

Data-driven approximation of Koopman operators and generators: Convergence rates and error bounds

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Abstract

Global information about dynamical systems can be extracted by analysing associated infinite-dimensional transfer operators, such as the Perron–Frobenius and Koopman operators as well as their infinitesimal generators. In practice, these operators typically need to be approximated from data. Popular approximation methods are *extended dynamic mode decomposition* (EDMD) and *generator extended mode decomposition* (gEDMD). We propose a unified framework that leverages Monte Carlo sampling to approximate the operator of interest on a finite-dimensional space spanned by a set of basis functions. Our framework contains EDMD and gEDMD as special cases, but can also be used to approximate more general operators. Our key contributions are proofs of the convergence of the approximating operator and its spectrum under non-restrictive conditions. Moreover, we derive explicit convergence rates and account for the presence of noise in the observations. Whilst all these results are broadly applicable, they also refine previous analyses of EDMD and gEDMD. We verify the analytical results with the aid of several numerical experiments.

1 Introduction

Dynamical systems are a vital tool to describe deterministic and stochastic processes in science and engineering: the motion of celestial bodies, dynamics of molecules, or the development of the human brain. Even the most complex dynamical systems can often be analysed by studying certain associated linear operators such as the Koopman operator, the Perron–Frobenius operator, and their generators [1, 2, 3, 4]. These operators have been used in a wide range of fields, such as molecular dynamics [5, 6], fluid dynamics [7, 8], and engineering [9, 10]. Koopman and Perron–Frobenius operators allow us to study the evolution of *observables*, such as the velocity, acceleration, or energy of the system, and *probability densities*. The generators of these operators are used to study the temporal rate of change of observables and densities, respectively.

As a result, the investigation of our dynamical system reduces to having access to a linear operator \mathcal{A} , which acts on observables or probability densities of our system. The goal of *data-driven methods* is to obtain an approximation $\hat{\mathcal{A}}_{NM}$ of \mathcal{A} using the information derived from studying the system using only a finite amount of observables ψ_1, \dots, ψ_N and training points $\mathbf{x}_1, \dots, \mathbf{x}_M$. These

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methods gained considerable interest in the literature in recent years, and various methods have been developed to address this problem; some of the most notable are *dynamic mode decomposition* (DMD) [11, 12, 13], which relies on a least-squares estimate of the Koopman operator using a set of linear basis functions, *extended dynamic mode decomposition* EDMD [14, 15], which can be regarded as a nonlinear generalization of DMD, and *generator extended dynamic mode decomposition* (gEDMD) [16, 17], which approximates the infinitesimal generator of the Koopman operator.

More recently, the convergence of these methods has been analysed. Convergence properties of EDMD were studied in [18], though no error bounds were given. The rate of convergence of gEDMD has been studied in [19, 20, 21]. However, all these works require strong assumptions that may be impossible to verify in practice. In this work, our goal is to resolve these limitations. Our main contributions are as follows:

1. **A common framework:** We introduce a unified framework to study methods for the data-driven analysis of dynamical systems (such as, but not limited to, EDMD and gEDMD). Within this framework, a linear operator \mathcal{A} is estimated using a Monte Carlo approximation, denoted by $\hat{\mathcal{A}}_{NM}$. This approximation utilises M Monte Carlo samples to estimate \mathcal{A}_N , which is the projection of \mathcal{A} onto the dictionary space $\mathcal{F}_N = \text{span}(\psi_1, \dots, \psi_N)$.
2. **Convergence:** We show that $\hat{\mathcal{A}}_{NM}$ is the projection of \mathcal{A} onto the space of empirical samples $\hat{\mathcal{F}}_{NM}$, almost sure convergence of $\hat{\mathcal{A}}_{NM}$ to \mathcal{A}_N , and convergence of eigenvalues and eigenfunctions of $\hat{\mathcal{A}}_{NM}$ along a subsequence.
3. **Error bounds:** We derive bounds for the approximation errors $\|\hat{\mathcal{A}}_{NM} - \mathcal{A}_N\|$ and $\|\hat{\mathcal{A}}_{NM} - \mathcal{A}\|$ and then extend these results to the case of noisy observations.
4. **Minimal assumptions:** The above results are derived under minimal assumptions, which are described at the end of Section 2.

The outline of the article is as follows: In Section 2, we introduce Koopman and Perron–Frobenius operators and the mathematical setting for our problem. In Sections 3, 4 and 6, we prove Contribution 2. In Section 5, we prove Contribution 3. In Section 7, we provide numerical simulations to illustrate our results. We conclude with a discussion and some recommendations based on the theoretical and numerical results in Section 8. Our approach in Sections 3 and 4 is heavily influenced by the results in [18], and our work in Section 5 is more closely related to that of [21, 22]. However, we develop these results under a more general framework in which an arbitrary operator is estimated and under weaker assumptions.

2 A general framework for data-based recovery of dynamics

In this section, we will introduce the required mathematical concepts and the notation used throughout the paper.

2.1 Notation

Let E be a generic vector space. We define a family of N vectors by $\Psi = \{\psi_n\}_{n=1}^N \subseteq E$. Given such a family of vectors, we define as usual $\text{span}(\Psi)$ to be the smallest vector space containing Ψ . An operator $\mathcal{T}: \text{span}(\Psi) \rightarrow \text{span}(\Psi)$ can be represented by a matrix which we denote by $\mathbf{T}^\Psi \in \mathbb{R}^{N \times N}$. It is given by

$$\mathcal{T}\psi_j = \sum_{i=1}^N \mathbf{T}_{ij}^\Psi \psi_i, \quad j = 1, \dots, N.$$

We denote the Euclidean norm of a vector $\mathbf{v} \in \mathbb{C}^N$ by $|\mathbf{v}|$. Given an operator $\mathcal{T}: \mathcal{D} \rightarrow \mathcal{F}$ between normed spaces and a matrix $\mathbf{T} \in \mathbb{C}^{N \times N}$, we denote the induced operator norms of \mathcal{T} and \mathbf{T} and

the Frobenius norm of \mathbf{T} by

$$\|\mathcal{T}\| := \sup_{\|\phi\|_{\mathcal{D}}=1} \|\mathcal{T}\phi\|_{\mathcal{F}}, \quad \|\mathbf{T}\| := \sup_{|\mathbf{v}|=1} |\mathbf{T}\mathbf{v}|, \quad \|\mathbf{T}\|_F := \sum_{i,j=1}^N |\mathbf{T}_{ij}|^2,$$

respectively.

We define random objects, such as random variables, stochastic processes, and random flows on a common underlying probability space $(\Omega, \mathfrak{A}, \mathbb{P})$, but usually simplify our presentation by ignoring this dependence. Moreover, we let $(\mathbb{X}, \mathfrak{B}(\mathbb{X}), \mu)$ be an additional probability space with $\mathfrak{B}(\mathbb{X})$ being the Borel σ -algebra on the topological space \mathbb{X} and denote the space of μ square-integrable functions on \mathbb{X} by $\mathcal{F} := L^2(\mathbb{X} \rightarrow \mathbb{C}, \mu)$.

In what follows, we will denote vectors by bold lowercase letters, matrices by bold uppercase letters, and operators by calligraphic letters. Moreover, \mathbf{x} are elements of \mathbb{X} and ψ_1, \dots, ψ_N denote dictionary functions. Finally, we will always use $i, j, n \in \{1, \dots, N\}$ to index the dictionary and $m \in \{1, \dots, M\}$ to index samples where $M, N \in \mathbb{N}$. For the sake of convenience, we include an overview of the notation used throughout the paper in Appendix C.

2.2 Dynamical systems and linear operators

Linear operators are a powerful tool for studying dynamical systems. Two such operators are the Koopman and Perron–Frobenius operators, along with their generators. Let \mathbb{X} be the state space and consider a deterministic discrete-time dynamical system $\Phi: \mathbb{X} \rightarrow \mathbb{X}$ defined by

$$\mathbf{x}_{\ell+1} = \Phi(\mathbf{x}_{\ell}), \quad \ell \in \mathbb{N}_0, \quad (1)$$

with an appropriate initial condition $\mathbf{x}_0 \in \mathbb{X}$. We refer to Φ as the *flow* of the dynamical system. In practice, we may not have access to Φ . In order to recover some information about the dynamical system, we may measure some quantity $f: \mathbb{X} \rightarrow \mathbb{C}$ of the system, such as its velocity, acceleration, or energy and investigate how it evolves. That is, we study

$$\mathcal{K}f(\mathbf{x}) := f(\Phi(\mathbf{x})), \quad (2)$$

where the operator $\mathcal{K}: L^\infty(\mathbb{X}) \rightarrow L^\infty(\mathbb{X})$ is known as the *Koopman operator*. Its adjoint \mathcal{K}^* is the *Perron–Frobenius operator*.

These ideas translate to continuous-time dynamical systems, such as

$$\mathbf{x}_t = \Phi^{t-s}(\mathbf{x}_s) \in \mathbb{X}, \quad s, t \in \mathbb{R}^+, s < t,$$

where now $\Phi^t: \mathbb{X} \rightarrow \mathbb{X}$ defines the flow in continuous time, and we study the time evolution of observables f through the *semigroup of Koopman operators* \mathcal{K}^t , $t \geq 0$, defined by

$$\mathcal{K}^t f(\mathbf{x}) := f(\Phi^t(\mathbf{x})).$$

The *infinitesimal generator* of the Koopman semigroup \mathcal{K}^t is then defined on $f \in C^2(\mathbb{X})$ as

$$\mathcal{L}f(\mathbf{x}) := \lim_{t \downarrow 0} \frac{1}{t} (\mathcal{K}^t f(\mathbf{x}) - f(\mathbf{x})).$$

The above operators can also be extended to stochastic dynamical systems, i.e., to systems in which the flow Φ or Φ^t is a random object mapping from $\Omega \times \mathbb{X}$ to \mathbb{X} . In this setting, we still refer to the Koopman operators and semigroups as well as the associated Perron–Frobenius operators and their generators by \mathcal{K} , \mathcal{K}^t , \mathcal{K}^* , $(\mathcal{K}^t)^*$, \mathcal{L} , and \mathcal{L}^* , respectively. In this case, the Koopman operators and semigroups are given by

$$\mathcal{K}f(\mathbf{x}) := \mathbb{E}[f(\Phi(\mathbf{x}))], \quad \mathcal{K}^t f(\mathbf{x}) := \mathbb{E}[f(\Phi^t(\mathbf{x}))]. \quad (3)$$

The corresponding Perron–Frobenius operators and the generators are then defined in an analogous fashion. A typical case is when $\mathbf{X}_t \in \mathbb{X}$ is a continuous time dynamical system evolving according to the stochastic differential equation

$$d\mathbf{X}_t = \mathbf{b}(\mathbf{X}_t)dt + \boldsymbol{\sigma}(\mathbf{X}_t)d\mathbf{W}_t, \quad \mathbf{X}_0 = \mathbf{x}. \quad (4)$$

By applying Itô’s formula, one can show that the generator \mathcal{L} associated with the stochastic differential equation (4) is given by

$$\mathcal{L}f = \mathbf{b} \cdot \nabla f + \frac{1}{2} \text{Tr}(\boldsymbol{\Sigma} \nabla^2 f), \quad (5)$$

where $\boldsymbol{\Sigma} := \boldsymbol{\sigma} \boldsymbol{\sigma}^\top$ [23]. In physical terms, \mathcal{L} describes the infinitesimal rate of change of observables f evolving under our dynamical system. That is, writing $u(t, \mathbf{x}) := \mathcal{K}^t f(\mathbf{x})$, we have

$$\partial_t u = \mathcal{L}u.$$

The above is called the Kolmogorov backward equation. Similarly, \mathcal{L}^* describes the evolution of probability distributions of our system. If X_t has density $\nu(t, \mathbf{x}) \in C_t^1 C_{\mathbf{x}}^2([0, T] \times \mathbb{X})$, i.e., is once differentiable in time and twice in space with bounded derivatives, it holds that

$$\partial_t \nu = \mathcal{L}^* \nu,$$

see [24, Theorem 5.3.2]. This is known as the *forward Kolmogorov equation* or *Fokker–Planck equation*. As a result, knowledge of \mathcal{L} gives us complete knowledge of the evolution of \mathbf{X} .

Through the expressions above, we see that the Koopman and Perron–Frobenius operators, along with their generators, are critical tools to describe how a dynamical system evolves.

2.3 Mathematical framework

We now move on to the data-driven approximation of an operator of interest, which we denote by \mathcal{A} . In what follows, this operator can be one of the operators we have introduced in the context of dynamical systems, i.e., \mathcal{K} or \mathcal{K}^* in discrete time and \mathcal{K}^t , $(\mathcal{K}^t)^*$, \mathcal{L} , or \mathcal{L}^* in continuous time, but our theory is not limited to these operators. As before, we consider the state space $(\mathbb{X}, \mathcal{B}, \mu)$ and write $\mathcal{F} := L^2(\mathbb{X}, \mu)$. The observables on which \mathcal{A} can be evaluated define the *domain* of \mathcal{A} , i.e.,

$$\mathcal{D} := \{f \in \mathcal{F} : \mathcal{A}f \in \mathcal{F}\}.$$

We say that \mathcal{A} is a *closed operator* if the graph of \mathcal{A} ,

$$\{(f, \mathcal{A}f) \in \mathcal{F} \times \mathcal{F} : f \in \mathcal{D}\},$$

is a closed subspace of $\mathcal{F} \times \mathcal{F}$. If \mathcal{A} is a closed operator, \mathcal{D} is a Hilbert space with the inner product

$$\langle f, g \rangle_{\mathcal{D}} := \langle f, g \rangle_{\mathcal{F}} + \langle \mathcal{A}f, \mathcal{A}g \rangle_{\mathcal{F}}, \quad \|f\|^2 := \langle f, f \rangle_{\mathcal{D}}, \quad \forall f, g \in \mathcal{D},$$

see [25] for more details. A direct consequence of the above definitions is that $\|f\|_{\mathcal{F}} \leq \|f\|_{\mathcal{D}}$ and $\mathcal{A}: \mathcal{D} \rightarrow \mathcal{F}$ is a continuous operator with $\|\mathcal{A}\| \leq 1$.

In practice, there are two main cases. If \mathcal{A} is continuous on \mathcal{F} , then $\mathcal{D} = \mathcal{F}$ and the norms $\|\cdot\|_{\mathcal{D}}$ and $\|\cdot\|_{\mathcal{F}}$ are equivalent. Otherwise, \mathcal{A} will typically be the infinitesimal generator of a strongly continuous semigroup (such as in (5)). In this case, \mathcal{D} will be dense in \mathcal{F} , see [26] for details. A common example is where \mathcal{D} is a weighted Sobolev space $H^k(\mathbb{X}, \mu)$ that contains all measurable functions $\psi: \mathbb{X} \rightarrow \mathbb{R}$ with finite norm

$$\|\psi\|_{H^k(\mathbb{X}, \mu)} = \sum_{|\alpha| \leq k} \left(\int_{\mathbb{X}} |D^\alpha \psi|^2 d\mu \right)^{1/2},$$

where D^α is the weak derivative of order α [27]. For example, if \mathcal{A} is the generator of a stochastic process, then $\mathcal{D} = H^2(\mathbb{X}, \mu)$. If the system is deterministic, on the other hand, then $\mathcal{D} = H^1(\mathbb{X}, \mu)$.

Our goal is to study a given dynamical system through the action of \mathcal{A} on observables $f \in \mathcal{D}$. A practical difficulty is that we will typically not know the value of $\mathcal{A}f(\mathbf{x})$ for every observable f and every point $\mathbf{x} \in \mathbb{X}$, as this would correspond to having an infinite amount of information about our system. The most we can hope for is to know this information for a finite amount of observables $\psi_1, \dots, \psi_N \subset \mathcal{D}$, called the *dictionary*, and a finite amount of training data points $\mathbf{x}_1, \dots, \mathbf{x}_M$, which are assumed to be sampled independently from some arbitrary probability measure μ . That is, our total information is

$$\{(\psi_n(\mathbf{x}_m), \mathcal{A}\psi_n(\mathbf{x}_m))\}_{m,n=1}^{M,N}. \quad (6)$$

Here, the terms $\mathcal{A}\psi_n(\mathbf{x}_m)$ may be evaluated exactly or approximated using existing techniques (e.g., finite differences, Kramers–Moyal expansions, etc.), see [16, 28]. Since \mathcal{A} is infinite-dimensional, this finite amount of information cannot fully describe \mathcal{A} except in simple cases. In general, the best we can hope is to obtain some approximation $\hat{\mathcal{A}}$ of \mathcal{A} .

Many approaches for the data-driven description of dynamics, such as DMD, EDMD, and gEDMD, can be described as trying to obtain the best approximation $\hat{\mathcal{A}}$ of \mathcal{A} given the limited data in (6). In fact, all of them can be subsumed under the framework that we will introduce below.

There are two aspects that need to be considered: a finite number of dictionary functions ψ_1, \dots, ψ_N that may not span the space \mathcal{F} and a finite number of samples $\mathbf{x}_1, \dots, \mathbf{x}_M$ that are not space-filling in \mathbb{X} . We now discuss the implications of these aspects, starting with the finite dictionary. Using the information in (6), the operator \mathcal{A} can be approximated on

$$\mathcal{F}_N := \text{span}(\Psi) = \text{span}(\psi_1, \dots, \psi_N)$$

by taking sampling-based approximations of the projection of \mathcal{A} onto \mathcal{F}_N . In all the preceding methods, this is done as follows: We would like our finite-dimensional approximation $\mathcal{A}_N: \mathcal{F}_N \rightarrow \mathcal{F}_N$ to \mathcal{A} to satisfy

$$[\mathbf{C}_N]_{ij} := \langle \mathcal{A}\psi_i, \psi_j \rangle_{L^2(\mu)} = \langle \mathcal{A}_N\psi_i, \psi_j \rangle_{L^2(\mu)} = [(\mathbf{A}_N^\Psi)^\top \mathbf{G}_N]_{ij}, \quad (7)$$

for all i, j , where

$$[\mathbf{C}_N]_{ij} := \langle \mathcal{A}\psi_i, \psi_j \rangle_{L^2(\mu)}, \quad [\mathbf{G}_N]_{ij} := \langle \psi_i, \psi_j \rangle_{L^2(\mu)}$$

are the *structure matrix* and the *Gram matrix* of \mathcal{A} and Ψ , respectively. If we could evaluate the above integrals exactly, we would obtain our approximation via

$$(\mathbf{A}_N^\Psi)^\top = \mathbf{C}_N \mathbf{G}_N^{-1}, \quad (8)$$

where the invertibility of the Gram matrix is equivalent to Ψ being linearly independent. The operator $\mathcal{A}_N: \mathcal{F}_N \rightarrow \mathcal{F}_N$ defined through (8) satisfies (7) and, as a result, is necessarily the projection of \mathcal{A} onto \mathcal{F}_N . That is, if we write $\mathcal{P}_{\mathcal{F}_N}$ for the projection onto \mathcal{F}_N ,

$$\mathcal{A}_N = \mathcal{P}_{\mathcal{F}_N} \mathcal{A}|_{\mathcal{F}_N}. \quad (9)$$

Due to the connection with the finite element method (FEM), (9) is often called the *Galerkin approximation* (or projection) of \mathcal{A} .

However, since we only have access to the information in (6), the best we can do is to use the samples $\mathbf{x}_1, \dots, \mathbf{x}_M \sim \mu$ and defining the *empirical structure matrix* and the *empirical Gram matrix* as

$$[\hat{\mathbf{C}}_{NM}]_{ij} := \frac{1}{M} \sum_{m=1}^M \overline{\psi_j(\mathbf{x}_m)} \mathcal{A}\psi_i(\mathbf{x}_m), \quad [\hat{\mathbf{G}}_{NM}]_{ij} := \frac{1}{M} \sum_{m=1}^M \psi_i(\mathbf{x}_m) \overline{\psi_j(\mathbf{x}_m)}, \quad (10)$$

respectively. Let us denote the *empirical measure* associated with $\{\mathbf{x}_1, \dots, \mathbf{x}_M\}$ by

$$\hat{\mu}_M := \frac{1}{M} \sum_{m=1}^M \delta_{\mathbf{x}_m},$$

then the above can also be written as

$$[\hat{\mathbf{C}}_{NM}]_{ij} = \langle \mathcal{A}\psi_i, \psi_j \rangle_{L^2(\hat{\mu}_M)}, \quad [\hat{\mathbf{G}}_{NM}]_{ij} = \langle \psi_i, \psi_j \rangle_{L^2(\hat{\mu}_M)}.$$

We define, analogously to (8),

$$\hat{\mathbf{A}}_{NM}^\top := \hat{\mathbf{C}}_{NM} \hat{\mathbf{G}}_{NM}^+. \quad (11)$$

Here, \mathbf{G}_{NM}^+ denotes the *Moore–Penrose pseudoinverse* [29] of \mathbf{G}_{NM} and by construction is such that (11) minimises the empirical error,

$$\left\| \hat{\mathbf{A}}_{NM}^\top \hat{\mathbf{G}}_{NM} - \hat{\mathbf{C}}_{NM} \right\|_F^2 := \sum_{i,j=1}^N \left| [\hat{\mathbf{A}}_{NM}^\top \hat{\mathbf{G}}_{NM}]_{ij} - [\hat{\mathbf{C}}_{NM}]_{ij} \right|^2.$$

We note that the Gram matrix \mathbf{G}_N is always invertible as the basis functions contained in Ψ are assumed to be linearly independent. However, its Monte Carlo approximation $\hat{\mathbf{G}}_{NM}$ may not be invertible. For this reason, the pseudoinverse is required and ensures that we obtain the matrix $\hat{\mathbf{A}}_{NM} \in \mathbb{C}^{N \times N}$. This can give rise to theoretical issues, such as the discontinuity of the map from a matrix to its pseudoinverse. These problems can be resolved with careful analysis. We will touch upon this in more detail in Theorem 3.1.

By the strong law of large numbers and the definitions in (7) and (10), almost surely

$$\lim_{M \rightarrow \infty} \hat{\mathbf{C}}_{NM} = \mathbf{C}_N, \quad \lim_{M \rightarrow \infty} \hat{\mathbf{G}}_{NM} = \mathbf{G}_N.$$

As a result, we expect $\hat{\mathbf{A}}_{NM}$ to converge to \mathbf{A}_N^Ψ as the number of data points goes to infinity. This will be studied in Section 3. Convergence to \mathcal{A} , when the number of basis functions goes to infinity, is studied in Sections 4 and 5, where also error bounds are established. Convergence to the spectrum of \mathcal{A} is studied in Section 6. In practice, one may not have access to the exact values of $\psi_n(\mathbf{x}_m), \mathcal{A}\psi_n(\mathbf{x}_m)$, but only to an approximation or a noisy measurement. To deal with this case, we also study in Subsection 5.1 the case where our data has some noise $\boldsymbol{\eta}, \boldsymbol{\xi}$, i.e., we have access to the data

$$\{(\psi_n(\mathbf{x}_m) + \eta_N^{m,n}, \mathcal{A}\psi_n(\mathbf{x}_m) + \xi_N^{m,n})\}_{m,n=1}^{M,N}.$$

We again show convergence of the approximations to the true dynamics in this case.

We stress once more that all the previously mentioned methods for data-driven recovery of dynamics (DMD, EDMD, and gEDMD) fall into this framework and are thus covered by the analysis. Here, we use minimal assumptions. More precisely, we require that the observables be linearly independent, sufficiently regular and that the data be i.i.d. (Assumptions 1 and 2). To show convergence and error bounds, it is also necessary that, as N goes to infinity, the basis functions ψ_1, \dots, ψ_N cover the whole space (Assumption 3 and 4) and are bounded (Assumption 5). Finally, for the case where the measurements are noisy, we assume that the noise is centred at zero and independent (Assumption 6).

3 Data-driven approximation as a projection

The following section is inspired by [18]. However, in our analysis we do not require the *empirical Gram matrix* $\hat{\mathbf{G}}_{NM}$ to be invertible. We discuss natural situations in which $\hat{\mathbf{G}}_{NM}$ may not be invertible throughout this section. We begin by imposing the basic assumptions that will be used in what follows.

Assumption 1. We assume the following:

- (a) The basis functions $\Psi = \{\psi_1, \dots, \psi_N\} \subset \mathcal{D}$ are linearly independent.
- (b) The functions $\{\psi_n, \mathcal{A}\psi_n\}_{n=1}^N$ are continuous μ almost everywhere.
- (c) The points $\{\mathbf{x}_m\}_{m=1}^M \subset \mathbb{X}$ are i.i.d. samples from μ .

Point 1(a) of Assumption 1 is necessary to ensure that the Gram matrix \mathbf{G}_N is invertible. To the best of the authors' knowledge, Point 1(b) cannot be found in the literature. However, it is required so that the pointwise evaluation in the Monte Carlo approximations (10) is well-defined. Lastly, Point 1(c) is the basic assumption underlying Monte Carlo approximations.

Observation 1. In the case where \mathcal{A} is a differential operator of order k and \mathbb{X} is an open subset of \mathbb{R}^d with uniformly Lipschitz boundary (for example if $\mathbb{X} = \mathbb{R}^d$ or if \mathbb{X} is any open subset with Lipschitz continuous boundary), the continuity of 1(b) requires continuity of the derivatives of order k of the observables. By Sobolev embedding, a sufficient condition is $\Psi \subset H^s(\mathbb{X}, \mu)$ for $s > k + d/2$ (see [30, Section 12.3]). For example, if \mathcal{A} is, the generator \mathcal{L} of the Koopman operator defined in (5), then, in general, we require that the second derivatives of Ψ be continuous almost everywhere. However, if the stochastic dynamics in (4) are reversible with respect to μ (for example, if μ is the Gibbs distribution), given smooth ψ, φ , we have

$$\langle \mathcal{A}\psi, \varphi \rangle_{L^2(\mu)} = -\frac{1}{2} \langle \Sigma \nabla \psi, \nabla \varphi \rangle_{L^2(\mu)}$$

as shown in [22]. As a result, we can define

$$[C_N]_{ij} := -\frac{1}{2} \langle \Sigma \nabla \psi_i, \nabla \psi_j \rangle_{L^2(\mu)}, \quad [\widehat{C}_{NM}]_{ij} := -\frac{1}{2} \langle \Sigma \nabla \psi_i, \nabla \psi_j \rangle_{L^2(\widehat{\mu}_M)}.$$

This amounts to an integration by parts and can also be carried out when μ is the Lebesgue measure. Consequently, we then only need the first derivatives of Ψ to be continuous almost everywhere. This is useful if one wants to use piecewise linear basis functions as in FEM, see Section 7 and, for example, [20].

As we will see in Theorem 3.1, the approximation $\widehat{\mathbf{A}}_{NM}$ is best defined on the *empirical space*

$$\widehat{\mathcal{F}}_M := L^2(\mathbb{X} \rightarrow \mathbb{C}, \widehat{\mu}_M).$$

Elements in \mathcal{F} are not in $\widehat{\mathcal{F}}_M$ as functions defined μ almost everywhere are not in general well-defined $\widehat{\mu}_M$ almost everywhere. However, if $\psi \in \mathcal{F}$ is continuous almost everywhere, we can view it as an element of $\widehat{\mathcal{F}}_M$ through the (non-injective) mapping

$$\psi \mapsto \widehat{\psi} := \sum_{m=1}^M \psi(\mathbf{x}_m) \delta_{\mathbf{x}_m} \in \widehat{\mathcal{F}}_M. \quad (12)$$

We also use the notation

$$\widehat{\Psi} := \{\widehat{\psi}_n\}_{n=1}^N \subset \widehat{\mathcal{F}}_M, \quad \widehat{\mathcal{F}}_{NM} := \text{span}(\widehat{\Psi}) \subset \widehat{\mathcal{F}}_M$$

to denote the basis Ψ and subspace \mathcal{F}_N , respectively, when viewed as objects in $\widehat{\mathcal{F}}_M$ using (12). We denote by $\widehat{\mathcal{A}}$ the operator induced by \mathcal{A} , i.e.,

$$\widehat{\mathcal{A}}\widehat{\psi} := \widehat{\mathcal{A}\psi}.$$

Note that $\widehat{\psi}$ and $\widehat{\mathcal{A}}\widehat{\psi}$ are only well-defined if ψ and $\mathcal{A}\psi$ are continuous almost everywhere. In our case, this is satisfied for all $\psi \in \mathcal{F}_N$ by Point 1(b) of Assumption 1. Using this notation, the Monte Carlo approximation of the stiffness and Gram matrices in (10) become

$$[\widehat{\mathbf{C}}_{NM}]_{ij} = \left\langle \widehat{\mathcal{A}}\widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)}, \quad [\widehat{\mathbf{G}}_{NM}]_{ij} = \left\langle \widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)}. \quad (13)$$

Here, the Gram matrix $\widehat{\mathbf{G}}_{NM}$ with respect to $\widehat{\Psi}$ is in general *not* invertible as $\widehat{\Psi}$ may no longer be linearly independent (consider for example the case $M = 1$ and $N = 2$). By construction, $\widehat{\mathcal{F}}_M$ is a Hilbert space, so we can define the projection of $\widehat{\mathcal{F}}_M$ onto $\widehat{\mathcal{F}}_{NM}$ by

$$\mathcal{P}_{\widehat{\mathcal{F}}_{NM}} : \widehat{\mathcal{F}}_M \rightarrow \widehat{\mathcal{F}}_{NM}.$$

We prove that our data-driven approximation $\widehat{\mathbf{A}}_{NM}$ corresponds to the projection of $\widehat{\mathcal{A}}$ onto $\widehat{\mathcal{F}}_{NM}$.

Theorem 3.1 (Empirical projection). *Let Ψ satisfy Assumption 1(b). Then the matrix $\widehat{\mathbf{A}}_{NM}$ which approximates $\widehat{\mathcal{A}}$ is, with probability 1, a matrix representation of the projection of $\widehat{\mathcal{A}}$ onto $\widehat{\mathcal{F}}_{NM}$. That is,*

$$\widehat{\mathbf{A}}_{NM} = \mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}|_{\widehat{\mathcal{F}}_{NM}},$$

where $\widehat{\mathbf{A}}_{NM}$ is the operator that has matrix representation $\widehat{\mathbf{A}}_{NM}$ on $\widehat{\Psi}$.

Proof. By Assumption 1(b), with probability 1, the matrices $\widehat{\mathbf{C}}_{NM}$ and $\widehat{\mathbf{G}}_{NM}$ in (13), and thus $\widehat{\mathbf{A}}_{NM}$ in (11), are well-defined. By construction, the data-driven approximation $\widehat{\mathbf{A}}_{NM}$ minimizes the empirical error, i.e.,

$$\widehat{\mathbf{A}}_{NM} \in \arg \min_{\widehat{\mathbf{A}} \in \mathbb{C}^{N \times N}} \left\| \widehat{\mathbf{C}}_{NM} - \widehat{\mathbf{A}}^\top \widehat{\mathbf{G}}_{NM} \right\|_F. \quad (14)$$

Now, by definition, we have

$$\mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}|_{\widehat{\mathcal{F}}_{NM}} : \widehat{\mathcal{F}}_{NM} \rightarrow \widehat{\mathcal{F}}_{NM}.$$

Furthermore, using basic properties of the projection, for all $i, j \in \{1, \dots, N\}$, we have

$$[\widehat{\mathbf{C}}_{NM}]_{ij} := \left\langle \widehat{\mathcal{A}}\widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)} = \left\langle \mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}\widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)}.$$

Equivalently, any matrix representation $\left(\mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}|_{\widehat{\mathcal{F}}_{NM}} \right)^{\widehat{\Psi}} \in \mathbb{C}^{N \times N}$ of $\mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}$ satisfies

$$\left\| \widehat{\mathbf{C}}_{NM} - \left\{ \left(\mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}|_{\widehat{\mathcal{F}}_{NM}} \right)^{\widehat{\Psi}} \right\}^\top \widehat{\mathbf{G}}_{NM} \right\|_F = 0. \quad (15)$$

From (14) and (15) we deduce that $\widehat{\mathbf{C}}_{NM} = \widehat{\mathbf{A}}_{NM}^\top \widehat{\mathbf{G}}_{NM}$. That is,

$$\left\langle \widehat{\mathcal{A}}\widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)} = [\widehat{\mathbf{A}}_{NM}^\top \widehat{\mathbf{G}}_{NM}]_{ij}, \quad \forall i, j \in \{1, \dots, N\}. \quad (16)$$

Define the data-driven operator $\widehat{\mathcal{A}}_{NM} : \widehat{\mathcal{F}}_{NM} \rightarrow \widehat{\mathcal{F}}_{NM}$ corresponding to $\widehat{\mathbf{A}}_{NM}$ via

$$\widehat{\mathcal{A}}_{NM} v := \sum_{i,k=1}^N c_i [\widehat{\mathbf{A}}_{NM}]_{ki} \widehat{\psi}_k, \quad \forall v = \sum_{i=1}^N c_i \widehat{\psi}_i \in \widehat{\mathcal{F}}_{NM}.$$

We want to use Lemma A.1 to see that $\widehat{\mathcal{A}}_{NM}$ is well-defined. To this end, consider $(c_1, \dots, c_N) \in \mathbb{C}^N$ such that $\sum_{i=1}^N c_i \widehat{\psi}_i = 0$. Then, for $j \in \{1, \dots, N\}$, we have

$$\begin{aligned} \sum_{i,k=1}^N \left\langle c_i [\widehat{\mathcal{A}}_{NM}]_{ki} \widehat{\psi}_k, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)} &= \sum_{i,k=1}^N c_i [\widehat{\mathcal{A}}_{NM}]_{ki} [\widehat{\mathbf{G}}_{NM}]_{kj} = \sum_{i=1}^N c_i [\widehat{\mathcal{A}}_{NM}^\top \widehat{\mathbf{G}}_{NM}]_{ij} \\ &= \sum_{i=1}^N c_i \left\langle \widehat{\mathcal{A}} \widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)} = \left\langle \widehat{\mathcal{A}} \sum_{i=1}^N c_i \widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)} \\ &= 0, \end{aligned}$$

where in the first equality, we used the definition of $\widehat{\mathbf{G}}_{NM}$, in the third, we used (16), and in the last, we used that $\sum_{i=1}^N c_i \widehat{\psi}_i = 0$. Since j was arbitrary, applying Lemma A.1, $\widehat{\mathcal{A}}_{NM}$ is a well-defined operator with matrix representation $\widehat{\mathcal{A}}_{NM}$. Furthermore, by construction of $\widehat{\mathcal{A}}_{NM}$ and (16), $\widehat{\mathcal{A}}_{NM}$ satisfies

$$\left\langle \widehat{\mathcal{A}} \widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)} = \left\langle \widehat{\mathcal{A}}_{NM} \widehat{\psi}_i, \widehat{\psi}_j \right\rangle_{L^2(\widehat{\mu}_M)}, \quad \forall i, j = 1, \dots, N. \quad (17)$$

Due to the general theory of Hilbert spaces, the only operator $\widehat{\mathcal{A}}_{NM}: \widehat{\mathcal{F}}_{NM} \rightarrow \widehat{\mathcal{F}}_{NM}$ satisfying (17) is $\mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}|_{\widehat{\mathcal{F}}_{NM}}$. As a result, $\widehat{\mathcal{A}}_{NM} = \mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}|_{\widehat{\mathcal{F}}_{NM}}$, which completes the proof. \square

We now show that if \mathcal{F}_N is invariant under the action of \mathcal{A} , then $\widehat{\mathcal{A}}_{NM}$ is an exact approximation of the Galerkin projection \mathcal{A}_N (9) of \mathcal{A} with probability 1.

Corollary 3.2 (Exact approximation). *If $\mathcal{A}\mathcal{F}_N \subset \mathcal{F}_N$, then, with probability 1,*

$$\widehat{\mathcal{A}}_{NM} = \widehat{\mathcal{A}}_N.$$

Let \mathbf{A}_N^Ψ be the matrix of $\mathcal{A}_N = \mathcal{A}|_{\mathcal{F}_N}$ in the basis Ψ . If additionally, $\widehat{\mathbf{G}}_{NM}$ is invertible, then

$$\widehat{\mathcal{A}}_{NM} = \mathbf{A}_N^\Psi.$$

Proof. Taking $\mathcal{A}_N = \mathcal{A}|_{\mathcal{F}_N}$ in place of \mathcal{A} in Theorem 3.1 and using that $\widehat{\mathcal{A}}_N: \widehat{\mathcal{F}}_{NM} \rightarrow \widehat{\mathcal{F}}_{NM}$,

$$\widehat{\mathcal{A}}_{NM} = \widehat{\mathcal{A}}_{N NM} = \mathcal{P}_{\widehat{\mathcal{F}}_{NM}} \widehat{\mathcal{A}}_N|_{\widehat{\mathcal{F}}_{NM}} = \widehat{\mathcal{A}}_N.$$

This proves the first part of the corollary, to see the second, note that if $\widehat{\mathbf{G}}_{NM}$ is invertible, then $\widehat{\Psi}$ form a basis of $\widehat{\mathcal{F}}_{NM}$ and matrix representations in $\widehat{\mathcal{F}}_{NM}$ and \mathcal{F}_N are the same. As a result, $\widehat{\mathcal{A}}_{NM} = \mathbf{A}_N^\Psi$. This completes the proof. \square

Theorem 3.1 is a generalisation of Theorem 1 in [18], where it was also required that $\widehat{\Psi}$ be linearly independent in $\widehat{\mathcal{F}}_M$ (or equivalently, that $\widehat{\mathbf{G}}_{NM}$ be invertible). However, this assumption is not altogether benign. The assumption will always fail when $M < N$ (as \mathcal{F}_M has dimension M) and also in many cases of interest, such as the following example.

Example 3.3 (Finite element basis of degree k). We want to approximate \mathcal{F} by the space of piecewise polynomials of degree up to k . That is, we decompose \mathbb{X} into disjoint subdomains $\{T_1, \dots, T_L\}$, i.e.,

$$\mathbb{X} = \bigsqcup_{l=1}^L T_l,$$

and take

$$\mathcal{F}_N = \left\{ v \in C(\mathbb{X}), \quad v|_{T_l} \in P_k, \forall l \in \{1, \dots, L\} \right\},$$

where P_k is the set of polynomials of degree up to k in each variable. This space has dimension $N = Lk^d$. A basis Ψ can be obtained by taking k^d nodes in each T_l to obtain a total of N nodes $\{\mathbf{a}_1, \dots, \mathbf{a}_N\}$ and taking the unique functions $\Psi = \{\psi_n\}_{n=1}^N \subset \mathcal{F}_N$ such that

$$\psi_i(\mathbf{a}_j) = \delta_{ij}, \quad \forall i, j \in \{1, \dots, N\}.$$

Here, typically, L is chosen so that each T_L has a diameter at most h . In this case, $L = \mathcal{O}(h^{-d})$ and $N = \mathcal{O}((k/h)^d)$. \triangle

In the above example, if there is a cell T_{l_0} which holds no data point, then $\hat{\psi}_{l_0} = 0$. As a result, $\hat{\Psi}$ will not be linearly independent in general. We now study the convergence of $\hat{\mathcal{A}}_{NM}$ to the projection of \mathcal{A} onto \mathcal{F}_N . This convergence uses the law of large numbers and requires that the empirical matrices have finite variances.

Assumption 2. The basis functions $\Psi = \{\psi_n\}_{n=1}^N$ satisfy $\psi_j \mathcal{A} \psi_i \in \mathcal{F}$ as well as $\psi_i^2 \in \mathcal{F}$ for all $i, j \in \{1, \dots, N\}$.

For example, the above assumption will hold by Assumption 1 if \mathbb{X} is a compact domain. Though $\hat{\Psi}$ are not linearly independent in general, they will be (almost surely) when we have a large enough training data set. This is shown in the following lemma.

Lemma 3.4. Suppose Assumptions 1 and 2 hold, then there exists an \mathbb{N} -valued random variable m_0 such that $\hat{\Psi} \subset \hat{\mathcal{F}}_M$ are almost surely linearly independent for all $M \geq m_0$.

Proof. By Assumption 1, we may apply the strong law of large numbers to deduce that, for all $i, j \in \{1, \dots, N\}$, when $M \rightarrow \infty$

$$[\hat{\mathbf{G}}_{NM}]_{ij} = \frac{1}{M} \sum_{m=1}^M \psi_i(\mathbf{x}_m) \overline{\psi_j(\mathbf{x}_m)} \xrightarrow{a.s.} \int \psi_i(\mathbf{x}) \overline{\psi_j(\mathbf{x})} d\mu(\mathbf{x}) = [\mathbf{G}_N]_{ij}.$$

Since the determinant is a continuous function and \mathbf{G}_N is the Gram matrix of a linearly independent set of functions, we have

$$\det(\hat{\mathbf{G}}_{NM}) \rightarrow \det(\mathbf{G}_N) \neq 0 \quad \text{a.s. for } M \rightarrow \infty,$$

from which it follows that there exists $m_0 \in \mathbb{N}$ such that

$$\left| \det(\hat{\mathbf{G}}_{NM}) - \det(\mathbf{G}_N) \right| < \det(\mathbf{G}_N) \quad \text{a.s. when } M \geq m_0.$$

Consequently,

$$\det(\hat{\mathbf{G}}_{NM}) \neq 0 \quad \text{a.s. when } M \geq m_0,$$

which proves the result. \square

Observation 2. Lemma 3.4 shows that, for sufficiently large M , $\hat{\Psi}$ form a basis of $\hat{\mathcal{F}}_{NM}$. As a result, for large M , we can, and will, identify \mathcal{F}_N with $\hat{\mathcal{F}}_{NM}$ through the mapping (12). In particular, for large enough M , we can view $\hat{\mathcal{A}}_{NM}$ as an operator on \mathcal{F}_N . Lemma 3.4 does not provide a bound on m_0 . In Section 5, we will derive a bound so that $\hat{\mathbf{G}}_{NM}$ can be made invertible with arbitrarily large probability by choosing M appropriately.

Using Lemma 3.4, we prove that in the infinite sample limit, the data-driven operator $\hat{\mathbf{A}}_{NM}$ converges to \mathcal{A}_N , i.e., the Galerkin projection of \mathcal{A} onto \mathcal{F}_N .

Theorem 3.5 (Convergence in data limit). *If Assumptions 1 and 2 hold, almost surely,*

$$\lim_{M \rightarrow \infty} \hat{\mathbf{A}}_{NM} = \mathbf{A}_N^\Psi,$$

where \mathbf{A}_N^Ψ is the matrix of \mathcal{A}_N with respect to Ψ .

Proof. Let m_0 be as in Lemma 3.4. For $M > m_0$, since $\hat{\mathbf{G}}_{NM}$ is invertible, its pseudoinverse is equal to its inverse, and, by the strong law of large numbers, we have

$$\left(\hat{\mathbf{A}}_{NM}\right)^\top = \hat{\mathbf{C}}_{NM} \hat{\mathbf{G}}_{NM}^{-1} \xrightarrow{a.s.} \mathbf{C}_N \mathbf{G}_N^{-1} = \left(\mathbf{A}_N^\Psi\right)^\top \quad \text{for } M \rightarrow \infty.$$

In other words, the matrix of $\hat{\mathcal{A}}_{NM}$ converges to that of \mathcal{A}_N . □

Corollary 3.6. *If Assumptions 1 and 2 hold, then, with probability 1,*

$$\lim_{M \rightarrow \infty} \left\| \hat{\mathcal{A}}_{NM} - \mathcal{A}_N \right\| = 0,$$

where $\|\cdot\|$ is the operator norm. In particular, for all $\psi \in \mathcal{F}_N$ and with probability 1

$$\lim_{M \rightarrow \infty} \left\| \hat{\mathcal{A}}_{NM} \psi - \mathcal{A}_N \psi \right\|_{\mathcal{F}_N} = 0,$$

where $\|\cdot\|_{\mathcal{F}_N}$ is any norm on \mathcal{F}_N .

Proof. The convergence in the operator norm is a direct consequence of the convergence of the matrix representations of Theorem 3.5. The second point follows from the fact that convergence in the operator norm implies pointwise convergence and that all norms on finite-dimensional spaces are equivalent. □

4 Convergence of the projections

In the previous section, we have shown that the data-driven approximation in (11) defines an operator $\hat{\mathcal{A}}_{NM}$ that converges to the Galerkin projection $\mathcal{A}_N = \mathcal{P}_{\mathcal{F}_N} \mathcal{A}|_{\mathcal{F}_N}$. In this section, our goal is to show that \mathcal{A}_N converges to \mathcal{A} . This was also done in [18], where it was assumed that the (Koopman) operator is bounded on \mathcal{F} and that $\{\psi_n\}_{n=1}^\infty$ form an orthonormal basis of \mathcal{F} . In many cases, however, \mathcal{A} will *not* be bounded (for example, if \mathcal{A} is the generator \mathcal{L} of the Koopman operator). Furthermore, the requirement that the basis be orthonormal is restrictive, and in practice, it is often preferable to work with a dictionary that does not have to be orthonormalised; a finite element basis, for instance, will often produce sparse operators, but it is not orthonormal. Additionally, the sampling measure μ is typically unknown, so it is not possible to orthonormalise with respect to the norm on \mathcal{F} .

We will work in a more general setting. Firstly, we require that \mathcal{F}_N converges to \mathcal{F} as $N \rightarrow \infty$. That is, as we take more basis functions, we fill \mathcal{F} .

Assumption 3. Assumption 1 holds and

$$\lim_{N \rightarrow \infty} \|\mathcal{P}_{\mathcal{F}_N} \phi - \phi\|_{\mathcal{F}} = 0, \quad \forall \phi \in \mathcal{F},$$

where $\mathcal{P}_{\mathcal{F}_N}$ is the projection of \mathcal{F} onto \mathcal{F}_N using the inner product on \mathcal{F} .

We will also need to approximate functions in the domain \mathcal{D} . This necessitates the following assumption.

Assumption 4. Assumption 1 holds, \mathcal{A} is a closed operator, and

$$\lim_{N \rightarrow \infty} \|\mathcal{P}_{\mathcal{D}_N} f - f\|_{\mathcal{D}} = 0, \quad \forall f \in \mathcal{D}.$$

Here, $\mathcal{P}_{\mathcal{D}_N}$ is the projection of \mathcal{D} onto \mathcal{F}_N using the inner product on \mathcal{D} .

If \mathcal{A} is bounded on \mathcal{F} , then $\mathcal{F} = \mathcal{D}$ and Assumptions 3 and 4 are equivalent. In general, though, this is not the case. One assumption may imply that functions are approximated well in $L^2(\mathbb{X}, \mu)$ and the other in $H^r(\mathbb{X}, \mu)$.

Example 4.1 (Orthonormal basis). Let $\{\psi_n\}_{n=1}^{\infty}$ be an orthonormal basis of \mathcal{F} and set $\Psi_N := \{\psi_1, \dots, \psi_N\}$. Given $f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) \in \mathcal{F}$,

$$\|\mathcal{P}_{\mathcal{F}_N} \phi - \phi\|_{\mathcal{F}}^2 = \sum_{n=N+1}^{\infty} c_n^2 \rightarrow 0 \quad (N \rightarrow \infty).$$

If \mathcal{A} is continuous on \mathcal{F} , then $\mathcal{D} = \mathcal{F}$ so that Assumption 3 holds. \triangle

The above assumptions only require that the subspaces \mathcal{F}_N are good approximations of \mathcal{F} and \mathcal{D} , with the error vanishing in the limit. We now introduce the notation

$$\mathcal{F}_{\infty} := \bigoplus_{n=1}^{\infty} \mathcal{F}_n = \bigcup_{n=1}^{\infty} \mathcal{F}_n.$$

Under the above assumptions, we can prove the convergence of the Galerkin approximation.

Theorem 4.2 (Convergence in dictionary limit). *Let Ψ_N satisfy Assumption 3, then*

$$\lim_{N \rightarrow \infty} \|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} \psi - \mathcal{A} \psi\|_{\mathcal{F}} = 0, \quad \forall \psi \in \mathcal{F}_{\infty}.$$

If additionally Assumption 4 holds, then

$$\lim_{N \rightarrow \infty} \|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A} f\|_{\mathcal{F}} = 0, \quad \forall f \in \mathcal{D}.$$

Proof. Using basic algebra and the fact that by definition $\mathcal{A}_N = \mathcal{P}_{\mathcal{F}_N} \mathcal{A}|_{\mathcal{F}_N}$, we obtain

$$\begin{aligned} \mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} - \mathcal{A} &= (\mathcal{A}_N - \mathcal{A}) \mathcal{P}_{\mathcal{D}_N} + \mathcal{A} \mathcal{P}_{\mathcal{D}_N} - \mathcal{A} \\ &= (\mathcal{P}_{\mathcal{F}_N} - \text{Id}) \mathcal{A} \mathcal{P}_{\mathcal{D}_N} + \mathcal{A} (\mathcal{P}_{\mathcal{D}_N} - \text{Id}) \\ &= (\mathcal{P}_{\mathcal{F}_N} - \text{Id}) \mathcal{A} + (\mathcal{P}_{\mathcal{F}_N} - \text{Id}) \mathcal{A} (\mathcal{P}_{\mathcal{D}_N} - \text{Id}) + \mathcal{A} (\mathcal{P}_{\mathcal{D}_N} - \text{Id}). \end{aligned}$$

Consider now $f \in \mathcal{D}$. Applying the triangle inequality and the fact that \mathcal{A} is continuous on its domain gives

$$\begin{aligned} \|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A} f\|_{\mathcal{F}} &\leq \|(\mathcal{P}_{\mathcal{F}_N} - \text{Id}) \mathcal{A} f\|_{\mathcal{F}} + \|(\mathcal{P}_{\mathcal{F}_N} - \text{Id}) \mathcal{A}\| \|\mathcal{P}_{\mathcal{D}_N} f - f\|_{\mathcal{D}} \\ &\quad + \|\mathcal{A}\| \|\mathcal{P}_{\mathcal{D}_N} f - f\|_{\mathcal{D}}. \end{aligned} \tag{18}$$

If $f \in \mathcal{F}_{\infty}$, then $\mathcal{P}_{\mathcal{D}_N} f = f$ for N large enough, and using Assumption 3 with $\phi := \mathcal{A} f$ proves the first part of the theorem. If $f \in \mathcal{D}$, then combining Assumption 3 and Assumption 4 concludes the proof. \square

The first part of Theorem 4.2 is useful in the case where we have a finite-dimensional space of observables we are interested in. In this case, these can be incorporated directly into \mathcal{F}_N . The second part of the theorem is useful when we want to know the evolution of every possible observable. The proof also shows that the order of convergence depends completely on the rate of convergence of $\mathcal{P}_{\mathcal{F}_N} f$ and $\mathcal{P}_{\mathcal{D}_N} f$ to f . We summarise this result in the following corollary.

Corollary 4.3. Consider Ψ_N satisfying Assumption 1 and such that $\|\mathcal{P}_{\mathcal{F}_N}\phi - \phi\|_{\mathcal{F}} = \mathcal{O}(N^{-\alpha})$ for all $\phi \in \mathcal{F}$. Then

$$\|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} \psi - \mathcal{A} \psi\|_{\mathcal{F}} = \mathcal{O}(N^{-\alpha}), \quad \forall \psi \in \mathcal{F}_{\infty}.$$

If additionally, \mathcal{A} is closed and $\|\mathcal{P}_{\mathcal{D}_N} f - f\|_{\mathcal{D}} = \mathcal{O}(N^{-\alpha})$ for all $f \in \mathcal{D}$, then

$$\|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A} f\|_{\mathcal{F}} = \mathcal{O}(N^{-\alpha}), \quad \forall f \in \mathcal{D},$$

where, in both cases, the hidden constant depends only linearly on $\|\mathcal{A}\|, \|\psi\|, \|f\|$.

Proof. This follows from inequality (18) and the observation that if $f \in \mathcal{F}_{\infty}$ then the second and third terms in this equation are identically zero for large enough N . \square

5 Joint limit in data and dictionary

In Sections 3 and 4, we studied the iterated limits of $\hat{\mathcal{A}}_{NM}$ when the size of the training data set M and the number of basis functions N go to infinity. In this section, we study the behaviour of $\hat{\mathcal{A}}_{NM}$ when M and N increase simultaneously.

In [19], the projection error was studied for various approximation spaces, such as reproducing kernel Hilbert spaces and those generated by finite-dimensional bases of wavelets. In [20], the authors work with the generator of an ordinary differential equation and derive a projection error in the context of a finite element basis. They also provide a finite-data error bound on the approximation of the generator in the case where the data is sampled from the Lebesgue measure. In [21], the authors derive an error bound for the approximation error of gEDMD under the assumptions that the Koopman semigroup is exponentially stable and the points are sampled from a probability measure invariant under the flow and from a single ergodic trajectory. The error bounds in [20, 21] both require M to be “sufficiently large” so that the empirical Gram matrix is invertible. However, no bound on how large M must be is given. In fact, a deterministic bound on M is impossible, but rather a probabilistic one is needed.

We work under relaxed assumptions, for example, we do not impose that the dictionary functions be orthonormal, we do not impose that $\mathbf{x}_1, \dots, \mathbf{x}_M$ be sampled from the Lebesgue measure, a measure invariant under the flow or even from the same trajectory, and we do not impose that the empirical Gram matrix be invertible. We first formulate an existence result of the following type:

Theorem 5.1 (Convergence in joint limit). *Let Ψ satisfy Assumptions 1, 2, and 3, then there exists a sequence $\{(N, M_N)\}_{N=1}^{\infty}$ such that for any $M'_N \geq M_N$ almost surely*

$$\lim_{N \rightarrow \infty} \left\| \hat{\mathcal{A}}_{NM'_N} \psi - \mathcal{A} \psi \right\|_{\mathcal{F}} = 0, \quad \forall \psi \in \mathcal{F}_{\infty}.$$

If additionally Assumption 4 is satisfied, then almost surely

$$\lim_{N \rightarrow \infty} \left\| \hat{\mathcal{A}}_{NM'_N} \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A} f \right\|_{\mathcal{F}} = 0, \quad \forall f \in \mathcal{D}.$$

Proof. Let $f \in \mathcal{D}$ and $\varepsilon > 0$. Using the triangle inequality, we have

$$\left\| \hat{\mathcal{A}}_{NM_N} \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A} f \right\|_{\mathcal{F}} \leq \left\| \hat{\mathcal{A}}_{NM_N} - \mathcal{A}_N \right\| \|\mathcal{P}_{\mathcal{D}_N} f\|_{\mathcal{D}} + \|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A} f\|_{\mathcal{F}}. \quad (19)$$

By Corollary 3.6, for any $N \in \mathbb{N}$, there exists almost surely M_N such that for all $M'_N \geq M_N$

$$\left\| \hat{\mathcal{A}}_{NM'_N} - \mathcal{A}_N \right\| < \frac{1}{2N}. \quad (20)$$

Let us set $N_0 > \varepsilon^{-1} \|f\|_{\mathcal{D}}$ and such that for $N \geq N_0$ we have

$$\|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A}f\|_{\mathcal{F}} < \frac{\varepsilon}{2}, \quad (21)$$

where (21) is possible due to Theorem 4.2 in both the case $f \in \mathcal{F}_\infty$ as well as $f \in \mathcal{D}$. As a result, we obtain from (19), (20), and (21) that for all $N \geq N_0$

$$\left\| \hat{\mathcal{A}}_{NM'_N} \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A}f \right\|_{\mathcal{F}} < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon,$$

where it was also used that $\|\mathcal{P}_{\mathcal{D}_N}\| = 1$. Since $\varepsilon > 0$ and f were arbitrary, this proves the theorem. \square

This existence result forms a good foundation. In practice, however, we may need an explicit dependence between M and N and explicit error bounds. Before we can proceed, we first need to state additional assumptions.

Assumption 5 (Boundedness of the basis functions). We assume that:

- (a) There exists γ_N such that μ almost everywhere $|\Psi_N(\mathbf{x})|^2 < \gamma_N$.
- (b) There exists γ_N such that μ almost everywhere $|\mathcal{A}\Psi_N(\mathbf{x})|^2 < \gamma_N$,

where in 5(b) the operator is applied componentwise.

Let us illustrate these assumptions with two examples.

Example 5.2 (Bounded dictionary). Suppose that for all $i \in \{1, \dots, N\}$ it holds that

$$\|\psi_i\|_\infty^2 < \gamma, \quad \|\mathcal{A}\psi_i\|_\infty^2 < \gamma.$$

Then Assumption 5 holds with $\gamma_N = N\gamma$. \triangle

Example 5.3 (Locally supported dictionary). Consider Ψ_N as before and assume that there exists some $K \in \mathbb{N}$ for which

$$\mu \left(\bigcap_{k=1}^K \text{supp}(\psi_{i_k}) \right) = 0, \quad \forall i_1, \dots, i_K \in \{1, \dots, N\}.$$

Then Assumption 5 holds with $\gamma_N = K\gamma$ (that is constant in N). This is, for example, the case if Ψ is a finite element basis and \mathcal{A} has order 0. \triangle

The first ingredient for our error analysis is an error bound for the Gram matrix \mathbf{G} .

Lemma 5.4 (Error estimate \mathbf{G}). Under Assumptions 1 and 5(a), given any $0 < \delta < \frac{1}{2} \|\mathbf{G}_N^{-1}\|^{-1}$ and $p \in (0, 1)$ and for all

$$M > (3 \|\mathbf{G}_N\| + 2\delta) \frac{2\gamma_N}{3\delta^2} \log \left(\frac{2N}{1-p} \right),$$

it holds that

$$\mathbb{P} \left[\hat{\mathbf{G}}_{NM} \text{ is invertible and } \left\| \hat{\mathbf{G}}_{NM}^{-1} - \mathbf{G}_N^{-1} \right\| < 2 \|\mathbf{G}_N^{-1}\|^2 \delta \right] \geq p.$$

Proof. Given $m \in \{1, \dots, M\}$, we define

$$\mathbf{S}_m := \frac{1}{M} \left(\Psi_N(\mathbf{x}_m) \Psi_N^\dagger(\mathbf{x}_m) - \mathbf{G}_N \right), \quad (22)$$

where \dagger denotes the Hermitian adjoint. By construction, we are in the conditions of Bernstein's inequality for the covariance in Corollary B.2 where, using the notation of this inequality, $\mathbf{g}_m = \mathbf{c}_m = \Psi_N(\mathbf{x}_m)$, $\mathbf{G} = \mathbf{C} = \mathbf{T} = \mathbf{G}_N$, $\gamma = \gamma_N$ and

$$\mathbf{Z} := \sum_{m=1}^M \mathbf{S}_m = \widehat{\mathbf{G}}_{NM} - \mathbf{G}_N.$$

As a result, for M as in the statement of the proposition, we obtain that

$$\mathbb{P}[\|\mathbf{Z}\| < \delta] \geq p.$$

Now, since $\delta < 1/\|\mathbf{G}_N^{-1}\|$ and \mathbf{G}_N is invertible, we deduce that, with probability greater or equal to p , the approximation $\widehat{\mathbf{G}}_{NM} = \mathbf{G}_N + \mathbf{Z}$ is also invertible with inverse given by the Neumann series

$$\widehat{\mathbf{G}}_{NM}^{-1} = \mathbf{G}_N^{-1} \sum_{k=0}^{\infty} (-\mathbf{Z}\mathbf{G}_N^{-1})^k.$$

Taking norms shows that, with probability greater or equal to p , $\widehat{\mathbf{G}}_{NM}$ is invertible and

$$\left\| \widehat{\mathbf{G}}_{NM}^{-1} - \mathbf{G}_N^{-1} \right\| \leq \|\mathbf{G}_N^{-1}\| \sum_{k=1}^{\infty} (\|\mathbf{G}_N^{-1}\| \delta)^k = \frac{\|\mathbf{G}_N^{-1}\|^2 \delta}{1 - \|\mathbf{G}_N^{-1}\| \delta} < 2 \|\mathbf{G}_N^{-1}\|^2 \delta.$$

This concludes the proof. \square

In an analogous fashion, we can bound the error due to using $\widehat{\mathbf{C}}_{NM}$ with an arbitrarily large probability. In fact, the result is more straightforward as we no longer have to deal with the matrix inversion necessary for $\widehat{\mathbf{G}}_{NM}$.

Lemma 5.5 (Error estimate \mathbf{C}). *Let Ψ satisfy Assumptions 1 and 5 and let $\delta > 0$ and $p \in (0, 1)$ be arbitrary. Write $[\mathbf{T}_N]_{ij} := \langle \mathcal{A}\psi_i, \mathcal{A}\psi_j \rangle$. Then, for all*

$$M > (3 \max\{\|\mathbf{G}_N\|, \|\mathbf{T}_N\|\} + 2\delta) \frac{2\gamma_N}{3\delta^2} \log\left(\frac{2N}{1-p}\right),$$

it holds that

$$\mathbb{P}\left[\left\|\widehat{\mathbf{C}}_{NM} - \mathbf{C}_N\right\| < \delta\right] \geq p.$$

Proof. The proof is similar to that of Lemma 5.4. Given $m \in \{1, \dots, M\}$, we define

$$\mathbf{S}_m := \frac{1}{M} \left(\mathcal{A}\Psi_N(\mathbf{x}_m) \Psi_N^\dagger(\mathbf{x}_m) - \mathbf{C}_N \right). \quad (23)$$

By construction, we are now able to apply Bernstein's inequality for the covariance defined in Corollary B.2, where $\mathbf{g}_m = \Psi_N(\mathbf{x}_m)$, $\mathbf{c}_m = \mathcal{A}\Psi_N(\mathbf{x}_m)$, $\mathbf{G} = \mathbf{G}_N$, $\mathbf{C} = \mathbf{C}_N$, $\mathbf{T} = \mathbf{T}_N$, $\gamma = \gamma_N$ and

$$\mathbf{Z} := \sum_{m=1}^M \mathbf{S}_m = \widehat{\mathbf{C}}_{NM} - \mathbf{C}_N.$$

As a result, for M as in the statement of the proposition, we obtain that

$$\mathbb{P}\left[\left\|\widehat{\mathbf{C}}_{NM} - \mathbf{C}_N\right\| < \delta\right] = \mathbb{P}[\|\mathbf{Z}\| < \delta] \geq p.$$

This concludes the proof. \square

Having bounded the error due to using $\widehat{\mathbf{G}}_{NM}$ and $\widehat{\mathbf{C}}_{NM}$ instead of \mathbf{G}_N and \mathbf{C}_N , we can now bound the error in approximating \mathcal{A}_N by $\widehat{\mathcal{A}}_{NM}$. To do so, we need to relate the bounds in the matrix norms back to the operator norms. As shown in the Lemma B.3, this depends on the condition number of \mathbf{G}_N , which can be written as

$$\kappa(\mathbf{G}_N) = \frac{\lambda_{\max}(\mathbf{G}_N)}{\lambda_{\min}(\mathbf{G}_N)},$$

since \mathbf{G}_N is Hermitian. The condition number is 1 for an orthonormal basis but can become very large for other bases, such as the basis of monomials. This will be discussed in more detail below.

Proposition 5.6 (Error estimate projection). *Let Ψ_N satisfy Assumptions 1 and 5. Let $0 < \delta < \frac{1}{2} \|\mathbf{G}_N^{-1}\|^{-1}$ and $p \in (0, 1)$.*

$$M > (3 \max \{\|\mathbf{G}_N\|, \|\mathbf{T}_N\|\} + 2\delta) \frac{2\gamma_N}{3\delta^2} \log \left(\frac{4N}{1-p} \right), \quad (24)$$

it holds that

$$\mathbb{P} \left[\left\| \widehat{\mathcal{A}}_{NM} - \mathcal{A}_N \right\| \leq 2\sqrt{\kappa(\mathbf{G}_N)}(1 + \|\mathbf{C}_N\| \|\mathbf{G}_N^{-1}\|) \|\mathbf{G}_N^{-1}\| \delta \right] \geq p.$$

Proof. By Lemmas 5.4 and 5.5, we deduce that for M as defined above it holds that

$$\widehat{\mathbf{G}}_{NM} \text{ is invertible, } \|\delta_{\mathbf{G}^{-1}}\| < 2 \|\mathbf{G}_N^{-1}\|^2 \delta, \text{ and } \|\delta_{\mathbf{C}}\| < \delta, \quad (25)$$

with probability greater or equal to p , where, in order to simplify the notation, we used

$$\delta_{\mathbf{G}^{-1}} := \widehat{\mathbf{G}}_{NM}^{-1} - \mathbf{G}_N^{-1}, \quad \delta_{\mathbf{C}} := \widehat{\mathbf{C}}_{NM} - \mathbf{C}_N.$$

Let us now restrict ourselves to the region of the probability space where (25) holds. First, let $\mathcal{T} := \widehat{\mathcal{A}}_{NM} - \mathcal{A}_N$, then

$$\mathbf{T}^{\Psi_N} = \widehat{\mathbf{C}}_{NM} \widehat{\mathbf{G}}_{NM}^{-1} - \mathbf{C}_N \mathbf{G}_N^{-1} = \mathbf{C}_N \delta_{\mathbf{G}^{-1}} + \delta_{\mathbf{C}} \mathbf{G}_N^{-1} + \delta_{\mathbf{G}^{-1}} \delta_{\mathbf{C}}.$$

As a result, by (25) and collecting the terms, we have

$$\|\mathcal{T}^{\Psi_N}\| \leq (2 + 2\|\mathbf{C}_N\| \|\mathbf{G}_N^{-1}\|) \|\mathbf{G}_N^{-1}\| \delta.$$

Now, applying Lemma B.3 yields

$$\|\mathcal{T}\| \leq 2\sqrt{\kappa(\mathbf{G}_N)}(1 + \|\mathbf{C}_N\| \|\mathbf{G}_N^{-1}\|) \|\mathbf{G}_N^{-1}\| \delta.$$

This concludes the proof. \square

The bound on the error in approximating the projection \mathcal{A}_N in the just proved proposition can be combined with an error in the approximation of \mathcal{A} through \mathcal{A}_N . This gives the following result.

Theorem 5.7 (Order of convergence). *Let Ψ_N satisfy Assumptions 1 and 5 and $N \in \mathbb{N}$ be arbitrary. Define $\rho_N := \sqrt{\kappa(\mathbf{G}_N)}(1 + \|\mathbf{C}_N\| \|\mathbf{G}_N^{-1}\|)$, let $\varepsilon \in (0, \rho_N)$ be arbitrary and write $\delta_N := \varepsilon / (2\rho_N \|\mathbf{G}_N^{-1}\|)$. Then, for all $p \in (0, 1)$ and*

$$M > (3 \max \{\|\mathbf{G}_N\|, \|\mathbf{T}_N\|\} + 2\delta_N) \frac{2\gamma_N}{3\delta_N^2} \log \left(\frac{4N}{1-p} \right),$$

it holds that

$$\mathbb{P} \left[\left\| \widehat{\mathcal{A}}_{NM} - \mathcal{A}_N \right\| \leq \varepsilon \right] \geq p.$$

Furthermore, if $f \in \mathcal{F}_\infty$ and $\|(\mathcal{P}_{\mathcal{F}_N} - Id)\phi\|_{\mathcal{F}} = \mathcal{O}(N^{-\alpha})$ for all $\phi \in \mathcal{F}$, or if $f \in \mathcal{D}$ and additionally $\|(\mathcal{P}_{\mathcal{D}_N} - Id)f\|_{\mathcal{D}} = \mathcal{O}(N^{-\alpha})$, then, for $N = \mathcal{O}(\varepsilon^{-1/\alpha})$ and M as defined above, it holds that

$$\mathbb{P} \left[\left\| \widehat{\mathcal{A}}_{NM} \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A} f \right\|_{\mathcal{F}} \leq \|\mathcal{A}\| \|f\|_{\mathcal{D}} \varepsilon \right] \geq p.$$

Proof. By construction, we have that $\delta_N < \frac{1}{2} \|\mathbf{G}_N^{-1}\|^{-1}$. Applying Proposition 5.6 with δ_N in the place of δ proves the first part of the theorem. To prove the second part, we use the triangle inequality to obtain

$$\left\| \hat{\mathcal{A}}_{NM} \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A}f \right\|_{\mathcal{F}} \leq \left\| \hat{\mathcal{A}}_{NM} - \mathcal{A}_N \right\| \|f\|_{\mathcal{D}} + \|\mathcal{A}_N \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A}f\|_{\mathcal{F}}. \quad (26)$$

To bound the first term on the right-hand side of (26), we use what was just proved. To bound the second term, we use (4.3) to obtain that, for \mathcal{A} and f nonzero,

$$\left\| \hat{\mathcal{A}}_{NM} \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A}f \right\|_{\mathcal{F}} \leq \varepsilon \|f\|_{\mathcal{D}} + C\varepsilon \|\mathcal{A}\| \|f\| \lesssim \|\mathcal{A}\| \|f\|_{\mathcal{D}} \varepsilon.$$

If \mathcal{A} or f are zero, on the other hand, it is clear that the error is zero. This concludes the proof. \square

This theorem allows us to estimate the cost of an approximation of \mathcal{A} with accuracy $\varepsilon > 0$ that holds with probability p . In terms of the order of convergence of $\hat{\mathcal{A}}_{NM}$ to \mathcal{A}_N , we have that

$$M = \mathcal{O}\left(\gamma_N \max\{\|\mathbf{G}_N\|, \|\mathbf{T}_N\|\} \kappa(\mathbf{G}_N) \|\mathbf{C}_N\|^2 \|\mathbf{G}_N^{-1}\|^4 \log\left(\frac{N}{1-p}\right) \varepsilon^{-2}\right). \quad (27)$$

Let us now consider two examples.

Example 5.8. If \mathbf{C}_N , \mathbf{G}_N , and $\kappa(\mathbf{G}_N)$ are bounded and $\gamma_N = \mathcal{O}(N)$, then, to obtain an error of ε ,

$$M = \mathcal{O}\left(-\frac{1}{\alpha} \log\left(\frac{\varepsilon}{1-p}\right) \varepsilon^{-2-1/\alpha}\right), \quad N = \mathcal{O}(\varepsilon^{-1/\alpha}).$$

The cost of obtaining $\hat{\mathcal{A}}_{NM}$ is

$$C(\varepsilon, p) = \mathcal{O}(MN^2 + N^3) = \mathcal{O}(MN^2) = \mathcal{O}\left(-\log\left(\frac{\varepsilon}{1-p}\right) \varepsilon^{-2-3/\alpha}\right). \quad \triangle$$

Example 5.9. If \mathbf{G}_N is sparse, it is likely that $\|\mathbf{G}_N^{-1}\|$ is not bounded. For example for a 1-dimensional FEM basis $\|\mathbf{G}_N^{-1}\| = \mathcal{O}(h_N^{-1}) = \mathcal{O}(N^{1/2})$ and from (27), if the remaining quantities are bounded, we obtain

$$M = \mathcal{O}\left(-\frac{1}{\alpha} \log\left(\frac{\varepsilon}{1-p}\right) \varepsilon^{-2-2/\alpha}\right), \quad N = \mathcal{O}(\varepsilon^{-1/\alpha}).$$

As a result, the cost of obtaining $\hat{\mathcal{A}}_{NM}$ is

$$C(\varepsilon, p) = \mathcal{O}(MN) = \mathcal{O}\left(\log\left(\frac{\varepsilon}{1-p}\right) \varepsilon^{-2-3/\alpha}\right).$$

This is equal to the cost in the previous example. \triangle

5.1 Accounting for measurement error

In practice, it is often not possible to evaluate the dictionary $(\psi_n)_{n=1}^N$ and operator applied to the dictionary functions $(\mathcal{A}\psi_n)_{n=1}^N$ precisely. The evaluations may be perturbed by measurement errors, or we may need to approximate the operator \mathcal{A} , as mentioned in the beginning of Section 2. This error will influence the accuracy of the approximation of \mathcal{A} , which is what we study throughout this section.

We will assume in what follows that instead of (6), we only have access to

$$\{\psi_n(\mathbf{x}_m) + \eta_N^{m,n}, \mathcal{A}\psi_n(\mathbf{x}_m) + \xi_N^{m,n}\}_{m,n=1}^{M,N}, \quad (28)$$

where $(\eta_N^{m,1}, \dots, \eta_N^{m,N}) =: \boldsymbol{\eta}_N^m$ and $(\xi_N^{m,1}, \dots, \xi_N^{m,N}) =: \boldsymbol{\xi}_N^m$ represent the measurement or evaluation error in dictionary and operator, respectively. Given this perturbed data, our data-driven approximation is given by

$$\tilde{\mathbf{A}}_{NM}^\top := \tilde{\mathbf{C}}_{NM} \tilde{\mathbf{G}}_{NM}^+,$$

with perturbed stiffness and Gram matrices given by

$$\begin{aligned} [\tilde{\mathbf{C}}_{NM}]_{ij} &:= \frac{1}{M} \sum_{m=1}^M \left(\mathcal{A}\psi_i(\mathbf{x}_m) + \boldsymbol{\xi}_N^{m,i} \right) \left(\psi_j(\mathbf{x}_m) + \boldsymbol{\eta}_N^{m,j} \right)^\dagger, \\ [\tilde{\mathbf{G}}_{NM}]_{ij} &:= \frac{1}{M} \sum_{m=1}^M \left(\Psi_i(\mathbf{x}_m) + \boldsymbol{\eta}_N^{m,i} \right) \left(\Psi_j(\mathbf{x}_m) + \boldsymbol{\eta}_N^{m,j} \right)^\dagger, \end{aligned}$$

respectively. In this section, we show how the error bounds in Lemmas 5.4 and 5.5 can be modified to account for this noise. This leads to an analogous error bound on the data-driven operator as in Proposition 5.6 and Theorem 5.7. We now describe the errors using random variables. The distribution of these random variables will need to satisfy a certain boundedness criterion, which we state below.

Assumption 6. The random variables $\{(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)\}_{m=1}^M$ have mean $\mathbf{0}$, are symmetric, independent, and independent of $\{\mathbf{x}_m\}_{m=1}^M$.

Given $\tilde{\gamma}_N \geq 0$ we will use the notation

$$\tilde{p}_N := \mathbb{P} \left[|(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N \right].$$

This assumption is satisfied by Gaussian measurement error and, by studying the cumulative distribution function of the χ^2 distribution, an explicit expression for \tilde{p}_N can be given. We do so in Example 5.12 below, after adopting our previous estimates to the setting of noisy data, starting with the result analogous to Proposition 5.6.

Proposition 5.10 (Error estimate noise). *Let $\Psi, \boldsymbol{\eta}_N, \boldsymbol{\xi}_N$ satisfy Assumptions 1, 5, and 6, and let $0 < \delta < \frac{1}{2} \|\mathbf{G}_N^{-1}\|$ and $p \in (0, 1), \tilde{p}_N \in (p, 1)$. Then, for all*

$$M > (3 \max \{\|\mathbf{G}_N\|, \|\mathbf{T}_N\|\} + 2\delta) \frac{2(\gamma_N + \tilde{\gamma}_N)}{3\delta^2} \log \left(\frac{4N}{1 - p/\tilde{p}_N} \right),$$

it holds that

$$\mathbb{P} \left[\left\| \tilde{\mathcal{A}}_{NM} - \mathcal{A}_N \right\| \leq 2\sqrt{\kappa(\mathbf{G}_N)}(1 + \|\mathbf{C}_N\| \|\mathbf{G}_N^{-1}\|) \|\mathbf{G}_N^{-1}\| \delta \right] \geq p,$$

Proof. We begin by restricting ourselves to realizations where $|\boldsymbol{\eta}_N^m|^2 \leq \tilde{\gamma}_N, |\boldsymbol{\xi}_N^m|^2 \leq \tilde{\gamma}_N$. More formally, we modify our probability space to $(\Omega, \mathcal{E}, \tilde{\mathbb{P}})$ where $\tilde{\mathbb{P}}$ is the conditional probability

$$\tilde{\mathbb{P}}(\mathbb{A}) := \frac{\mathbb{P} \left[\mathbb{A} \cap \left\{ |(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N, \forall m \right\} \right]}{\mathbb{P} \left[\left\{ |(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N, \forall m \right\} \right]}.$$

Given $k \in \{1, \dots, N\}$, by the independence of \mathbf{x}_k of $\{(\boldsymbol{\xi}_N^m, \boldsymbol{\eta}_N^m)\}_{m=1}^M$, for all $\mathbb{A} \in \mathcal{B}(\mathbb{R}^d)$, we have

$$\tilde{\mathbb{P}}(\mathbf{x}_k \in \mathbb{A}) := \frac{\mathbb{P} \left[\mathbf{x}_k \in \mathbb{A} \cap \left\{ |(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N, \forall m \right\} \right]}{\mathbb{P} \left[\left\{ |(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N, \forall m \right\} \right]} = \mathbb{P}[\mathbf{x}_k \in \mathbb{A}] \cdot 1 = \mu(\mathbb{A}).$$

That is, also $\mathbf{x}_k \sim \mu$ under the probability measure $\tilde{\mathbb{P}}$. Additionally, the family $\{\mathbf{x}_m\}_{m=1}^M$ is independent under $\tilde{\mathbb{P}}$ as well. This is because, given $\mathbb{A}_1, \dots, \mathbb{A}_M \in \mathcal{B}(\mathbb{R}^d)$, we have

$$\begin{aligned}\tilde{\mathbb{P}}(\{\mathbf{x}_m \in \mathbb{A}_m, \forall m\}) &= \frac{\mathbb{P}\left[\{\mathbf{x}_m \in \mathbb{A}_m, \forall m\} \cap \left\{ |(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N, \forall m \right\}\right]}{\mathbb{P}\left[\left\{ |(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N, \forall m \right\}\right]} \\ &= \mathbb{P}[\{\mathbf{x}_m \in \mathbb{A}_m, \forall m\}] \cdot 1 = \mu(\mathbb{A}_1) \cdots \mu(\mathbb{A}_M),\end{aligned}$$

where in the second and last equality we used the independence stated in Assumption 6. Similarly, one can also show that $\{\mathbf{x}_m\}_{m=1}^M$ are independent of $\{(\boldsymbol{\xi}_N^m, \boldsymbol{\eta}^m)\}_{m=1}^M$ and that $\{(\boldsymbol{\xi}_N^m, \boldsymbol{\eta}^m)\}_{m=1}^M$ are i.i.d. with distribution

$$\tilde{\mathbb{P}}[(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m) \in \mathbb{A} \times \mathbb{B}] = \frac{\mathbb{P}\left[\{(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m) \in \mathbb{A} \times \mathbb{B}\} \cap \left\{ |(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N \right\}\right]}{\mathbb{P}\left[\left\{ |(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N \right\}\right]}, \quad \forall m \in \{1, \dots, M\}.$$

Using this result, since $(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)$ is symmetric and centred at $\mathbf{0}$ under \mathbb{P} , we obtain that $(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)$ also has mean $\mathbf{0}$ under $\tilde{\mathbb{P}}$. In conclusion,

$$\{(\mathbf{g}_m, \mathbf{c}_m)\}_{m=1}^M := \{\Psi_N(\mathbf{x}_m) + \boldsymbol{\eta}_N^m, \mathcal{A}\Psi_N(\mathbf{x}_m) + \boldsymbol{\eta}_N^m\}_{m=1}^M, \quad (29)$$

are i.i.d. (under $\tilde{\mathbb{P}}$) with

$$\mathbf{G}_N = \mathbb{E}[\mathbf{g}\mathbf{g}^\dagger], \quad \mathbf{T}_N = \mathbb{E}[\mathbf{c}\mathbf{c}^\dagger], \quad \mathbf{C}_N := \mathbb{E}[\mathbf{c}\mathbf{g}^\dagger], \quad (30)$$

and by definition of $\tilde{\mathbb{P}}$ and the triangle inequality for all $m \in \{1, \dots, M\}$, it holds that

$$\tilde{\mathbb{P}}[|\mathbf{g}_m|^2 \leq \gamma_N + \tilde{\gamma}_N \text{ and } |\mathbf{c}_m|^2 \leq \gamma_N + \tilde{\gamma}_N] = 1. \quad (31)$$

Now, analogously to (22) and (23), we define

$$\begin{aligned}\mathbf{S}_m^{\mathbf{G}} &:= \frac{1}{M}(\Psi_N(\mathbf{x}_m) + \boldsymbol{\eta}_N^m)(\Psi_N(\mathbf{x}_m) + \boldsymbol{\eta}_N^m)^\dagger - \mathbf{G}_N, \\ \mathbf{S}_m^{\mathbf{C}} &:= \frac{1}{M}(\mathcal{A}\Psi_N(\mathbf{x}_m) + \boldsymbol{\eta}_N^m)(\Psi_N(\mathbf{x}_m) + \boldsymbol{\eta}_N^m)^\dagger - \mathbf{C}_N.\end{aligned} \quad (32)$$

By the independence of \mathbf{g}_m and \mathbf{c}_m in (29), their mean value in (30) and the bound in (31), we may apply Bernstein's inequality for the covariance defined in Corollary B.2 to (32), which implies that

$$\begin{aligned}\tilde{\mathbb{P}}\left[\left\|\tilde{\mathbf{G}}_{NM} - \mathbf{G}_N\right\| \geq \delta\right] &\leq 2N \exp\left(\frac{-M\delta^2/2}{(\gamma_N + \tilde{\gamma}_N)(\|\mathbf{G}_N\| + 2\delta/3)}\right), \\ \tilde{\mathbb{P}}\left[\left\|\tilde{\mathbf{C}}_{NM} - \mathbf{C}_N\right\| \geq \delta\right] &\leq 2N \exp\left(\frac{-M\delta^2/2}{(\gamma_N + \tilde{\gamma}_N)(\max\{\|\mathbf{T}_N\|, \|\mathbf{G}_N\|\} + 2\delta/3)}\right).\end{aligned}$$

Solving for M we obtain that, for M as in the problem statement

$$p \leq \tilde{p}_N \tilde{\mathbb{P}}\left[\left\|\tilde{\mathbf{G}}_{NM} - \mathbf{G}_N\right\| < \delta, \text{ and } \left\|\tilde{\mathbf{C}}_{NM} - \mathbf{C}_N\right\| < \delta\right]. \quad (33)$$

Now, by definition of $\tilde{\mathbb{P}}$, we have that $\tilde{p}_N \tilde{\mathbb{P}} \leq \mathbb{P}$. Using this in (33) shows that, for M as above

$$p \leq \mathbb{P}\left[\left\|\tilde{\mathbf{G}}_{NM} - \mathbf{G}_N\right\| < \delta, \text{ and } \left\|\tilde{\mathbf{C}}_{NM} - \mathbf{C}_N\right\| < \delta\right].$$

The result follows identically to the proof of Proposition 5.6. \square

The generalisation of Theorem 5.7 to the case with noise can be proved in the same way as said theorem, but this time using Proposition 5.10 instead of Proposition 5.6. This gives the following result.

Theorem 5.11 (Order of convergence with noise). *Let $\Psi, \boldsymbol{\eta}_N, \boldsymbol{\xi}_N$ satisfy Assumptions 1, 5, and 6 and $N \in \mathbb{N}$ be arbitrary. Define $\rho_N := \sqrt{\kappa(\mathbf{G}_N)}(1 + \|\mathbf{C}_N\| \|\mathbf{G}_N^{-1}\|)$, let $\varepsilon \in (0, \rho_N)$ be arbitrary and write $\delta_N := \varepsilon / (2\rho_N \|\mathbf{G}_N^{-1}\|)$. Then, for all $p \in (0, 1)$, $\tilde{p}_N \in (p, 1)$ and*

$$M > (3 \max \{\|\mathbf{G}_N\|, \|\mathbf{T}_N\|\} + 2\delta_N) \frac{2(\gamma_N + \tilde{\gamma}_N)}{3\delta_N^2} \log \left(\frac{4N}{1 - p/\tilde{p}_N} \right),$$

it holds that

$$\mathbb{P} \left[\left\| \hat{\mathcal{A}}_{NM} - \mathcal{A}_N \right\| \leq \varepsilon \right] \geq p.$$

Furthermore, if $f \in \mathcal{F}_\infty$ and $\|(\mathcal{P}_{\mathcal{F}_N} - Id)\phi\|_{\mathcal{F}} = \mathcal{O}(N^{-\alpha})$ for all $\phi \in \mathcal{F}$, or if $f \in \mathcal{D}$ and additionally $\|(\mathcal{P}_{\mathcal{D}_N} - Id)f\|_{\mathcal{D}} = \mathcal{O}(N^{-\alpha})$, then, for $N = \mathcal{O}(\varepsilon^{-1/\alpha})$ and M as defined above, it holds that

$$\mathbb{P} \left[\left\| \hat{\mathcal{A}}_{NM} \mathcal{P}_{\mathcal{D}_N} f - \mathcal{A} f \right\|_{\mathcal{F}} \leq \|\mathcal{A}\| \|f\|_{\mathcal{D}} \varepsilon \right] \geq p.$$

Thus, Theorem 5.11 shows an order of convergence of $\hat{\mathcal{A}}_{NM}$ to \mathcal{A}_N of

$$M = \mathcal{O} \left((\gamma_N + \tilde{\gamma}_N) \max \{\|\mathbf{G}_N\|, \|\mathbf{T}_N\|\} \kappa(\mathbf{G}_N) \|\mathbf{C}_N\|^2 \|\mathbf{G}_N^{-1}\|^4 \log \left(\frac{N}{1 - p/\tilde{p}_N} \right) \varepsilon^{-2} \right). \quad (34)$$

We now discuss this result in the context of Gaussian noise.

Example 5.12. Let $(\boldsymbol{\eta}_N, \boldsymbol{\xi}_N) \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_{2N \times 2N})$. Then, $\sigma^{-2} |\boldsymbol{\eta}_N|^2 \sim \chi_N^2, \sigma^{-2} |\boldsymbol{\xi}_N|^2 \sim \chi_N^2$. Suppose Ψ satisfies Assumption 5(a) with $\gamma_N = 2N$ and write $\tilde{\gamma}_N := \sigma^2 \gamma_N$. Then, for all m

$$\mathbb{P} \left[|(\boldsymbol{\eta}_N^m, \boldsymbol{\xi}_N^m)|^2 \leq \tilde{\gamma}_N \right] = 1 - F_N(\gamma_N) \leq \left(\frac{\gamma_N}{N} e^{1 - \gamma_N/N} \right)^{N/2} = (2/e)^{N/2},$$

where in the inequality we used a tail bound property of the χ^2 distribution. As a result, we obtain that $\tilde{p}_N \geq 1 - (2/e)^{N/2} \approx 1$. This shows that, in this case, the effect of the noise on the theoretical error bound is small, effectively multiplying it by a factor of 2 (compare (27) with (34) where $\tilde{\gamma}_N = \gamma_N$). \triangle

6 Convergence of eigenvalues and eigenfunctions

In Sections 3, 4, and 5, we established the convergence of the data-driven operators $\hat{\mathcal{A}}_{NM}$ when M goes to infinity, the convergence of the Galerkin approximations \mathcal{A}_N when N goes to infinity, and the joint convergence of $\hat{\mathcal{A}}_{NM}$ when N, M go to infinity, respectively. This section establishes convergence results for the eigenvalues and eigenfunctions of the approximations $\hat{\mathcal{A}}_{NM}$ and \mathcal{A}_N .

Eigenvalues and eigenfunctions of transfer operators play a vital role in the global analysis of complex dynamical systems. The dominant eigenvalues are related to the slowest timescales of the underlying system and the corresponding eigenfunctions contain important information about slowly evolving spatiotemporal patterns and have been, for instance, used to detect stable conformations of molecules or gyres in the ocean, see [6, 7] for more details.

We again discuss large data and large dictionary limits, first separately and then jointly, establishing three convergence results below. We first remind the reader of the definition of weak convergence in a Hilbert space. Let $(f_n)_{n=1}^\infty$ be a sequence taking values in a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ and $f \in \mathcal{H}$. Then $(f_n)_{n=1}^\infty$ converges weakly to f , denoted by $f_n \xrightarrow{w} f$, if

$$\langle f_n, g \rangle_{\mathcal{H}} \rightarrow \langle f, g \rangle_{\mathcal{H}} \text{ for every } g \in \mathcal{H}.$$

We now establish a convergence result for eigenpairs in the large data limit.

Theorem 6.1 (Convergence of eigensystem in data limit). *Suppose Ψ satisfies Assumption 1(b) and let (λ_M, f_M) be a sequence of eigenvalue and normalised eigenfunction pairs of $\hat{\mathcal{A}}_{NM}$, i.e.,*

$$\|f_M\|_{\mathcal{D}} = 1, \quad \hat{\mathcal{A}}_{NM}f_M = \lambda_M f_M.$$

Then there almost surely exists a subsequence of eigenvalue and normalised eigenfunction pairs $(\lambda_{M_i}, f_{M_i})_{i \in \mathbb{N}}$ such that

$$\lambda_{M_i} \rightarrow \lambda, \quad f_{M_i} \xrightarrow{w} f \in \mathcal{F}_N \subset \mathcal{D}, \quad \text{when } M_i \rightarrow \infty,$$

where the weak convergence is with respect to the inner product on \mathcal{D} . Furthermore, if $f \neq 0$ and Assumptions 1 and 2 hold, then (λ, f) is an eigenvalue and eigenfunction pair of $\mathcal{A}_N := \mathcal{P}_{\mathcal{F}_N} \mathbb{A}|_{\mathcal{F}_N}$.

Proof. It holds that (f_M) is a bounded subsequence of $\mathcal{F}_N \subset \mathcal{D}$, so by the Banach–Alaoglu Theorem it has a weakly convergent subsequence, see [31, Section 16.2, Theorem 6]. In our finite-dimensional case, this weak convergence is equivalent to convergence in the norm $\|\cdot\|_{\mathcal{D}}$. Additionally, for each M , $\hat{\mathcal{A}}_{NM}$ is bounded and thus the sequence of eigenvalues (λ_M) is also bounded and has a convergent subsequence. Consequently, there exists a subsequence of eigenvalue and normalised eigenfunction pairs (λ_{M_i}, f_{M_i}) such that

$$\lambda_{M_i} \rightarrow \lambda, \quad f_{M_i} \rightarrow f, \quad \text{when } M_i \rightarrow \infty.$$

Supposing that Assumptions 1 and 2 hold, we want to show that $\mathcal{A}_N f = \lambda f$. We have

$$\mathcal{A}_N f = \mathcal{A}_N(f - f_{M_i}) + \mathcal{A}_N f_{M_i}. \quad (35)$$

The first summand converges to zero because $f_{M_i} \rightarrow f$ and \mathcal{A}_N is bounded on \mathcal{D} . Expanding the second summand, we have

$$\lim_{i \rightarrow \infty} \mathcal{A}_N f_{M_i} = \lim_{i \rightarrow \infty} (\mathcal{A}_N - \hat{\mathcal{A}}_{NM_i})f_{M_i} + \lim_{i \rightarrow \infty} \hat{\mathcal{A}}_{NM_i}f_{M_i} = \lim_{i \rightarrow \infty} \lambda_i f_{M_i} = \lambda f,$$

where in the second equality we used Corollary 3.6 and in the third we used the convergence of (λ_{M_i}, f_{M_i}) . Taking limits in (35) concludes the proof. \square

We now move on to the convergence result in the large dictionary limit.

Theorem 6.2 (Convergence of eigensystem in dictionary limit). *Suppose there exists a sequence (λ_N, f_N) of eigenvalue and normalized eigenfunction pairs of \mathcal{A}_N , i.e.,*

$$\|f_N\|_{\mathcal{D}} = 1, \quad \mathcal{A}_N f_N = \lambda_N f_N.$$

Then there exists a subsequence of eigenvalue and normalised eigenfunction pairs $(\lambda_{N_i}, f_{N_i})_{i \in \mathbb{N}}$ such that

$$\lambda_{N_i} \rightarrow \lambda, \quad f_{N_i} \xrightarrow{w} f, \quad \text{when } N_i \rightarrow \infty,$$

where $f \in \mathcal{D}$ and the weak convergence is with respect to the inner product on \mathcal{D} . Furthermore, if $f \neq 0$ and Assumption 3 holds, then (λ, f) is an eigenvalue and eigenfunction pair of \mathcal{A} .

Proof. It holds that (f_N) is a bounded subsequence of \mathcal{D} . Additionally, for each N , \mathcal{A}_N is bounded. Thus, the sequence of eigenvalues (λ_N) is also bounded and has a convergent subsequence. Consequently, there exists a subsequence of eigenvalue and normalised eigenfunction pairs (λ_{N_i}, f_{N_i}) such that

$$\lambda_{N_i} \rightarrow \lambda, \quad f_{N_i} \xrightarrow{w} f, \quad \text{when } N_i \rightarrow \infty.$$

Supposing that Assumption 3 holds, we want to show that $\mathcal{A}f = \lambda f$ or, equivalently, that $\langle \mathcal{A}f, g \rangle_{\mathcal{F}} = \langle \lambda f, g \rangle_{\mathcal{F}}$ for all $g \in \mathcal{D}$. We have

$$\langle \mathcal{A}f, g \rangle_{\mathcal{F}} = \langle \mathcal{A}(f - f_{N_i}), g \rangle_{\mathcal{F}} + \langle \mathcal{A}f_{N_i}, g \rangle_{\mathcal{F}}. \quad (36)$$

Now, on the one hand, since $f_{N_i} \xrightarrow{w} f$ in \mathcal{D}

$$\lim_{i \rightarrow \infty} \langle \mathcal{A}(f - f_{N_i}), g \rangle_{\mathcal{F}} = \lim_{i \rightarrow \infty} \langle f - f_{N_i}, \mathcal{A}^*g \rangle_{\mathcal{D}} = 0. \quad (37)$$

On the other hand,

$$\begin{aligned} \lim_{i \rightarrow \infty} \langle \mathcal{A}f_{N_i}, g \rangle_{\mathcal{F}} &= \lim_{i \rightarrow \infty} \left\langle \left(\text{Id} - \mathcal{P}_{\mathcal{F}_{N_i}} \right) \mathcal{A}f_{N_i}, g \right\rangle_{\mathcal{F}} + \lim_{i \rightarrow \infty} \langle \mathcal{A}_{N_i} f_{N_i}, g \rangle_{\mathcal{F}} \\ &= \lim_{i \rightarrow \infty} \langle \lambda_i f_{N_i}, g \rangle_{\mathcal{F}} = \langle \lambda f, g \rangle_{\mathcal{F}}, \end{aligned} \quad (38)$$

where in the first equality we used that by definition $\mathcal{A}_{N_i} = \mathcal{P}_{\mathcal{F}_{N_i}} \mathcal{A}|_{\mathcal{F}_{N_i}}$, in the second we used that $(\text{Id} - \mathcal{P}_{\mathcal{F}_{N_i}}) \mathcal{A}f_{N_i} \rightarrow 0$ by Assumption 3 and in the third we used the convergence of (λ_{N_i}, f_{N_i}) . Taking limits in (36) and using (37) and (38) concludes the proof. \square

From Theorem 5.1, we finally obtain the following result regarding the convergence of eigenvalues and eigenfunctions in the joint large data and dictionary limit.

Theorem 6.3 (Joint data and dictionary limit of eigensystem). *Let Ψ satisfy Assumption 1(b) and let $(\lambda_{NM}, f_{NM})_{(N,M) \in \mathbb{N}^2}$ be a sequence of eigenvalue and normalized eigenfunction pairs of $\hat{\mathcal{A}}_{NM}$. Then there almost surely exists a subsequence of eigenvalue and normalised eigenfunction pairs $(\lambda_{N_i M_{N_i}}, f_{N_i M_{N_i}})$ such that, for any sequence $M'_{N_i} \geq M_{N_i}$, almost surely*

$$\lambda_{N_i M'_{N_i}} \rightarrow \lambda, \quad f_{N_i M'_{N_i}} \xrightarrow{w} f, \quad \text{when } N_i \rightarrow \infty,$$

where $f \in \mathcal{D}$ and the weak convergence is with respect to the inner product on \mathcal{D} . Furthermore, if $f \neq 0$ and Assumptions 1, 2, 3, and 4 hold, then (λ, f) is an eigenvalue and eigenfunction pair of \mathcal{A} .

Proof. The first part follows from (λ_{NM}) and (f_{NM}) being bounded sequences of \mathbb{C} and $\mathcal{F}_N \subset \mathcal{D}$, respectively. Let $(\lambda_{N_i, M_i}, f_{N_i, M_i})$ be such a convergent sequence and suppose that Assumptions 1, 2, 3, and 4 hold. Then, by Theorem 5.1, there exists a subsubsequence (N_i, M_{N_i}) such that, for any $M'_{N_i} \geq M_{N_i}$, almost surely, for any $g \in \mathcal{D}$,

$$\left(\hat{\mathcal{A}}_{N_i M'_{N_i}} - \mathcal{A} \right) : (\mathcal{F}_{N_i}, \|\cdot\|_D) \rightarrow (\mathcal{F}, \|\cdot\|_{\mathcal{F}})$$

converges to zero pointwise when $N_i \rightarrow \infty$. It holds that

$$\langle \mathcal{A}f, g \rangle_{\mathcal{F}} = \left\langle \mathcal{A} \left(f - f_{N_i, M'_{N_i}} \right), g \right\rangle_{\mathcal{F}} + \left\langle (\mathcal{A} - \mathcal{A}_{N_i, M'_{N_i}}) f_{N_i, M'_{N_i}}, g \right\rangle_{\mathcal{F}} + \left\langle \mathcal{A}_{N_i, M'_{N_i}} f_{N_i, M'_{N_i}}, g \right\rangle_{\mathcal{F}}.$$

For $N_i \rightarrow \infty$, the first summand converges to zero because \mathcal{A} is bounded and $f_{N_i, M'_{N_i}} \xrightarrow{w} f$, the second summand does the same because of how (N_i, M'_{N_i}) was chosen, and the third summand converges to $\langle \lambda f, g \rangle_{\mathcal{F}}$ because $\lambda_{N_i M'_{N_i}} \rightarrow \lambda$. Thus,

$$\langle \mathcal{A}f, g \rangle_{\mathcal{F}} = \langle \lambda f, g \rangle_{\mathcal{F}}$$

for all $g \in \mathcal{D}$, which concludes the proof. \square

7 Numerical experiments

We will now illustrate the derived convergence results and error bounds and test their sharpness.

7.1 Benchmark problems

We analyse transfer operators associated with deterministic and stochastic systems of the form (4). In particular, we consider:

1. The ODE defined by

$$\mathbf{b}(\mathbf{x}) = \begin{bmatrix} \gamma x_1 \\ \delta(x_2 - x_1^2) \end{bmatrix}, \quad (39)$$

with $\gamma = -0.8, \delta = -0.7$.

2. The overdamped Langevin dynamics corresponding to the two-dimensional double-well potential $V(x) = (x_1^2 - 1)^2 + x_2^2$ with anisotropic diffusion, whose drift and diffusion terms are given by

$$\mathbf{b}(\mathbf{x}) = \begin{bmatrix} 4x_1 - 4x_1^3 \\ -2x_2 \end{bmatrix}, \quad \boldsymbol{\sigma}(\mathbf{x}) = \begin{bmatrix} 0.7 & x_1 \\ 0 & 0.5 \end{bmatrix}, \quad (40)$$

respectively.

3. The one-dimensional Ornstein–Uhlenbeck process given by

$$b(x) = -x, \quad \sigma(x) = \sqrt{\frac{1}{2}}, \quad (41)$$

This SDE has a unique invariant distribution $\mathcal{N}(0, \frac{1}{4})$.

For each of the dynamical systems, we aim to reconstruct the Koopman operator or its infinitesimal generator from data. We will specify the precise setup below. In each case, we compute the normalized error

$$\varepsilon_N := \frac{\|\mathbf{A}_N - \widehat{\mathbf{A}}_{NM}\|}{\|\mathbf{A}_N\|} \quad (42)$$

of the data-driven matrix $\widehat{\mathbf{A}}_{NM}$ with respect to the true Galerkin projection \mathbf{A}_N in (5), where we consider as a proxy for \mathbf{A}_N the result of gEDMD with a large number of data points. In the two-dimensional case, we use the domain $\mathbb{X} = [-2, 2] \times [-1, 1]$ and in the one-dimensional case, we define $\mathbb{X} = [-2, 2]$. For the three dynamical systems introduced above, we now study three different scenarios: the large data limit, the large dictionary limit, and the large data limit when using noisy data.

7.2 Numerical results as the number of data points tends to infinity

In our first experiment, we choose as basis functions monomials of order up to k , defined by

$$\Psi^{\text{MON}} = \{\mathbf{x}^\alpha\}_{|\alpha| \leq k},$$

and Gaussians centred at a collection of equidistant grid points $\{\mathbf{p}_n\}_{n=1}^N$, i.e.,

$$\Psi^{\text{GSN}} = \left\{ \exp\left(-\frac{\|\mathbf{x} - \mathbf{p}_n\|^2}{2\theta^2}\right) \right\}_{n=1}^N,$$

where for two-dimensional problems we use

$$\{\mathbf{p}_n\}_{n=1}^N = \left\{ \left(\frac{i}{2} - 2, \frac{j}{2} - 1 \right), i = 0, \dots, 8, j = 0, \dots, 4 \right\},$$

and for one-dimension problems

$$\{\mathbf{p}_n\}_{n=1}^N = \left\{ \frac{i}{2} - 2, i = 0, \dots, 8 \right\}.$$

We also use a finite element method (FEM) basis of piecewise linear functions with 0 boundary condition on a uniform mesh. That is, if we write $\{\mathbf{v}_j\}_{j=1}^N$ for the non-boundary vertices of the mesh, we have that ψ^{FEM} are the only continuous piecewise linear functions that satisfy

$$\psi_i^{\text{FEM}}(\mathbf{v}_j) = \delta_{ij}, \quad \forall i, j = 1, \dots, N,$$

and write $\Psi^{\text{FEM}} = \{\psi_n^{\text{FEM}}\}_{n=1}^N$. The basis functions in Ψ^{FEM} are only once weakly differentiable. However, the structure matrix \mathbf{C} can still be calculated for second-order operators using Observation 1.

We set the maximum degree of the monomials to $k = 8$ so that $N = \binom{k+d}{k}$. That is, $N = 45$ when the dimension is $d = 2$ and $N = 9$ when $d = 1$. Additionally, we take a uniform mesh with 45 and 9 non-boundary nodes in the 2D and 1D cases, respectively. In this way, there are the same number of observables in Ψ^{MON} , Ψ^{GSN} and Ψ^{FEM} . We then set $\theta = \frac{1}{2N}$ so that the basis functions are well separated. That is, $\theta < \frac{1}{2} \min_{i \neq j} \|\mathbf{p}_i - \mathbf{p}_j\|$. The points $\mathbf{x}_1, \dots, \mathbf{x}_M$ are sampled uniformly and independently from \mathbb{X} .

We apply the data-driven algorithm (11) to approximate the Koopman semigroup, and the Koopman and Perron–Frobenius generators associated with (39), (40), and (41) for an increasing number of data points using $M = 2^8, 2^9, \dots, 2^{19}$ and compute (42), where, since in general we do not have access to \mathbf{A}_N , we approximate it by $\hat{\mathbf{A}}_{NM}$ with $M = 2^{20}$. We repeat this process 50 times for each M to calculate the average normalized operator error ε . In Figure 1, we plot in log-log scale the relationship between M and ε , including a 95% confidence interval for the error. To serve as a reference, we show dashed lines with slope $-\frac{1}{2}$ and -1 , respectively.

As can be seen, for all choices of basis functions and all systems, the error has a slope of approximately $-\frac{1}{2}$. This is in accordance with Corollary 5.7 as when N is fixed we obtain $\varepsilon = \mathcal{O}(M^{-1/2})$. In Figures 1b and 1c, we see that the error of the approximation using FEM basis functions is quite large. This is to be expected as for small M it is possible for an element of the mesh to have few points. If this is the case, the empirical Gram matrix is close to singular (see the comments around Example 3.3). This also results in initially large confidence interval for the error, which, when represented on a log-log plot, creates a strong visual effect. The error decays at the expected rate. In Figure 1d, the error using monomial basis functions becomes zero. This is because the subspace spanned by the monomial basis functions is invariant under the Koopman generator of the OU system, see Corollary 3.2.

7.3 Numerical results as the number of dictionary elements tends to infinity

We now study the effect of the number of dictionary elements on the operator error. To do so, we consider as our basis functions the dictionary comprising Gaussian functions from the previous subsection. We partition the domain into N equally sized quadrants and define $\{\mathbf{p}_n\}_{n=1}^N$ to be the centres of these quadrants. We apply the data-driven algorithms with $M = 10^4$ data points. We repeat this process 50 times and calculate the average normalized operator error where again \mathbf{A}_N is approximated by $\hat{\mathbf{A}}_{NM}$ with $M = 10^5$. We then increase N from 4 to 1024. In this case, the monomial basis functions are not chosen as for higher orders, the matrix \mathbf{G}_N becomes ill-conditioned

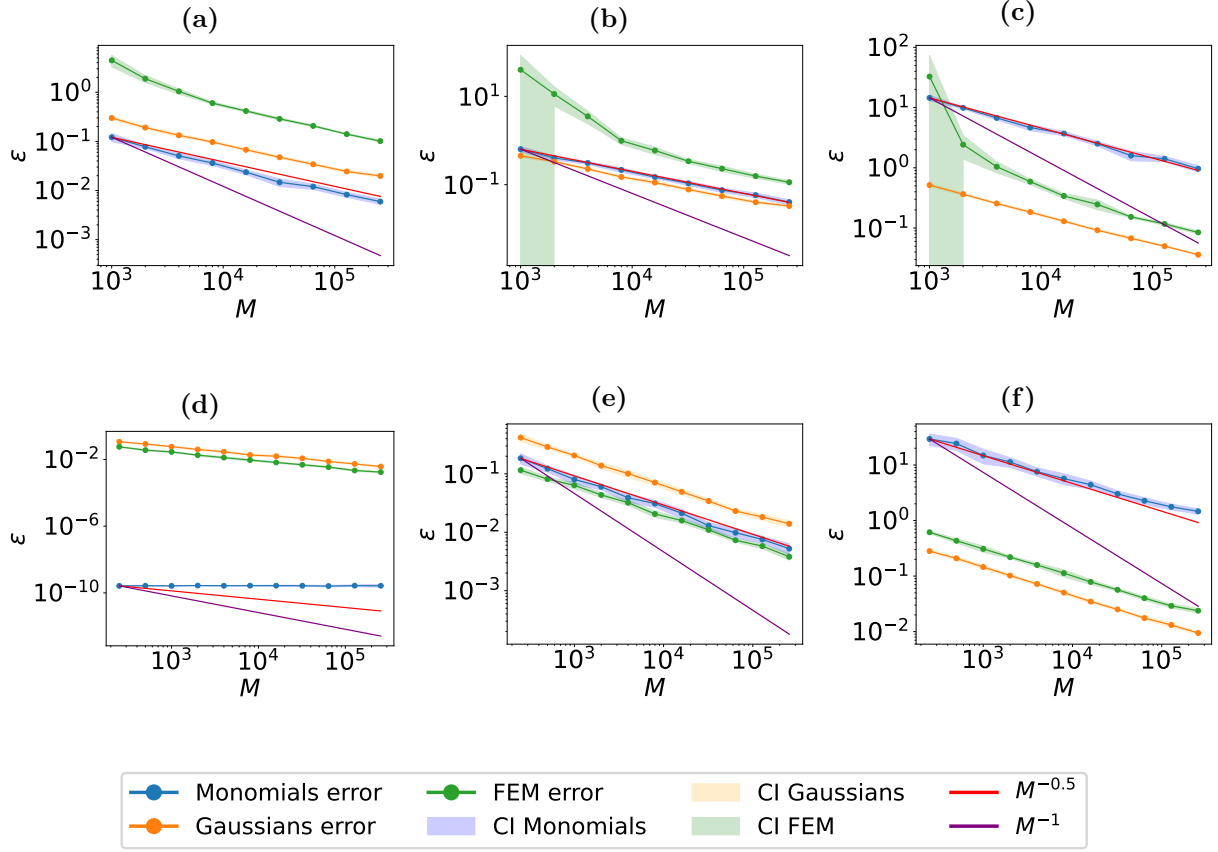


Figure 1: Average normalized error $\varepsilon := \mathbb{E}[\|\hat{\mathbf{A}}_{MN} - \mathbf{A}_N\| / \|\mathbf{A}_N\|]$ as a function of the number of data points M for: the Koopman generator of the ODE (39) in Figure 1a, the Koopman generator and Koopman operator for the double-well potential (40) in Figures 1b and 1c, and the Koopman generator, the Perron–Frobenius generator and the Koopman operator for the OU process in Figures 1d, 1e, and 1f. In all cases, monomials up to order 8 and the same number of Gaussian observables and FEM basis functions are used. The red and purple lines represent the slopes $-1/2$ and -1 , respectively. The blue, red and green lines represent the average error over 50 simulations of the above approximations. The shaded areas represent the 95% confidence intervals for the respective errors.

(for example, for monomials of order 10 in two dimensions, we have that $\kappa(\mathbf{G}_N) \geq 10^{28}$). When approximating the Koopman operator for the OU process, we also use the piecewise linear FEM basis functions Ψ^{FEM} . However, these are not used for gEDMD as the theoretical error requires the calculation of $\mathbf{T}_{ij} = \langle \mathcal{L}\psi_i, \mathcal{L}\psi_j \rangle$. For gEDMD, \mathcal{L} is a second order operator and ψ_i^{FEM} are not twice differentiable. Since we plot normalised errors, we cap the theoretical bound in Corollary 5.7 in the plots at one. As can be seen in Figure 2, the error increases with the number of observables as expected in view of Corollary 5.7. We observe that the theoretical bound on the error increases faster than the simulation error. This indicates that perhaps there is some underlying structure which could make the bounds tighter. Additionally, we see that the confidence interval for the FEM basis functions becomes larger as the number of basis functions increases. This is because of the increased likelihood that very few particles end up in some interval of the partition. This leads to close to a singular mass matrix and a large condition number. See the comments around Example 3.3.

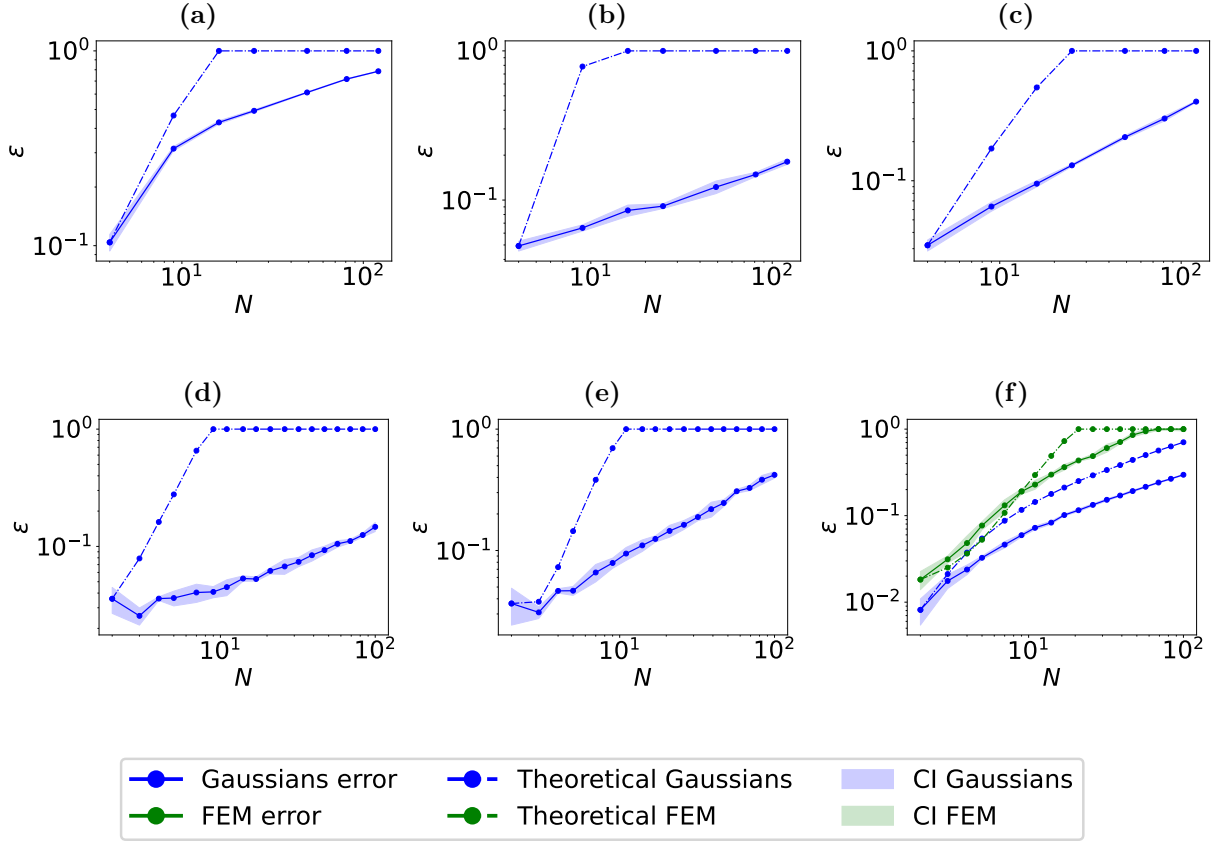


Figure 2: Average normalized error $\varepsilon := \mathbb{E}[\|\hat{\mathbf{A}}_{MN} - \mathbf{A}_N\| / \|\mathbf{A}_N\|]$ and the theoretical error bound in Corollary 5.7 as a function of the number of observables N for the Koopman generator of the ODE (39) in Figure 2a, the Koopman generator and Koopman operator for the double-well system (40) in Figures 2b and 2c, and the Koopman generator, the Perron–Frobenius, and Koopman operator for the OU process (41) using up to 1024 Gaussian functions in Figures 2d, 2e, and 2f.

7.4 Numerical results with noise

In this section, we repeat the experiments carried out in Section 7.2 with the addition of a noise term as in (28), where we take normal i.i.d. noise, i.e.,

$$(\boldsymbol{\eta}_n, \boldsymbol{\xi}_n) \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_{2n \times 2n}).$$

We increase the noise using $\sigma = 10^{-3}, 10^{-2}, 10^{-1}$ and study its effect on the normalised error. To limit the number of plots, we restrict ourselves to gEDMD for the ODE (39) and gEDMD for the Perron–Frobenius operator associated with the Ornstein–Uhlenbeck process.

As we can see, the Gaussian and FEM observables are more resilient to increased noise. The FEM basis functions perform the best in the presence of noise. This is expected as we evaluated the FEM basis functions exactly to 0 on all points outside of their support and only added noise to the non-zero ones. The lower resilience of the monomials compared to the other two is due to the fact that the condition number of the Gram matrix of the monomials is larger and thus the inverse of the Gram matrix is very sensitive to noise. In the second and third rows of Figure 3, the monomials are slightly more resilient to the noise. This, however, is due to the fact that, since the dimension of the domain is 1 instead of 2, there are fewer monomials and thus the condition number of the Gram matrix is smaller. It can be seen that even when the error without noise is exactly zero (see Figure 1d), the monomial basis functions are not resilient to noise.

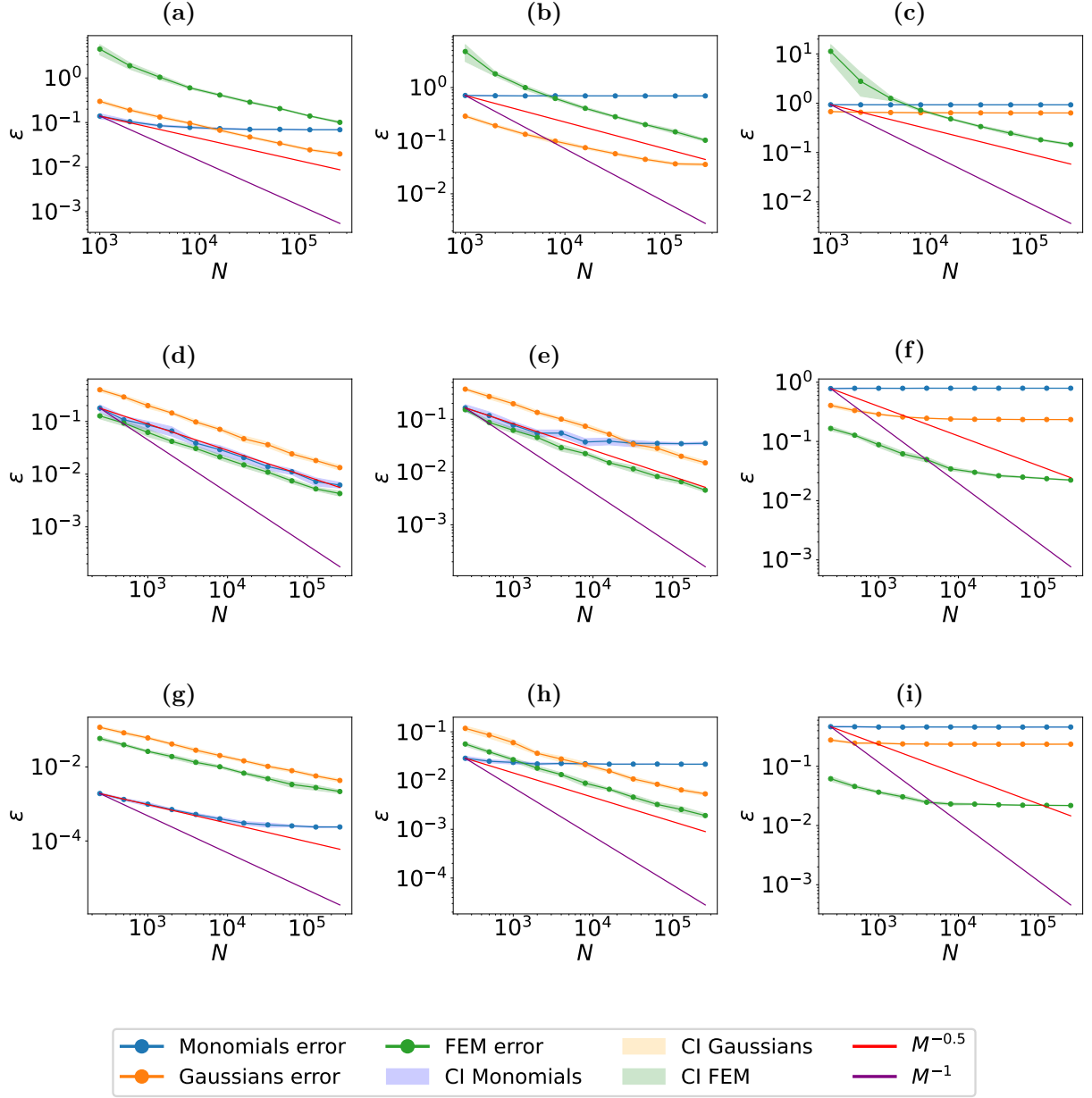


Figure 3: Average normalized error $\varepsilon := \mathbb{E}[\|\hat{\mathbf{A}}_{MN} - \mathbf{A}_N\| / \|\mathbf{A}_N\|]$ as a function of the number of data points M . In Figures 3a, 3b, and 3c, we take $\sigma = 10^{-3}, 10^{-2}, 10^{-1}$, respectively, and approximate the Koopman generator of the ODE. In Figures 3d, 3e, 3f and in 3g, 3h, 3i we also take $\sigma = 10^{-3}, 10^{-2}, 10^{-1}$ and now approximate the Perron-Frobenius operator and Koopman generator of (41), respectively. In all cases, monomials up to order 8 and the same number of Gaussian observables and FEM basis functions are used. The red and purple lines represent the slopes $-\frac{1}{2}$ and -1 , respectively. The blue, red and green lines represent the error averaged over 50 simulations of the above approximations. The shaded areas represent the 95% confidence intervals for the respective errors.

8 Conclusion

In this article, we have investigated the approximation of an operator \mathcal{A} from point evaluations of a dictionary to which the operator has been applied. That is, we have assumed that we have training data of the form

$$\{(\psi_n(\mathbf{x}_m), \mathcal{A}\psi_n(\mathbf{x}_m))\}_{m,n=1}^{M,N},$$

where the evaluations could additionally be subject to random noise. After describing the estimation procedure for linear operators from data, we have presented a thorough convergence and error analysis in the dictionary limit ($N \rightarrow \infty$), the data limit ($M \rightarrow \infty$), and their joint limit ($N, M \rightarrow \infty$). We have studied the convergence of the full operators as well as their spectra.

Throughout this work, we have usually thought of the approximation of transfer operators in the context of dynamical systems, such as Koopman operators, Perron–Frobenius operators, and their generators. The framework we have presented is clearly not limited to such operators. Indeed, it generalises approximation techniques for transfer operators, such as EDMD and gEDMD, to general operators. EDMD and gEDMD fall naturally into our framework and we have shown significant new convergence results and error analyses for these methods. Additionally, we have verified our analytical results in numerical experiments.

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A When does a matrix determine an operator?

As discussed in Section 2.1, a matrix may not always define an operator when it is interpreted as acting on a set of vectors that are not linearly independent. The following lemma gives necessary and sufficient conditions for such an operator to be well-defined.

Lemma A.1. *Let $\mathbf{T} \in \mathbb{C}^{N \times N}$ and consider $\Psi = \{\psi_n\}_{n=1}^N$ and $V = \text{span}(\Psi)$. Given*

$$v = \sum_{j=1}^n c_j \psi_j \in V,$$

define

$$\mathcal{T}v := \sum_{i,j=1}^N c_j \mathbf{T}_{ij} \psi_i, \tag{43}$$

then $\mathcal{T}: V \rightarrow V$ is a well-defined linear operator if and only if for all $(c_1, \dots, c_N) \in \mathbb{C}^N$ it holds that

$$\sum_{i=1}^N c_i \psi_i = 0 \implies \sum_{i,j=1}^N c_j \mathbf{T}_{ij} \psi_i = 0. \tag{44}$$

Here, $\mathbf{T} = \mathbf{T}^\Psi$, that is, \mathbf{T} is a matrix representation of \mathcal{T} with respect to Ψ .

Proof. Suppose that condition (44) holds. To see that \mathcal{T} is well-defined, we check that, if $v \in V$ has two representations

$$v = \sum_{j=1}^N b_j \psi_j = \sum_{j=1}^N b'_j \psi_j,$$

then \mathcal{T} is equal on both representations. That is,

$$\sum_{i,j=1}^N b_j \mathbf{T}_{ij} \psi_i - \sum_{i,j=1}^N b'_j \mathbf{T}_{ij} \psi_i = \sum_{i,j=1}^N (b_j - b'_j) \mathbf{T}_{ij} \psi_i = 0.$$

This holds, as can be seen by using (44) with $c_j := b_j - b'_j$. The fact that $\mathcal{T}: V \rightarrow V$ is linear follows from the definition in (43). The reverse implication is a consequence of the linearity of \mathcal{T} as, if $v = \sum_{j=1}^N c_j \psi_j = 0$, then

$$0 = \mathcal{T}v = \sum_{i,j=1}^N c_j \mathbf{T}_{ij} \psi_i.$$

Finally, to check that if (44) holds, then $\mathbf{T} = \mathbf{T}^\Psi$ it suffices to take $v = \psi_j$ in (43). □

B Bernstein inequality

The following results can be found in [32, page 8].

Theorem B.1. *Let $\mathbf{S}_1, \dots, \mathbf{S}_M \in \mathbb{C}^{N \times N}$ be independent, random matrices such that*

$$\mathbb{E}[\mathbf{S}_m] = \mathbf{0} \text{ and } \|\mathbf{S}_m\| \leq L, \quad \forall m \in \{1, \dots, M\}.$$

Consider the sum

$$\mathbf{Z} = \sum_{m=1}^M \mathbf{S}_m,$$

and let $\nu(\mathbf{Z})$ denote the matrix variance statistic of the sum:

$$\nu(\mathbf{Z}) = \max \left\{ \|\mathbb{E}(\mathbf{Z}\mathbf{Z}^\dagger)\|, \|\mathbb{E}(\mathbf{Z}^\dagger\mathbf{Z})\| \right\}.$$

Then for every $\delta > 0$

$$\mathbb{P}\{\|\mathbf{Z}\| \geq \delta\} \leq 2N \exp \left(\frac{-\delta^2/2}{\nu(\mathbf{Z}) + L\delta/3} \right), \quad \forall \delta \geq 0.$$

Corollary B.2 (Bernstein inequality for the covariance). *Let \mathbf{c} and \mathbf{g} be two random vectors in \mathbb{C}^n such that almost everywhere*

$$|\mathbf{c}|^2 \leq \gamma, \quad |\mathbf{g}|^2 \leq \gamma.$$

Let $\{\mathbf{c}_m\}_{m=1}^M, \{\mathbf{g}_m\}_{m=1}^M$ be copies of \mathbf{c} and \mathbf{g} respectively and such that $\{\mathbf{c}_m \mathbf{g}_m^\dagger\}_{m=1}^M$ are independent. Define the matrices,

$$\begin{aligned} \mathbf{G} &:= \mathbb{E}[\mathbf{g}\mathbf{g}^\dagger], \quad \mathbf{T} := \mathbb{E}[\mathbf{c}\mathbf{c}^\dagger], \quad \mathbf{C} := \mathbb{E}[\mathbf{c}\mathbf{g}^\dagger], \\ \mathbf{S}_m &:= \frac{1}{M} \left(\mathbf{c}_m \mathbf{g}_m^\dagger - \mathbf{C} \right), \quad \mathbf{Z} := \sum_{m=1}^M \mathbf{S}_m. \end{aligned}$$

Then

$$\mathbb{P}\{\|\mathbf{Z}\| \geq \delta\} \leq 2N \exp \left(\frac{-M\delta^2/2}{\gamma(\max\{\|\mathbf{T}\|, \|\mathbf{G}\|\} + 2\delta/3)} \right).$$

Furthermore, for all $p \in (0, 1)$ and for all

$$M > (3 \max\{\|\mathbf{G}\|, \|\mathbf{T}\|\} + 2\delta) \frac{2\gamma}{3\delta^2} \log \left(\frac{2N}{1-p} \right),$$

it holds that

$$\mathbb{P}\{\|\mathbf{Z}\| < \delta\} \geq p.$$

Proof. By construction, \mathbf{S}_m are independent with mean zero so that we can apply Bernstein's inequality B.1. We have

$$\|\mathbf{S}_m\| \leq \frac{1}{M} \left(\|\mathbf{c}_m \mathbf{g}_m^\dagger\| + \|\mathbf{C}\| \right) = \frac{1}{M} \left(\|\mathbf{c}_m\| \|\mathbf{g}_m^\dagger\| + \|\mathbb{E}[\mathbf{c}\mathbf{g}^\dagger]\| \right) \leq \frac{2\gamma}{M} =: L.$$

Next, we bound the matrix variance statistic $\nu(\mathbf{Z})$. First,

$$\mathbb{E}[\mathbf{S}_m \mathbf{S}_m^\dagger] = \frac{1}{M^2} \mathbb{E} \left[\|\mathbf{g}_m\|^2 \mathbf{c}_m \mathbf{c}_m^\dagger - \mathbf{c}_m \mathbf{g}_m^\dagger \mathbf{C}^\dagger - \mathbf{C} \mathbf{c}_m \mathbf{g}_m^\dagger + \mathbf{C} \mathbf{C}^\dagger \right] \preceq \frac{1}{M^2} \left(\gamma \mathbf{T} - \mathbf{C} \mathbf{C}^\dagger \right) \preceq \frac{\gamma}{M^2} \mathbf{T},$$

where we used the notation $\mathbf{D} \preceq \mathbf{E}$ to signify that $\mathbf{E} - \mathbf{D}$ is positive semi-definite. Similarly,

$$\mathbb{E}[\mathbf{S}_m^\dagger \mathbf{S}_m] = \frac{1}{M^2} \mathbb{E} \left[\|\mathbf{c}_m\|^2 \mathbf{g}_m \mathbf{g}_m^\dagger - \mathbf{C}^\dagger \mathbf{c}_m \mathbf{g}_m^\dagger - \mathbf{c}_m \mathbf{g}_m^\dagger \mathbf{C} + \mathbf{C} \mathbf{C}^\dagger \right] \preceq \frac{1}{M^2} (\gamma \mathbf{G} - \mathbf{C} \mathbf{C}^\dagger) \preceq \frac{\gamma}{M^2} \mathbf{G}.$$

Now, since \mathbf{S}_m are independent with mean zero, we obtain that

$$\nu(\mathbf{Z}) = \max \left\{ \|\mathbb{E}(\mathbf{Z} \mathbf{Z}^\dagger)\|, \|\mathbb{E}(\mathbf{Z}^\dagger \mathbf{Z})\| \right\} \leq \frac{\gamma}{M} \max \{\|\mathbf{T}\|, \|\mathbf{G}\|\}.$$

Applying Bernstein's inequality [B.1](#), we obtain

$$\mathbb{P}\{\|\mathbf{Z}\| \geq \delta\} \leq 2N \exp \left(\frac{-M\delta^2/2}{\gamma(\max\{\|\mathbf{T}\|, \|\mathbf{G}\|\} + 2\delta/3)} \right).$$

Setting the right-hand side of the above to $1 - p$ and solving for M concludes the proof. \square

Lemma B.3. *Given $\mathcal{T}: \mathcal{F}_N \rightarrow \mathcal{F}_N$ it holds that $\|\mathcal{T}\| \leq \sqrt{\kappa(\mathbf{G}_N)} \|\mathbf{T}^\Psi\|$.*

Proof. To establish a bound, we begin by orthonormalising Ψ_N by considering

$$\tilde{\Psi}_N := \mathbf{G}_N^{-1/2} \Psi_N. \quad (45)$$

Now, given $\psi \in \mathcal{F}_N$, we can write $\psi = \tilde{\mathbf{c}} \cdot \tilde{\Psi}_N$ for some $\tilde{\mathbf{c}} \in \mathbb{C}^N$. Using that $\tilde{\Psi}_N$ is orthonormal, and the expression for the change of basis matrix given by [\(45\)](#) shows that

$$\|\mathcal{T}\psi\|_{\mathcal{F}} = \|\mathbf{T}^{\tilde{\Psi}_N} \tilde{\mathbf{c}}\| = \|\mathbf{G}_N^{-1/2} \mathbf{T}^{\Psi_N} \mathbf{G}_N^{1/2} \tilde{\mathbf{c}}\| \leq \|\mathbf{G}_N^{-1/2}\| \|\mathbf{T}^{\Psi_N}\| \|\mathbf{G}_N^{1/2}\| |\tilde{\mathbf{c}}|. \quad (46)$$

Now, given a matrix \mathbf{B} , its operator norm in the Euclidean metric is

$$\|\mathbf{B}\|^2 = \lambda_{\max}(\mathbf{B} \mathbf{B}^\dagger).$$

Applying this to $\mathbf{G}_N^{1/2}$ and $\mathbf{G}_N^{-1/2}$ and substituting back into [\(46\)](#) completes the proof. \square

C Table of notation

The notation used throughout the manuscript is summarised in [Table 1](#).

Table 1: Overview of the notation.

Symbol	Description
\mathbb{X}	state space of the dynamical system
μ	probability measure on \mathbb{X}
$\mathcal{F} = L^2(\mathbb{X}, \mu)$	ambient space
$\mathcal{A}: \mathcal{D} \subset \mathcal{F} \rightarrow \mathcal{F}$	target linear operator
\mathcal{D}	domain of the operator \mathcal{A}
$\ \cdot\ _{\mathcal{F}}, \ \cdot\ _{\mathcal{D}}$	norms on the function spaces \mathcal{F} and \mathcal{D}
$\{\psi_n\}_{n=1}^N$	dictionary or set of functions used to approximate \mathcal{A}
Ψ_N	first N elements ψ_1, \dots, ψ_N of the dictionary
$\{\mathbf{x}_m\}_{m=1}^M$	data sampled i.i.d. from μ used to approximate \mathcal{A}
$\mathcal{F}_N = \text{span}(\Psi_N)$	finite-dimensional subspace on which \mathcal{A} is approximated
$\mathcal{F}_{\infty} = \bigoplus_{n=1}^{\infty} \mathcal{F}_n$	infinite-dimensional space spanned by the dictionary
$\mathcal{P}_{\mathcal{F}_N}$	projection operator onto \mathcal{F}_N using inner product on \mathcal{F}
$\mathcal{P}_{\mathcal{D}_N}$	projection operator onto \mathcal{D}_N using inner product on \mathcal{D}
$\mathcal{A}_N = \mathcal{P}_{\mathcal{F}_N} \mathcal{A} _{\mathcal{F}_N}$	Galerkin projection of \mathcal{A} onto \mathcal{F}_N
$\hat{\mathcal{A}}_{NM}$	approximation of \mathcal{A} and \mathcal{A}_N using M samples and N basis functions
\mathbf{T}^{Ψ}	matrix representation of the operator \mathcal{T} using the basis given by Ψ
$\mathbf{C}_N, \mathbf{G}_N$	structure matrix of \mathcal{A} and Gram matrix w.r.t. the basis Ψ_N
$\hat{\mathbf{C}}_{NM}, \hat{\mathbf{G}}_{NM}$	empirical structure and Gram matrices
$\hat{\mu}_M = \frac{1}{M} \sum_{m=1}^M \delta_{\mathbf{x}_m}$	empirical measure associated with the M samples
$\hat{\mathcal{F}}_M = L^2(\mathbb{X}, \hat{\mu}_M)$	empirical space associated with the M samples
$\hat{\phi} = \sum_{m=1}^M \phi(\mathbf{x}_m) \delta_{\mathbf{x}_m}$	function $\phi \in \mathcal{F}$ when viewed in $\hat{\mathcal{F}}_M$
$\hat{\Psi}_N$	first N elements of the dictionary when viewed in $\hat{\mathcal{F}}_M$
$\hat{\mathcal{F}}_{NM} = \text{span}(\hat{\Psi}_N) \subset \mathcal{F}_M$	span of dictionary in empirical space
$\hat{\mathcal{T}}$	operator \mathcal{T} viewed as acting on $\hat{\mathcal{F}}_M$
$\boldsymbol{\eta}_N, \boldsymbol{\xi}_N$	additive noise in the samples and observations
$\tilde{\mathcal{A}}_{NM}, \tilde{\mathbf{C}}_{NM}, \tilde{\mathbf{G}}_{NM}$	approximations of $\mathcal{A}_N, \mathbf{C}_N, \mathbf{G}_N$ when noise is present
$\Phi: \mathbb{X} \rightarrow \mathbb{X}$	flow of the dynamical system
$\mathcal{K}, \mathcal{K}^*$	Koopman operator and its adjoint
$\mathcal{L}, \mathcal{L}^*$	infinitesimal generator of the Koopman operator and its adjoint