set of the observables so that the equivariance of the underlying system carries over to the level of observables. The next assumptions (A2) and (A3) are in the same spirit; the second ensures that the group operation can shift from state to observation level and the third assumes left equivariance of the system dynamics.³ Finally, (A4) ensures that the underlying distribution is invariant with respect to group actions. That is, acting on states does not change the probability.

Our main result is now as follows:

Theorem 3.1. *Under (A1), (A2), (A3) and (A4), there is an equivariant EDMD matrix.*

³Note that assumption (A3) already implies equivariance of the Koopman operator: One can define a group action on observables of the form $f : Y \rightarrow \mathbb{C}$ by $(g \cdot f)(y) := f(g^{-1} \cdot y)$. The Koopman operator then satisfies $\mathcal{K}(g \cdot f) = g \cdot (\mathcal{K}f)$ (see Theorem III.1 in Salova et al. (2019)).

(Before going into the proof, note that the minimization problem (1) can have multiple solutions if no further restriction are applied. However, under suitable conditions, the solution is unique (see, e.g., (Philipp et al., 2024, Lemma C.2)). In that case, according to this theorem, the unique optimal EDMD matrix must be equivariant.)

Proof. Introduce $\mathbf{u} = \psi(\mathbf{y})$ and $\mathbf{u}^+ = \mathcal{K}\psi(\mathbf{y})$, and define $\ell(K) = \mathbb{E}_{\mathbf{y} \sim P}[\|K\mathbf{u} - \mathbf{u}^+\|^2]$, so that an EDMD matrix satisfies $K \in \arg \min_{K \in \mathbb{C}^{O \times O}} \ell(K)$. It suffices to fix an arbitrary K and to show that there is an equivariant matrix K' such that $\ell(K) \geq \ell(K')$.

Let $S \subseteq O$ be a set of orbit representatives. Since G defines a free action on O by (A1), the mapping $(s, g) \mapsto s \cdot g$ constitutes a bijection between $S \times G$ and O (see also Remark 1). Hence,

$$\ell(K) = \sum_{g \in G} \sum_{s \in S} \mathbb{E}_{\mathbf{y} \sim P}[(K\mathbf{u})_{s \cdot g} - \mathbf{u}_{s \cdot g}^+]^2. \quad (12)$$

Select the group element that minimizes the inner sum:

$$g_\star \in \arg \min_{g \in G} \sum_{s \in S} \mathbb{E}_{\mathbf{y} \sim P}[(K\mathbf{u})_{s \cdot g} - \mathbf{u}_{s \cdot g}^+]^2.$$

We then define K' by setting

$$K'_{s \cdot g, s' \cdot h} := K_{s \cdot g_\star, s' \cdot h g_\star^{-1}},$$

and note that it is indeed equivariant. Then, for arbitrary $g \in G$ and $s \in S$,

$$\begin{aligned} (K'\psi(g \cdot \mathbf{y}))_{s \cdot g_\star g^{-1}} &= \sum_{(s', h) \in S \times G} K'_{s \cdot g_\star g^{-1}, s' \cdot h} \psi_{s' \cdot h}(g \cdot \mathbf{y}) \\ &= \sum_{(s', h) \in S \times G} K'_{s \cdot g_\star, s' \cdot h g} \psi_{s' \cdot h g}(\mathbf{y}) \end{aligned} \quad (13)$$

$$= \sum_{(s', h) \in S \times G} K_{s \cdot g_\star, s' \cdot h g} \psi_{s' \cdot h g}(\mathbf{y}) \quad (14)$$

$$= \sum_{(s', h) \in S \times G} K_{s \cdot g_\star, s' \cdot h} \psi_{s' \cdot h}(\mathbf{y}) \quad (15)$$

$$= (K\psi(\mathbf{y}))_{s \cdot g_\star}. \quad (16)$$

Equation (13) uses (A2) and equivariance of K' . Then (14) follows by definition of K' . Finally, (15) holds by the substitution $h \mapsto h g_\star^{-1}$. Hence,

$$\ell(K) \geq \sum_{(s, g) \in S \times G} \mathbb{E}_{\mathbf{y} \sim P}[(K\mathbf{u})_{s \cdot g_\star} - \mathbf{u}_{s \cdot g_\star}^+]^2 \quad (17)$$

$$= \sum_{(s, g) \in S \times G} \mathbb{E}_{\mathbf{y} \sim P}[(K'\psi(g \cdot \mathbf{y}))_{s \cdot (g_\star g^{-1})} - \psi_{s \cdot g_\star}(\Phi(\mathbf{y}))]^2 \quad (18)$$

$$= \sum_{(s, g) \in S \times G} \mathbb{E}_{\mathbf{y} \sim P}[(K'\psi(g \cdot \mathbf{y}))_{s \cdot (g_\star g^{-1})} - \psi_{s \cdot (g_\star g^{-1})}(\Phi(g \cdot \mathbf{y}))]^2 \quad (19)$$

$$= \sum_{(s, g) \in S \times G} \mathbb{E}_{\mathbf{y} \sim P}[(K'\mathbf{u})_{s \cdot (g_\star g^{-1})} - \mathbf{u}_{s \cdot (g_\star g^{-1})}^+]^2 \quad (20)$$

$$= \sum_{(s, g) \in S \times G} \mathbb{E}_{\mathbf{y} \sim P}[(K'\mathbf{u})_{s \cdot g} - \mathbf{u}_{s \cdot g}^+]^2 = \ell(K').$$

Equation (17) is obtained when bounding the outer sum in (12) from below by substituting $g \mapsto g_\star$. Then, (18) holds by (16) and definition of \mathbf{u}^+ . Applying (A3) and (A2), we get (19). Then we can apply the substitution $g \cdot \mathbf{y} \mapsto \mathbf{y}$ inside the expectation by (A4), and reintroduce \mathbf{u} and \mathbf{u}^+ . Finally, we reorder the summation using the substitution $g \mapsto g^{-1} g_\star$. \square

Constructing observables. In order to construct observables satisfying [\(A1\)](#) and [\(A2\)](#), one can start with an arbitrary finite set S and a set of *generating* observables $\chi : Y \rightarrow \mathbb{C}^S$ that are then expanded using the group. Letting $O = S \times G$, we obtain a full set of observables by setting $\psi : Y \rightarrow \mathbb{C}^O$, where $\psi_{(s,g)}(y) = \chi_s(g \cdot y)$. Indeed, G defines a free right-group action on O via $(s, h) \cdot g = (s, hg)$, and we see that it satisfies [\(A2\)](#):

$$\psi_{(s,h)}(g \cdot y) = \chi_s(h \cdot (g \cdot y)) = \chi_s((hg) \cdot y) = \psi_{(s,hg)}(y) = \psi_{(s,h) \cdot g}(y).$$

This argument also works the other way around: We can obtain a set of generating observables given that ψ satisfies [\(A1\)](#) and [\(A2\)](#): In that case, since G acts freely on O , there is a finite set of orbit-representatives $S \subseteq O$ such that $(s, g) \mapsto s \cdot g$ is a bijection between $S \times G$ and O . Therefore, one can define a selection of generating observables by setting $\chi_s(y) = \psi_s(y)$, $s \in S$, and recover $\psi_{s \cdot g}(y)$ using [\(A2\)](#) and the identity $\psi_s(g \cdot y) = \chi_s(g \cdot y)$. (Constructing observables this way appears to be similar to that of [Salova et al. \(2019\)](#).)

Example 3.1. *Suppose the state space Y contains functions of the form $y : [0, 1) \rightarrow \mathbb{R}$. The group $G = \mathbb{Z}_n$ can act on Y via periodic shifts: For $g \in G$, define*

$$(g \cdot y)(x) := y(x - g/n \bmod 1).$$

In order to obtain a set of generating observables, one may define $S = \{1, 2, 3\}$ and

$$\chi(y) = [y(0) \quad y(0)^2 \quad y(0)^3].$$

That is, $\chi(y)$ simply observes the state's value at the origin in various ways. The full set of observables $\psi : Y \rightarrow \mathbb{C}^O$ is obtained when shifting the state periodically and then observing it at the origin by means of χ . Practically, this has the same effect as observing the original state at different coordinates: Viewing $\psi(y)$ as a matrix in $\mathbb{C}^{|G| \times |S|}$:

$$\psi(y) = \begin{bmatrix} \chi(0 \cdot y) \\ \chi((n-1) \cdot y) \\ \chi((n-2) \cdot y) \\ \vdots \\ \chi(1 \cdot y) \end{bmatrix} = \begin{bmatrix} y(0) & y(0)^2 & y(0)^3 \\ y(1/n) & y(1/n)^2 & y(1/n)^3 \\ y(2/n) & y(2/n)^2 & y(2/n)^3 \\ \vdots & \vdots & \vdots \\ y(1 - 1/n) & y(1 - 1/n)^2 & y(1 - 1/n)^3 \end{bmatrix}.$$

Training. Instead of constructing a full equivariant EDMD matrix, we can compute its convolution kernel instead. That is, we can solve the problem

$$\min_{A: G \rightarrow \mathbb{C}^{S \times S}} \mathbb{E}[\|A * \mathbf{u} - \mathbf{u}^+\|^2],$$

where \mathbf{u} and \mathbf{u}^+ are $G \rightarrow \mathbb{C}^S$ -valued random variables with an arbitrary distribution. A convenient way is to do it in Fourier space. Using Plancherel's identity ([Lemma 2](#)) and the convolution theorem ([11](#)), one has

$$\mathbb{E}[\|A * \mathbf{u} - \mathbf{u}^+\|^2] = \frac{1}{|G|} \sum_{\rho \in \widehat{G}} d_\rho \mathbb{E}[\|\widehat{A}(\rho) \widehat{\mathbf{u}}(\rho) - \widehat{\mathbf{u}^+}(\rho)\|_F^2],$$

where $\|\cdot\|_F$ is the Frobenius norm. When minimizing the right-hand side, notice that the $\{\widehat{A}(\rho) : \rho \in \widehat{G}\}$ are independent. Hence, we can individually solve $|\widehat{G}|$ least-squares problems:

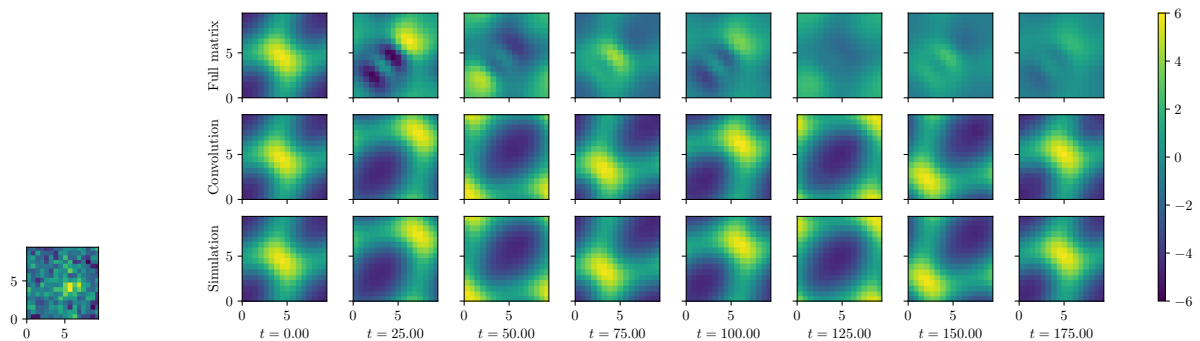
$$\min_{\widehat{A}(\rho) \in \mathbb{C}^{|S|d_\rho \times |S|d_\rho}} \mathbb{E}[\|\widehat{A}(\rho)\widehat{\mathbf{u}}(\rho) - \widehat{\mathbf{u}}^+(\rho)\|_F^2], \quad (21)$$

i.e., one for every representation. To recover A , one can apply the inverse Fourier transform.

Eigenfunctions. One commonly approximates eigenfunctions of the Koopman operator by taking left eigenpairs (λ, v) of the EDMD matrix, i.e., $v^T K = \lambda v^T$, and introducing $f(y) = v^T \psi(y) = \sum_{o \in O} v_o \psi_o(y)$ (see, e.g., Williams et al. (2015)) to approximate an eigenfunction. Indeed, one has

$$\mathcal{K}f(y) = \mathcal{K}(v^T \psi)(y) = v^T \mathcal{K}\psi(y) \approx v^T K\psi(y) = \lambda v^T \psi(y) = \lambda f(y).$$

If the EDMD matrix is equivariant, then one can simply compute eigenpairs of its “transposed” convolution kernel using the approach from Section 2.3.



(a) Initial state.

(b) System dynamics and predicted trajectories in the low-data regime.

Figure 2: Experimental setup: The Kuramoto–Sivashinsky equation is solved in two spatial dimensions with periodic boundary conditions. Starting from the shown initial state, the system converges to a periodic attractor (bottom row), and its evolution is predicted using a group-convolutional and a full-matrix EDMD approach.

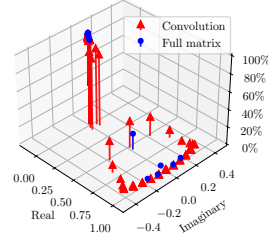
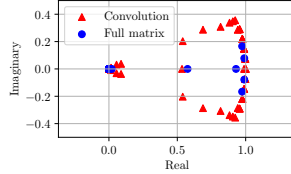
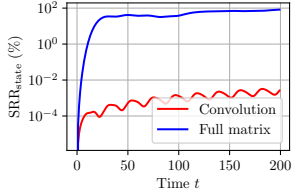
3.1. Experiments: Partial-differential equations with periodic boundary conditions

The goal of this section is to demonstrate the convolutional EDMD approach on the two-dimensional Kuramoto-Sivashinsky (KS) equation (2). Insofar, we utilize the results Section 3 and show how to 1) construct observables using the notion of generating observables, 2) how to learn a convolution kernel in Fourier space, and 3) how to approximate eigenfunctions of the Koopman operator by computing eigenvectors of convolutions.⁴

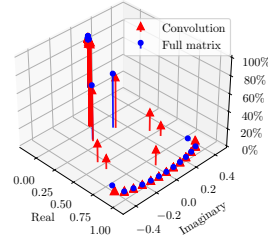
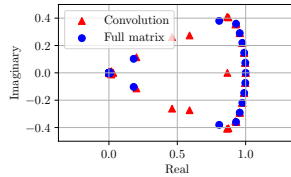
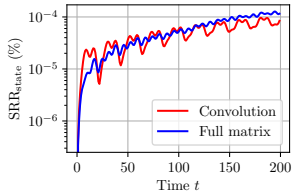
Before going into details, let us remark on some methodical aspects. The error (1) is generally smaller if the EDMD matrix is left unconstrained, i.e., forcing it to be equivariant can only increase it. But there are two advantages that come with equivariant matrices:

⁴Code and detailed description available online, <https://github.com/graps1/convolutional-edmd>.

Low-data regime



Large-data regime



Deviation from true trajectory as a function of time over the test set.

Eigenvalues of the approximated eigenfunctions in the complex plane.

The SRR of each approximated eigenfunction plotted against the location of its eigenvalue.

Table 1: Experimental comparison of the convolutional with the full-matrix EDMD approach in the low and large data-regimes: Model performance over time (left column), eigenvalues (center column), quality of eigenfunctions (right column).

Firstly, the additional structure means that fewer parameters are learned, and thus, if the expectation in (1) is approximated using only few data points, an equivariant approach may compute better solutions. Secondly, if the group is large and if the Fourier transform can be computed efficiently, then convolutions may provide a computational advantage over a full-scale EDMD matrix. Therefore, we conduct one experiment in the “low-data” and one experiment in the “large-data” regime. For each case, we learn both an equivariant EDMD matrix that is represented by a convolution kernel, and a full-scale EDMD matrix that is left unconstrained.

Setup. The PDE is simulated on a small periodic domain of size $\Omega = [0, L) \times [0, L)$, $L = 3\pi$. The dynamics of the KS equation become chaotic for larger domain sizes, but for our chosen initial condition (see Figure 2a) and domain size, the solution tends to a periodic wave that travels from the lower left to the upper right corner (see the lower row in Figure 2b). We assume that its states are of the form $y(t) \in Y \subseteq C^\infty(\Omega)$ for $t \geq 0$ and that a flow $\Phi : Y \rightarrow Y$ is given, which solves the equation given by \mathcal{N} in (2) in time steps of $\delta = 1$. Because of the periodic boundary conditions and independence of the spatial coordinate, this PDE is equivariant with respect to the group $G = \mathbb{Z}_n \times \mathbb{Z}_n$, $n \in \mathbb{N}$, acting on $y \in Y$ via

$$(g \cdot y)(x) = y(x - gL/n \pmod L).$$

One can then show that equivariance holds for the PDE-operator \mathcal{N} , which carries over to the PDE’s flow (see, e.g., [Harder et al. \(2024\)](#)). Here, periodicity of the boundary conditions is important. We simulate the system’s trajectory starting from the initial state (Figure 2a) until it settles onto its attractor, and record the trajectory for another 300 steps. For the low-data regime, we select only 20 input-output pairs from the training data, and for the large-data regime, we select all training samples. Another 200 separate samples make up the test data, used for evaluation.

Observables. For each experiment, we construct observables by selecting 5 random coordinates $x_s \in \Omega$ for $s \in S := \{1, \dots, 5\}$, at which we simply measure the state of the PDE,

$$\chi : Y \rightarrow \mathbb{C}^S, \quad \chi_s(\mathbf{y}) := y(x_s).$$

This defines a set of *generating* observables that are expanded to a full set of base observables indexed by $O = S \times G$ using the approach of Section 3:

$$\psi : Y \rightarrow \mathbb{C}^O, \quad \psi_{(s,g)}(\mathbf{y}) := \chi_s(g \cdot \mathbf{y}).$$

The underlying group is set to $G = \mathbb{Z}_4 \times \mathbb{Z}_4$, so there are $|S||G| = 5 \cdot 16 = 80$ base observables in total. Therefore, the complete EDMD matrix has $80^2 = 6,400$ parameters, while a convolution kernel has $|S|^2|G| = 5^2 \cdot 16 = 400$. For the plot in Figure 2b, we discretized the spatial domain into $16 \times 16 = 256$ equispaced nodes. The discretized state at time t is then given by $\bar{\mathbf{y}}(t) \in \mathbb{R}^{256}$. In order to reconstruct $\bar{\mathbf{y}}(t)$ from $\psi(\mathbf{y}(t))$, we solve an additional least-squares problem

$$\min_{B \in \mathbb{R}^{256 \times |O|}} \mathbb{E}_{\mathbf{y} \sim P_{\text{test}}} [\|B\psi(\mathbf{y}) - \bar{\mathbf{y}}\|_F^2]$$

and apply B to the EDMD prediction of $\psi(\mathbf{y}(t))$ to infer $\bar{\mathbf{y}}(t)$.

Training. Following Section 3, one can learn the optimal convolution kernel in Fourier space, which amounts to $|\hat{G}| = |G| = 16$ small problems. Since G is abelian, the generalized Fourier transform is simply a two-dimensional discrete Fourier transform (see end of Section 2.3), with fast implementations widely available. Additionally, we solve the single large problem (1) for the full EDMD matrix.

Eigenvalues and eigenfunctions. Eigenvalues are computed using Proposition 1, and eigenfunctions are approximated by computing eigenpairs of the “transposed” convolution. To demonstrate the correctness of the approximated eigenfunctions, one defines the *squared relative residual* (SRR), see [Colbrook et al. \(2023\)](#):

$$\text{SRR}_{\text{eig}}(\lambda, f) = 100\% \cdot \frac{\mathbb{E}_{\mathbf{y} \sim P_{\text{test}}} [|\mathcal{K}f(\mathbf{y}) - \lambda f(\mathbf{y})|^2]}{\mathbb{E}_{\mathbf{y} \sim P_{\text{test}}} [|f(\mathbf{y})|^2]}, \quad (22)$$

where $f \in L^2_p(Y)$ and $\lambda \in \mathbb{C}$. We approximate the SRR by averaging over the test samples.

Evaluation. For each training trajectory, we use both EDMD models to predict the future state over the prediction horizon, starting from the last training sample of the same trajectory. We compare the predicted states to the result of running the full-order model. To compare the generated states, we employ another squared relative residual, this time as a function of time t : If $\varphi(t)$ for $t = 0, \delta, 2\delta, \dots$ is the predicted trajectory (that is, $\varphi(t) = K\varphi(t - \delta)$ for full EDMD and $\varphi(t) = A * \varphi(t - \delta)$ for the convolutional approach, with $\varphi(0) = \psi(y(0))$ in both cases), then

$$\text{SRR}_{\text{state}}(t) = 100\% \cdot \frac{\|\varphi(t) - \psi(y(t))\|^2}{\|\psi(y(t))\|^2}. \quad (23)$$

Results. In the *low-data regime*, the convolutional approach is able to capture the system dynamics with low error, see Figure 2b, whereas the full-matrix EDMD approach fails to learn; its eigenvalues have magnitude smaller than one, leading to a decay of the system state. The deviation from the true trajectory is depicted in the left column of Table 1 and underlines the significantly improved performance of the convolutional approach. Additionally, we can see that it accurately captures most of the eigenvalue spectrum (center column, top row) compared to the eigenvalues in the large-data regime (center column, bottom row). The leading eigenfunctions of the convolutional approach have a high quality in terms of the SRR, see the right column, and do not improve much with more data. In the *large-data regime*, both approaches work well, but the convolutional EDMD approach has lower error, even though both performances are comparable to the convolutional approach in the low-data regime. (A figure such as Figure 2b for the large-data regime is left out for brevity since the error is not recognizable by eye.) Here, the eigenvalues of both convolutional and full-matrix approach are in strong agreement, especially for the ones that have large magnitude, and both approaches perform similarly in terms of the SRR of their computed eigenfunctions.

4. Conclusion

We have shown that enforcing group-equivariant structures in the EDMD matrix can be useful for a few reasons. For example, one needs less data since the number of free parameters is reduced, and one may improve computational speed by means of fast (generalized) Fourier transforms. In view of practical applications we have illustrated that a convolutional approach may provide an advantage in the low-data regime by conducting experiments on the two-dimensional Kuramoto–Sivashinsky equation. Indeed, as we have argued, using an equivariant structure is also well-justified in face of Theorem 3.1. For future work, there are two main avenues that one can pursue: Firstly, one could investigate systems that are only “semi”-equivariant, for example, equivariant PDEs that have Dirichlet or Neumann instead of periodic boundary conditions. For the second avenue, one could investigate finite-data error bounds: The improved convergence of a convolutional method (when varying the number of data points) over a full-EDMD approach is likely better in theory too, and not only in practice.

5. Acknowledgments

S.P. and H.H. acknowledge financial support by the project “SAIL: SustAInable Life-cycle of Intelligent Socio-Technical Systems” (Grant ID NW21-059D), which is funded by the program “Netzwerke 2021” of the Ministry of Culture and Science of the State of Northrhine Westphalia, Germany. F.P. was funded by the Carl Zeiss Foundation within the project DeepTurb–Deep Learning in and from Turbulence. He was further supported by the free state of Thuringia and the German Federal Ministry of Education and Research (BMBF) within the project THInKI–Thüringer Hochschulinitiative für KI im Studium.

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