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Vladimir Kostic, Karim Lounici, H el ene Halconruy, Timoth ee Devergne,
Pietro Novelli, Massimiliano Pontil

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Learning the Infinitesimal Generator of Stochastic Diffusion Processes

Vladimir R. Kostic
Istituto Italiano di Tecnologia
University of Novi Sad
vladimir.kostic@iit.it

Karim Lounici
CMAP-Ecole Polytechnique
karim.lounici@polytechnique.edu

Helene Halconruy
Telecom Sud-Paris
helene.halconruy@telecom-sudparis.eu

Timothee Devergne
Istituto Italiano di Tecnologia
timothee.devergne@iit.it

Massimiliano Pontil
Istituto Italiano di Tecnologia
University College London
massimiliano.pontil@iit.it

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Abstract

We address data-driven learning of the infinitesimal generator of stochastic diffusion processes, essential for understanding numerical simulations of natural and physical systems. The unbounded nature of the generator poses significant challenges, rendering conventional analysis techniques for Hilbert-Schmidt operators ineffective. To overcome this, we introduce a novel framework based on the energy functional for these stochastic processes. Our approach integrates physical priors through an energy-based risk metric in both full and partial knowledge settings. We evaluate the statistical performance of a reduced-rank estimator in reproducing kernel Hilbert spaces (RKHS) in the partial knowledge setting. Notably, our approach provides learning bounds independent of the state space dimension and ensures non-spurious spectral estimation. Additionally, we elucidate how the distortion between the intrinsic energy-induced metric of the stochastic diffusion and the RKHS metric used for generator estimation impacts the spectral learning bounds.

1 Introduction

Continuous-time processes are often modeled using ordinary differential equations (ODEs), assuming deterministic dynamics. However, real systems in science and engineering that are modeled by ODEs are subject to unfeasible-to-model influences, necessitating the extension of deterministic models through *stochastic differential equations* (SDEs), see [33, 35] and references therein. SDEs are advantageous for modeling inherently random phenomena. For instance, in finance, they specify the stochastic process governing asset behavior, a crucial step in constructing pricing models for financial derivatives [34]. In atomistic simulations, where SDEs are used to model the evolution of atomic systems subjected to thermal fluctuations via the Boltzmann distribution [30].

A diverse range of SDEs can be represented as $dX_t = a(X_t)dt + b(X_t)dW_t$, where $X_0 = x$. Here, W denotes a (possibly multi-dimensional) Brownian motion, and the functions a and b are commonly known as the *drift* and *diffusion* coefficients, respectively. Determining these coefficients from one or more trajectories, whether discretized or continuous, has been a key pursuit in "diffusion statistics" since the 1980s, as seen in works like [18, 24, 25]. However, uncovering the drift and diffusion coefficients alone does not reveal all the intrinsic properties of a complex system, such as the metastable states of Langevin dynamics in atomistic simulations [see e.g. 42, and references therein]. Consequently, there has been a shift and growing interest in the Infinitesimal Generator (IG) of an SDE, as its spectral decomposition offers a more in-depth understanding of system dynamics and behavior, thus providing a comprehensive picture beyond the mere identification of coefficients.

Recovering the spectral decomposition of the IG can theoretically be achieved by exploiting the well-studied Transfer Operators (TO) [see 21, and references therein]. TOs represent the average evolution of state functions (observables) over time and, being linear and amenable to spectral decomposition under certain conditions, they offer a valuable means to interpret and analyze nonlinear systems. However, they require evenly sampled data at a high rate, which may be impractical. Additionally, TO approaches are purely data-driven, complicating the incorporation of partial or full knowledge of an SDE into the learning process. Thus, there is growing interest in learning the IG directly from data, as it can handle uneven sampling and integrate SDE knowledge. The challenge lies in the IG being an unbounded operator, unlike TO which are often well-approximated by Hilbert-Schmidt operators with comprehensive statistical theory [22]. Unfortunately, the existing statistical theory collapses when applied to unbounded operators, prompting the need to completely rethink the problem

Related work Extensive research has explored learning dynamical systems from data [see the monographs 7, 26, and references therein]. Analytical models for dynamics are often unavailable, motivating the need for data-driven methods. Two prominent approaches have emerged: deep learning-based methods [5, 11, 29], effective for learning complex data representations but lacking statistical analysis, and kernel methods [2, 6, 9, 16, 17, 20–22, 43], offering solid statistical guarantees for the estimation of the TO but requiring careful selection of the kernel function. A related question, tackling the challenging problem of learning invariant subspaces of the TO, has recently led to the development of several methodologies [17, 27, 31, 39, 45, 44], some of which are based on deep canonical correlation analysis [3, 23]. In comparison, there have been significantly fewer works on learning the IG and only in very specific settings. In [48] a deep learning approach is developed for Langevin diffusion, while [19] presents an extended dynamical mode decomposition method for learning the generator and clarifies its connection to Galerkin's approximation. However, neither of these two works provides any learning guarantees. In this respect the only previous work we are aware of are [1], revising the Galerkin method for Laplacian diffusion, [15], presenting a kernel approach for general diffusion SDE with full knowledge of drift and diffusion coefficients, and [36] addressing Langevin diffusion. As highlighted in Appendix E.6, the bounds and analysis in these works are either restricted to specific SDEs or are incomplete. Notably, none of these works proposed

an adequate framework to handle the unboundedness of the IG, resulting in an incomplete theoretical analysis and suboptimal rates, sometimes explicitly depending on state space dimension. Moreover, the estimators proposed in these works are prone to spurious eigenvalues and do not offer guarantees on the accurate estimation of eigenvalues and eigenfunctions.

Contributions In summary, our main contributions are: **1)** Underpinning a framework for learning the generator of stochastic diffusion processes in reproducing kernel Hilbert space, using a novel energy risk functional; **2)** Proposing a reduced-rank estimator with dimension-free learning bounds; **3)** Establishing first-of-its-kind spectral learning bounds for generator learning; **4)** Demonstrating the practical advantages of our approach over previous methods.

2 Background and the problem

Our drive to estimate the eigenvalues of the infinitesimal generator for an SDE like (1) stems from its crucial role in characterizing dynamics in physical systems. This operator's closed form (3), relies on the drift a and diffusion coefficient b , where we have partial knowledge: b is assumed to be known, but a is not. To compensate for the lack of prior knowledge about a , we introduce the system's *energy* as an additional known quantity. Below, we detail the mathematical concepts framing the problem (generator, spectrum, energy) exemplified through the Langevin and Cox-Ingersoll-Ross processes. For detailed list of notation used throughout the paper we refer Table 7 in the appendix.

Transfer operator and infinitesimal generator A variety of physical, biological, and financial systems evolve through stochastic processes $X = (X_t)_{t \in \mathbb{R}_+}$, where $X_t \in \mathcal{X} \subset \mathbb{R}^d$ denotes the system's state at time t . A commonly employed model for such dynamics is captured by *stochastic differential equations* (SDEs) of the form

$$dX_t = a(X_t)dt + b(X_t)dW_t \quad \text{and} \quad X_0 = x, \quad (1)$$

where $x \in \mathcal{X}$, $W = (W_t^1, \dots, W_t^p)_{t \in \mathbb{R}_+}$ is a \mathbb{R}^p -dimensional ($p \in \mathbb{N}$) standard Brownian motion, the *drift* $a : \mathcal{X} \rightarrow \mathbb{R}^d$, and the *diffusion* $b : \mathcal{X} \rightarrow \mathbb{R}^{d \times p}$ are assumed to be globally Lipschitz and sub-linear, so that the SDE (1) admits an unique solution $X = (X_t)_{\geq 0}$ with values in $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$. Processes akin to equations like (1) are diverse, spanning models like Langevin and Cox-Ingersoll-Ross processes (see examples below), with broad applications in science and engineering. The process X is a continuous-time Markov process with almost surely continuous sample paths whose dynamics is described by a family of probability densities $(p_t)_{t \in \mathbb{R}_+}$ and *transfer operators* $(A_t)_{t \in \mathbb{R}_+}$ such that for all $t \in \mathbb{R}_+$, $E \in \mathcal{B}(\mathcal{X})$, $x \in \mathcal{X}$ and measurable function $f : \mathcal{X} \rightarrow \mathbb{R}$,

$$\mathbb{P}(X_t \in E | X_0 = x) = \int_E p_t(x, y) dy \quad \text{and} \quad A_t f = \int_{\mathcal{X}} f(y) p_t(\cdot, y) dy = \mathbb{E}[f(X_t) | X_0 = \cdot]. \quad (2)$$

Evaluating $A_t f$ at x yields the expectation of f starting from x and evolving until time t , making the transfer operator crucial for understanding X dynamics. The family $(A_t)_{t \in \mathbb{R}_+}$ satisfies the fundamental semigroup equation $A_{t+s} = A_t \circ A_s$, for $s, t \in \mathbb{R}_+$. Here, we focus on the transfer operator's effect on the set $\mathcal{L}_\pi^2(\mathcal{X})$, a choice driven by the existence of an invariant measure π for A_t on $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$ which satisfies $A_t^* \pi = \pi$ for all $t \in \mathbb{R}_+$. Then, the process X is characterized by the infinitesimal generator L defined for every $f \in \mathcal{L}_\pi^2(\mathcal{X})$ such that the limit $Lf = \lim_{t \rightarrow 0^+} (A_t f - f)/t$ exists in $\mathcal{L}_\pi^2(\mathcal{X})$. The operator L is closed on its domain $\text{dom}(L)$ which is equal to the Sobolev space

$$\mathcal{W}_\pi^{1,2}(\mathcal{X}) = \{f \in \mathcal{L}_\pi^2(\mathcal{X}) \mid \|f\|_{\mathcal{W}}^2 = \|f\|_{\mathcal{L}_\pi^2}^2 + \|\nabla f\|_{\mathcal{L}_\pi^2}^2 < \infty\}.$$

For SDE dynamics of the form (1), we can prove (see A.2 for details) that L is the second-order differential operator given, for any $f \in \mathcal{L}_\pi^2(\mathcal{X})$, $x \in \mathcal{X}$, by

$$Lf(x) = \nabla f(x)^\top a(x) + \frac{1}{2} \text{Tr}[b(x)^\top (\nabla^2 f(x)) b(x)], \quad (3)$$

where $\nabla^2 f = (\partial_{ij}^2 f)_{i \in [d], j \in [p]}$ denotes the Hessian matrix of f .

Spectral decomposition Knowing only the drift a and diffusion b is not enough to compute (2) or to understand quantitative aspects of dynamical phase transitions, such as time scales and metastable states. The eigenvalues and eigenvectors of the generator are crucial for capturing these effects. To address the possible unbounded nature of L , one can turn to an auxiliary operator, the resolvent, which, under certain conditions, shares the same eigenfunctions as L and becomes compact. When it exists and is continuous for some $\mu \in \mathbb{C}$, the operator $L_\mu = (\mu I - L)^{-1}$ is the *resolvent* of L and the corresponding *resolvent set* is defined by

$$\rho(L) = \{\mu \in \mathbb{C} \mid (\mu I - L) \text{ is bijective and } L_\mu \text{ is continuous}\}$$

We assume L has a *compact resolvent*, meaning $\rho(L) \neq \emptyset$ and there exists $\mu_0 \in \rho(L)$ such that $(\mu_0 I - L)^{-1}$ is compact. Under this assumption, and given that $(L, \text{dom}(L))$ is self-adjoint, we can prove the spectral decomposition of the generator (see A.1 for details) as follows:

$$L = \sum_{i \in \mathbb{N}} \lambda_i f_i \otimes f_i \quad (4)$$

where $(\lambda_i)_{i \in \mathbb{N}}$ are the eigenvalues of L , and the corresponding eigenfunctions $f_i \in \mathcal{L}_\pi^2(\mathcal{X})$, forming an orthonormal basis $(f_i)_{i \in \mathbb{N}}$, are also eigenfunctions of the transfer operator A_t .

Dirichlet forms and energy To handle the initial lack of knowledge about the drift a , we assume to have access to another quantity, called the *energy*, defined as $\mathfrak{E}(f) = \lim_{t \rightarrow 0} \int_{\mathcal{X}} (f(f - A_t f)) / t d\pi$ for all functions $f \in \mathcal{L}_\pi^2(\mathcal{X})$ for which this limit exists, defining in the way the domain $\text{dom}(\mathfrak{E})$. The associated *Dirichlet form* is the bilinear form defined by polarization for any $f, g \in \text{dom}(\mathfrak{E})$ by

$$\mathfrak{E}(f, g) = - \int_{\mathcal{X}} f(Lg) d\pi = \int_{\mathcal{X}} (-Lf)g d\pi. \quad (5)$$

For every $f \in \text{dom}(\mathfrak{E})$, we have $\mathfrak{E}(f) = \mathfrak{E}(f, f)$. As for every $i \in \mathbb{N}$, $0 \leq \mathfrak{E}(f_i, f_i) = - \int_{\mathcal{X}} f_i(\lambda_i f_i) d\pi = -\lambda_i$, we check that the eigenvalues of L are negative. To relate L to Dirichlet form, we assume there exists a *Dirichlet operator* $B = s^\top \nabla$ where $s = [s_1 \mid \dots \mid s_p] : x \in \mathcal{X} \mapsto s(x) = [s_1(x) \mid \dots \mid s_p(x)] \in \mathbb{R}^{d \times p}$ is a smooth function s.t. $Lf = s(s^\top \nabla f) = s(Bf)$ and so that

$$\int_{\mathcal{X}} (-Lf)g d\pi = \int_{\mathcal{X}} (s(x)s(x)^\top \nabla f(x))^\top \nabla g(x) \pi(dx) = \int_{\mathcal{X}} (Bf(x))^\top (Bg(x)) \pi(dx).$$

We get that for any $f \in \text{dom}(\mathfrak{E})$

$$\mathfrak{E}(f) = \int_{\mathcal{X}} \|s^\top \nabla f\|^2 d\pi = \mathbb{E}_{x \sim \pi} [\|Bf(x)\|^2], \quad (6)$$

which is reminiscent of the expected value of the *kinetic energy* in quantum mechanics [13]. To illustrate this, we specify the generator and the associated Dirichlet gradient form for two processes: Overdamped Langevin and Cox-Ingersoll-Ross.

Example 1 (Langevin). Let $k_b, T \in \mathbb{R}_+^*$. The overdamped Langevin equation driven by a potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ is given by $dX_t = -\nabla V(X_t)dt + \sqrt{2(k_b T)}dW_t$ and $X_0 = x$, where k_b and T respectively represent the coefficient of friction and the temperature of the system. Its infinitesimal generator L is defined by $Lf = -\nabla V^\top \nabla f + (k_b T)\Delta f$, for $f \in \mathcal{W}_\pi^{1,2}(\mathcal{X})$. Since $\int (-Lf)g d\pi = -\int \left[\nabla \left((k_b T) \nabla f(x) \frac{e^{-(k_b T)^{-1}V(x)}}{Z} \right) \right] g(x) dx = (k_b T) \int \nabla f^\top \nabla g d\pi = \int f(-Lg) d\pi$, generator L is self-adjoint and associated to a gradient Dirichlet form with $s(x) = (k_b T)^{1/2}(\delta_{ij})_{i \in [d], j \in [p]}$.

Example 2 (Cox-Ingersoll-Ross process). Let $d = 1$, $a, b \in \mathbb{R}$, $\sigma \in \mathbb{R}_+^*$. The Cox-Ingersoll-Ross process is solution of the SDE $dX_t = (a + bX_t)dt + \sigma\sqrt{X_t}dW_t$ and $X_0 = x$. Its infinitesimal generator L is defined for $f \in \mathcal{L}_\pi^2(\mathcal{X})$ by $Lf = (a + bx)\nabla f + \frac{\sigma^2 x}{2}\Delta f$. By integration by parts, we can check that the generator L satisfies $\int (-Lf)g d\pi = \int \frac{\sigma^2 x}{2} f'(x)g'(x) \pi(dx) = \int f(-Lg) d\pi$, and it is associated to a gradient Dirichlet form with $s(x) = \sigma\sqrt{x}/\sqrt{2}$.

Learning in reproducing kernel Hilbert spaces (RKHSs) Throughout the paper we let \mathcal{H} be an RKHS and let $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be the associated kernel function. We let $\phi : \mathcal{X} \rightarrow \mathcal{H}$ be a feature map [38] such that $k(x, x') = \langle \phi(x), \phi(x') \rangle$ for all $x, x' \in \mathcal{X}$. We consider RKHSs satisfying $\mathcal{H} \subset \mathcal{L}_\pi^2(\mathcal{X})$ [38, Chapter 4.3], so that one can approximate $L : \mathcal{L}_\pi^2(\mathcal{X}) \rightarrow \mathcal{L}_\pi^2(\mathcal{X})$ with an operator $G : \mathcal{H} \rightarrow \mathcal{H}$. Notice that despite $\mathcal{H} \subset \mathcal{L}_\pi^2(\mathcal{X})$, the two spaces have different metric structures, that is for all $f, g \in \mathcal{H}$, one in general has $\langle f, g \rangle_{\mathcal{H}} \neq \langle f, g \rangle_{\mathcal{L}_\pi^2}$. In order to handle this ambiguity, we introduce the injection operator $S_\pi : \mathcal{H} \rightarrow \mathcal{L}_\pi^2(\mathcal{X})$ such that for all $f \in \mathcal{H}$, the object $S_\pi f$ is the element of $\mathcal{L}_\pi^2(\mathcal{X})$ which is pointwise equal to $f \in \mathcal{H}$, but endowed with the appropriate \mathcal{L}_π^2 norm.

Then, the infinitesimal generator restricted to \mathcal{H} is simply LS_π which can be estimated by $S_\pi G$ for some $G \in \text{HS}(\mathcal{H})$. This approach is based on the embedding $\ell\phi : \mathcal{X} \rightarrow \mathcal{H}$ of the generator in the RKHS that can be defined for kernels $k \in \mathcal{C}^2(\mathcal{X} \times \mathcal{X})$ whenever one knows drift and diffusion coefficients, see B, so that the reproducing property $\langle \ell\phi(x), h \rangle_{\mathcal{H}} = [LS_\pi h](x)$ holds. Based on this observation [15] developed empirical estimators of LS_π that essentially minimize the risk $\|LS_\pi - S_\pi G\|_{\text{HS}(\mathcal{H}, \mathcal{L}_\pi^2)}^2 = \mathbb{E}_{x \sim \pi} \|\ell\phi(x) - G^* \phi(x)\|_{\mathcal{H}}^2$. In scenarios where drift and diffusion coefficients are not known, then $\ell\phi$ becomes non-computable. However if the process has the Dirichlet form (6), one can still empirically estimate the Galerkin projection $(S_\pi^* S_\pi)^\dagger S_\pi^* LS_\pi$ onto \mathcal{H} , as considered in [1], which in fact minimizes the same risk. Yet this approach is problematic due to the unbounded nature of the generator and the associated estimators typically suffer from a large number of spurious eigenvalues around zero, making the estimation of physically most relevant eigenfunctions unreliable even for self-adjoint generators. Conversely, classical numerical methods can compute the leading part of a spectrum without spuriousness issues, suggesting that data-driven approaches should achieve similar reliability. In this paper, we address this problem by designing a novel notion of risk, leading to principled estimators designed to surmount these challenges.

3 Novel statistical learning framework

In this section, we tackle the challenges in developing suitable generator estimators highlighted earlier. To this end, we introduce a risk metric for resolvent estimation that can be efficiently minimized empirically, leading to good spectral estimation. Since L and $(\mu I - L)^{-1}$ share the same eigenfunctions, the main idea is to learn the (compact) resolvent, which can be effectively approximated by finite-rank operators, instead of learning the generator directly. However, this approach is challenging due to the lack of closed analytical forms for the action of the resolvent.

First, given $\mu > 0$, in order to approximate the action of the resolvent on the RKHS by some operator $G : \mathcal{H} \rightarrow \mathcal{H}$, we introduce its embedding $\chi_\mu : \mathcal{X} \rightarrow \mathcal{H}$ via the reproducing property

$\langle \chi_\mu(x), h \rangle_{\mathcal{H}} = [(\mu I - L)^{-1} S_\pi h](x)$, formally given by $\chi_\mu(x) = \int_0^\infty \mathbb{E}[\phi(X_t) e^{-\mu t} dt | X_0 = x]$, see B for details. Using this notation, we aim to estimate $[(\mu I - L)^{-1} S_\pi h](x) \approx [Gh](x)$, $h \in \mathcal{H}$, i.e. the objective is to estimate $\chi_\mu(x) \approx G^* \phi(x)$ π -a.e.

An obvious metric for the risk would be the mean square error (MSE) w.r.t. distribution π of the data. However, this becomes intractable since in general χ_μ is not computable in closed form when either full or partial knowledge of the process is at hand.

To mitigate this issue, we introduce a different ambient space in which we study the resolvent

$$\mathcal{W}_\pi^\mu(\mathcal{X}) = \{f \in \text{dom}(L) \mid \|f\|_{\mathcal{W}_\pi^\mu(\mathcal{X})}^2 \equiv \mathfrak{E}_\mu[f] = \langle f, (\mu I - L)f \rangle_{\mathcal{L}_\pi^2} < \infty\},$$

where the norm now balances the energy of an observable $f: \mathcal{X} \rightarrow \mathbb{R}$ w.r.t. the invariant distribution $\|f\|_{\mathcal{L}_\pi^2}^2$ and its energy w.r.t. the transient dynamics $-\langle f, Lf \rangle_{\mathcal{L}_\pi^2}$. Indeed

$$\mathfrak{E}_\mu[f] = \mathbb{E}_{x \sim \pi} [\mu |f(x)|^2 - f(x)[Lf](x)] = \mathbb{E}_{x \sim \pi} [\mu |f(x)|^2 + \|s(x)^\top \nabla f(x)\|^2], \quad (7)$$

where the last equality holds for Dirichlet gradient form (6), in which case $\mathcal{W}_\pi^\mu(\mathcal{X})$ is simply a weighted Sobolev space. Importantly, this energy functional can be empirically estimated from data sampled from π , whenever full knowledge, that is drift and diffusion coefficients of the SDE (1), or partial knowledge, i.e. the diffusion coefficient and Dirichlet operator B in (6), is at hand. With that in mind, instead of the standard MSE, we introduce the energy-based risk functional as

$$\min_{G: \mathcal{H} \rightarrow \mathcal{H}} \mathcal{R}(G) = \mathfrak{E}_\mu[\|\chi_\mu(\cdot) - G^* \phi(\cdot)\|_{\mathcal{H}}]. \quad (8)$$

Denoting by $Z_\mu: \mathcal{H} \rightarrow \mathcal{W}_\pi^\mu(\mathcal{X})$ the canonical injection, (8) can be equivalently written as

$$\mathcal{R}(G) = \|(\mu I - L)^{-1} Z_\mu - Z_\mu G\|_{\text{HS}(\mathcal{H}, \mathcal{W})}^2 = \|(\mu I - L)^{-1/2} S_\pi - (\mu I - L)^{1/2} S_\pi G\|_{\text{HS}(\mathcal{H}, \mathcal{L}_\pi^2)}^2, \quad (9)$$

where we abbreviated $\mathcal{W} = \mathcal{W}_\pi^\mu(\mathcal{X})$ and used $Z_\mu^* = S_\pi^*(\mu I - L)$, recalling that Hilbert-Schmidt and spectral norms for operators $A: \mathcal{H} \rightarrow \mathcal{W}$, are $\|A\|_{\text{HS}(\mathcal{H}, \mathcal{W})} = \sqrt{\text{tr}(A^*(\mu I - L)A)}$ and $\|A\|_{\mathcal{H} \rightarrow \mathcal{W}} = \sqrt{\lambda_1(A^*(\mu I - L)A)} \geq \mu^{-1/2} \|A\|_{\mathcal{H} \rightarrow \mathcal{L}_\pi^2}$.

Therefore, (9) implies that the regularized energy norm, while dominating the classical \mathcal{L}_π^2 one, exerts a *balancing effect* on the estimation of the resolvent. This leads us to the first general result regarding the well-posedness of this framework.

Proposition 1. *Given $\mu > 0$, let $\mathcal{H} \subseteq \mathcal{W}_\pi^\mu(\mathcal{X})$ be the RKHS associated to kernel $k \in \mathcal{C}^2(\mathcal{X} \times \mathcal{X})$ such that $Z_\mu \in \text{HS}(\mathcal{H}, \mathcal{W}_\pi^\mu(\mathcal{X}))$, and let $P_{\mathcal{H}}$ be the orthogonal projector onto the closure of $\text{Im}(Z_\mu) \subseteq \mathcal{W}_\pi^\mu(\mathcal{X})$. Then for every $\varepsilon > 0$ there exists a finite rank operator $G: \mathcal{H} \rightarrow \mathcal{H}$ such that $\mathcal{R}(G) \leq \|(I - P_{\mathcal{H}})(\mu I - L)^{-1} Z_\mu\|_{\text{HS}(\mathcal{H}, \mathcal{W})}^2 + \varepsilon$. Consequently, when k is universal, $\mathcal{R}(G) \leq \varepsilon$.*

The previous proposition reveals that whenever the hypothetical domain is dense in the true domain and the injection operator is Hilbert-Schmidt, there is no irreducible risk and one can find arbitrarily good finite rank approximations of the generator's resolvent. Note that $Z_\mu \in \text{HS}(\mathcal{H}, \mathcal{W}_\pi^\mu(\mathcal{X}))$ is equivalent to $Z_\mu^* Z_\mu = S_\pi^*(\mu I - L) S_\pi$ being a trace class operator, which is assured for our Examples 1 and 2, see the discussion in E.

Now, to address how minimization of the risk impacts the estimation of the spectral decomposition, let us define the *operator norm error* and the *metric distortion* functional, respectively, as

$$\mathcal{E}(G) = \|(\mu I - L)^{-1} Z_\mu - Z_\mu G\|_{\mathcal{H} \rightarrow \mathcal{W}}, \quad G \in \text{HS}(\mathcal{H}), \quad \text{and} \quad \eta(h) = \|h\|_{\mathcal{H}} / \|h\|_{\mathcal{W}}, \quad h \in \mathcal{H}. \quad (10)$$

Proposition 2. Let $\widehat{G} = \sum_{i \in [r]} (\mu - \widehat{\lambda}_i)^{-1} \widehat{h}_i \otimes \widehat{g}_i$ be the spectral decomposition of $\widehat{G}: \mathcal{H} \rightarrow \mathcal{H}$, where $\widehat{\lambda}_i \geq \widehat{\lambda}_{i+1}$ and let $\widehat{f}_i = S_\pi \widehat{h}_i / \|S_\pi \widehat{h}_i\|_{\mathcal{L}_\pi^2}$, for $i \in [r]$. Then for every $\mu > 0$ and $i \in [r]$

$$\frac{|\lambda_i - \widehat{\lambda}_i|}{|\mu - \lambda_i| |\mu - \widehat{\lambda}_i|} \leq \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i) \quad \text{and} \quad \|\widehat{f}_i - f_i\|_{\mathcal{L}_\pi^2}^2 \leq \frac{2 \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)}{\mu [\text{gap}_i - \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)]_+}, \quad (11)$$

where gap_i is the difference between i -th and $(i+1)$ -th eigenvalue of $(\mu I - L)^{-1}$.

Note that the estimation of the eigenfunctions is first obtained in the norm with respect to the energy space, and then transformed to the \mathcal{L}_π^2 -norm, as $\|f\|_{\mathcal{W}} \geq \sqrt{\mu} \|f\|_{\mathcal{L}_\pi^2}$, $f \in W_{\mu, \gamma}$. Therefore, by controlling the operator norm error and metric distortion (refer to C), we can guarantee accurate spectral estimation. Consequently, this allows us to approximately solve the SDE (1) starting from an initial condition.

$$\mathbb{E}[h(X_t) | X_0 = x] = [e^{Lt} S_\pi h](x) \approx \sum_{i \in [r]} e^{\widehat{\lambda}_i t} \langle \widehat{g}_i, h \rangle_{\mathcal{H}} \widehat{h}_i(x). \quad (12)$$

4 Empirical risk minimization

In this section we address empirical risk minimization (ERM), deriving two main estimators. The first one minimizes empirical risk with Tikhonov regularization, while the second introduces additional regularization in the form of rank constraints.

To present the estimator, we denote the covariance operator w.r.t. \mathcal{L}_π^2 by $C = S_\pi^* S_\pi = \mathbb{E}_{x \sim \pi} [\phi(x) \otimes \phi(x)]$, the cross-covariance operator $T = S_\pi^* L S_\pi$, capturing correlations between input and the outputs of the generator, and the covariance operator $W_\mu = Z_\mu^* Z_\mu = S_\pi^* (\mu I - L) S_\pi$ w.r.t. energy space \mathcal{W} . All operators can be estimated from data, depending on the available prior knowledge. In this work we focus on the case when

Dirichlet gradient form is known. Then we can define the embedding of the Dirichlet operator $B = s^\top \nabla: \mathcal{L}_\pi^2(\mathcal{X}) \rightarrow [\mathcal{L}_\pi^2(\mathcal{X})]^p$ into RKHS $d\phi: \mathcal{X} \rightarrow \mathcal{H}^p$ via the reproducing property as $\langle d\phi(x), h \rangle_{\mathcal{H}} = [B S_\pi h](x) = s(x)^\top D h(x) \in \mathbb{R}^p$, $h \in \mathcal{H}$. More precisely, we have that $d\phi(x)$ is a p -dimensional vector with components $d_k \phi(x)$, where $d_k \phi: \mathcal{X} \rightarrow \mathcal{H}$ is given via reproducing property $\langle d_k \phi(x), h \rangle_{\mathcal{H}} = s_k(x)^\top D h(x)$, $k \in [p]$. Hence, in this case we have that

$$T = -\mathbb{E}_{x \sim \pi} [d\phi(x) \otimes d\phi(x)] = -\sum_{k \in [p]} \mathbb{E}_{x \sim \pi} [d_k \phi(x) \otimes d_k \phi(x)]. \quad (13)$$

Moreover, defining $w\phi: \mathcal{X} \rightarrow \mathcal{H}^{p+1}$ by $w\phi(x) = [\sqrt{\mu} \phi(x), d_1 \phi(x), \dots, d_p \phi(x)]^\top \in \mathbb{R}^{p+1}$, we get

$$W_\mu = \mathbb{E}_{x \sim \pi} [\mu \phi(x) \otimes \phi(x) + d\phi(x) \otimes d\phi(x)] = \mathbb{E}_{x \sim \pi} [w\phi(x) \otimes w\phi(x)]. \quad (14)$$

Regularized risk Let us first introduce the regularized risk defined for some $\gamma > 0$ by

$$\mathcal{R}_\gamma(G) = \|(\mu I - L)^{-1/2} S_\pi - (\mu I - L)^{1/2} S_\pi G\|_{\text{HS}(\mathcal{H}, \mathcal{L}_\pi^2)}^2 + \gamma \mu \|G\|_{\text{HS}(\mathcal{H})}^2, \quad G \in \text{HS}(\mathcal{H}), \quad (15)$$

which, after some algebra, can be written as

$$\begin{aligned} \mathcal{R}_\gamma(G) &= \text{tr} [G^* (\mu C - T + \mu \gamma I) G - 2CG + S_\pi^* (\mu I - L)^{-1} S_\pi] \\ &= \underbrace{\|W_{\mu, \gamma}^{-1/2} C - W_{\mu, \gamma}^{1/2} G\|_{\text{HS}(\mathcal{H})}^2}_{\text{variance term}} + \underbrace{\mathfrak{E}_\mu[\chi_\mu(\cdot)] - \|W_{\mu, \gamma}^{-1/2} C\|_{\text{HS}(\mathcal{H})}^2}_{\text{bias term}} \end{aligned}$$

where $W_{\mu, \gamma} = W_\mu + \mu \gamma I$ is the regularized covariance w.r.t. \mathcal{W} .

Hence, assuming the access to the dataset $\mathcal{D}_n = (x_i)_{i \in [n]}$ made of i.i.d. samples from the invariant distribution π , replacing the regularized energy \mathfrak{E}_μ with its empirical estimate $\widehat{\mathfrak{E}}_\mu$ leads to the regularized empirical risk functional expressed as

$$\widehat{\mathcal{R}}_\gamma(G) = \|\widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C} - \widehat{W}_{\mu,\gamma}^{1/2}G\|_{\text{HS}(\mathcal{H})}^2 + \widehat{\mathfrak{E}}_\mu[\chi_\mu(\cdot)] - \|\widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C}\|_{\text{HS}(\mathcal{H})}^2, \quad (16)$$

where $W_{\mu,\gamma}$ and C are estimated by their empirical counterparts $\widehat{W}_{\mu,\gamma}$ and \widehat{C} , respectively, via (13).

Therefore, our regularized empirical risk minimization approach reduces to

$$\min_G \|\widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C} - \widehat{W}_{\mu,\gamma}^{1/2}G\|_{\text{HS}(\mathcal{H})}^2, \quad (17)$$

and we analyze two different estimators, the first one $\widehat{G}_{\mu,\gamma}$ is obtained by minimizing regularized empirical risk (17) over all $G \in \text{HS}(\mathcal{H})$, and, hence, the name *Kernel Ridge Regression* (KRR) of the generators resolvent. The second one $\widehat{G}_{\mu,\gamma}^r$ minimizes (17) subject to the (hard) constraint that G is at most of (a priori fixed) rank $r \in \mathbb{N}$ and, hence, is named *Reduced Rank Regression* (RRR) of the generator's resolvent. Notice that when $r = n$, the two estimators coincide. After some algebra, one sees that both minimization problems have closed form solutions

$$\widehat{G}_{\mu,\gamma} = \widehat{W}_{\mu,\gamma}^{-1}\widehat{C} \quad \text{and} \quad \widehat{G}_{\mu,\gamma}^r = \widehat{W}_{\mu,\gamma}^{-1/2}[\widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C}]_r, \quad (18)$$

where $[\cdot]_r$ denotes the r -truncated SVD of a compact operator.

To conclude this section, we show how to compute the eigenvalue decomposition of (18). To this end, we define the sampling operators $\widehat{S}: \mathcal{H} \rightarrow \mathbb{R}^n$ and $\widehat{Z}_\mu: \mathcal{H} \rightarrow \mathbb{R}^{(1+p)n}$ by

$$(\widehat{S}h)_i = \frac{1}{\sqrt{n}}h(x_i), i \in [n], \quad \text{and} \quad (\widehat{Z}_\mu h)_{kn+i} = \begin{cases} \frac{\sqrt{\mu}}{\sqrt{n}}h(x_i), & k=0, i \in [n], \\ \frac{1}{\sqrt{n}}s_k(x_i)^\top Dh(x_i), & k \in [p], i \in [n]. \end{cases}$$

Further, let $K = n^{-1}[k(x_i, x_j)]_{i,j \in [n]} \in \mathbb{R}^{n \times n}$ be kernel Gram matrix, and introduce the Gram matrices $N \in \mathbb{R}^{n \times pn}$ and $M \in \mathbb{R}^{pn \times pn}$ whose elements, for $k \in [1+p], i, j \in [n]$ are

$$N_{i,(k-1)n+j} = n^{-1}\langle \phi(x_i), d_k \phi(x_j) \rangle_{\mathcal{H}} \quad \text{and} \quad M_{(k-1)n+i, (\ell-1)n+j} = n^{-1}\langle d_k \phi(x_i), d_\ell \phi(x_j) \rangle_{\mathcal{H}}. \quad (19)$$

We note that although we have introduced the above matrices via inner products in \mathcal{H} , they can be readily computed via the kernel and its gradients knowing the Dirichlet form, see D.

Theorem 1. *Given $\mu > 0$ and $\gamma > 0$, let $J_{\mu,\gamma} = K - N(M + \gamma\mu I)^{-1}N^\top + \gamma I$. Let $(\widehat{\sigma}_i^2, v_i)_{i \in [r]}$ be the leading eigenpairs of the following generalized eigenvalue problem*

$$\mu^{-1}(J_{\mu,\gamma} - \gamma I)Kv_i = \widehat{\sigma}_i^2 J_{\mu,\gamma} v_i, \quad v_i^\top K v_j = \delta_{ij}, \quad i, j \in [r]. \quad (20)$$

Denoting $V_r = [v_1 | \dots | v_r] \in \mathbb{R}^{n \times r}$ and $\Sigma_r = \text{diag}(\widehat{\sigma}_1, \dots, \widehat{\sigma}_r)$, if $(\nu_i, w_i^\ell, w_i^r)_{i \in [r]}$ are eigentriplets of matrix $V_r^\top V_r \Sigma_r^2 \in \mathbb{R}^{r \times r}$, then the eigenvalue decomposition the RRR estimator $\widehat{G}_{\mu,\gamma}^r = \widehat{Z}_\mu U_r V_r^\top \widehat{S}$ is given by $\widehat{G}_{\mu,\gamma}^r = \sum_{i \in [r]} (\mu - \widehat{\lambda}_i)^{-1} \widehat{h}_i \otimes \widehat{g}_i$, where $\widehat{\lambda}_i = \mu - 1/\nu_i$, $\widehat{g}_i = \nu_i^{-1/2} \widehat{S}^* V_r w_i^\ell$ and $\widehat{h}_i = \widehat{Z}_\mu^* U_r w_i^r$ for $U_r = (\mu\gamma)^{-1} [\mu^{-1/2} I | -N(M + \gamma\mu I)^{-1}]^\top (K V_r - \mu V_r \Sigma_r^2) \in \mathbb{R}^{(1+p)n \times r}$.

The main computational cost of our method, in view of (12), to solve SDE (1) lies in the implicit inversion of $J_{\mu,\gamma}$ when solving (20). When computed with direct solvers this inversion is of the order $\mathcal{O}(n^3 p^3)$, however leveraging on the fact that $\mu J_{\mu,\gamma}$ is Schur's complement of the $(1+p)n \times (1+p)n$ symmetric positive definite matrix and using classical iterative solvers, like Lanczos or the generalized Davidson method, when $r \ll n$ this cost can significantly be reduced to $\mathcal{O}(r n^2 p^2)$, c.f. [14].

5 Spectral learning bounds

Recalling Prop. 2, in order to obtain the bounds on eigenvalues and eigenfunctions of the generator, it suffices to analyze the learning rates for the operator norm error \mathcal{E} and metric distortion η . For this purpose, we analyze the operator norm error of empirical estimator $\widehat{G}_{\mu,\gamma}^r$ using the decomposition

$$\mathcal{E}(\widehat{G}) \leq \underbrace{\|(\mu I - L)^{-1}Z_\mu - Z_\mu G_{\mu,\gamma}\|_{\mathcal{H} \rightarrow \mathcal{W}}}_{\text{regularization bias}} + \underbrace{\|Z_\mu(G_{\mu,\gamma} - G_{\mu,\gamma}^r)\|_{\mathcal{H} \rightarrow \mathcal{W}}}_{\text{rank reduction bias}} + \underbrace{\|Z_\mu(G_{\mu,\gamma}^r - \widehat{G}_{\mu,\gamma}^r)\|_{\mathcal{H} \rightarrow \mathcal{W}}}_{\text{estimator's variance}},$$

where $G_{\mu,\gamma} = W_{\mu,\gamma}^{-1}C$ is the minimizer of the full (i.e. without rank constraint) Tikhonov regularized risk and $G_{\mu,\gamma}^r = W_{\mu,\gamma}^{-1/2}[[W_{\mu,\gamma}^{-1/2}C]]_r$ is the population version of the empirical estimator $\widehat{G}_{\mu,\gamma}^r$.

Note that, while the last two terms in the above decomposition depend on the estimator, the first term depends only on the choice of \mathcal{H} and the regularity of L w.r.t. \mathcal{H} . In this work we focus on the classical kernel-based learning where one chooses a universal kernel [38, Chapter 4] and controls the regularization bias with a regularity condition. For details see Rem. 2 of App. E.2. Let $\mu > 0$ be a prescribed parameter, we make following assumptions to quantify the difficulty of the learning problem:

- (BK) Boundedness.** There exists $c_{\mathcal{W}} > 0$ such that $\text{ess sup}_{x \sim \pi} \|w\phi(x)\|^2 \leq c_{\mathcal{W}}$, i.e. $w\phi \in \mathcal{L}_\pi^\infty(\mathcal{X}, \mathcal{H}^{1+p})$;
- (RC) Regularity.** For some $\alpha \in (0, 2]$ there exists $c_\alpha > 0$ such that $C^2 \leq c_\alpha^2 W_\mu^{1+\alpha}$;
- (SD) Spectral Decay.** There exists $\beta \in (0, 1]$ and $c_\beta > 0$ s.t. $\lambda_j(W_\mu) \leq c_\beta j^{-1/\beta}$, for all $j \in J$.

The above assumptions, discussed in more details in App E.1, are in the spirit of state-of-the-art analysis of statistical learning theory of classical regression in RKHS spaces [12], recently extended to regression of transfer operators [28, 22]. In our setting, instead of relying on the injection into \mathcal{L}_π^2 as in the case of transfer operators, the relevant object is the injection Z_μ into the energy space \mathcal{W} .

The first assumption **(BK)** is the main limiting factor of our approach. Indeed, since $\|w\phi(x)\|^2 = \mu\|\phi(x)\|^2 + \sum_{k \in [p]} \|d_k \phi(x)\|^2$, apart from needing the kernel to be bounded, we also need the Dirichlet form embedding to be bounded. Essentially, this means that the Dirichlet coefficients are not growing too fast w.r.t. the kernel's gradients decay. Having this, we assure that $Z_\mu \in \text{HS}(\mathcal{H}, \mathcal{W}_\pi^\mu(\mathcal{X}))$ which implies the operator norm error can be controlled.

Another key difference between generator and transfer operator regression is that the covariance w.r.t. the domain of the operator becomes $W_\mu = Z_\mu^* Z_\mu$ instead of $C = S_\pi^* S_\pi$. On the other hand, the "cross-covariance" that captures now RKHS cross-correlations of the resolvent w.r.t domain is simply $Z_\mu^*(\mu I - L)^{-1}Z_\mu = S_\pi^*(\mu I - L)(\mu I - L)^{-1}S_\pi = C$. With this in mind, **(RC)** corresponds to the regularity condition in [22] and it quantifies the relationship between the hypothesis class (bounded operators in *RKHS*) and the object of interest $(\mu I - L)^{-1}$. Indeed, if L has eigenfunctions that belong to α -interpolation space between \mathcal{H} and $\mathcal{W}_\pi^\mu(\mathcal{X})$, **(RC)** holds true. In particular, if $f_i \in \mathcal{H}$ for all $i \geq 2$ (constant eigenfunction excluded), one has that $\alpha \geq 1$ (c.f. Proposition 7 in App. E.1).

Finally, **(SD)** quantifies the "size" of the hypothetical domain \mathcal{H} within the true domain $\mathcal{W}_\pi^\mu(\mathcal{X})$ via the *effective dimension* $\text{tr}(W_{\mu,\gamma}^{-1}W_\mu) \leq c_\beta(\mu\gamma)^{-\beta}$, which, due to **(BK)**, leads to another notion, known as the embedding property, quantifying the relationship between \mathcal{H} and essentially bounded functions in the domain of the operator

- (KE) Kernel Embedding.** There exists $\tau \in [\beta, 1]$ and such that

$$c_\tau = \text{ess sup}_{x \sim \pi} \sum_{j \in \mathbb{N}} \sigma_j^{2\tau} [\mu |z_j(x)|^2 - z_j(x)[Lz_j](x)] < +\infty, \quad (21)$$

where $Z_\mu = \sum_{j \in J} \sigma_j z_j \otimes h_j$ is the SVD of the injection operator $Z_\mu: \mathcal{H} \rightarrow \mathcal{W}_\pi^\mu(\mathcal{X})$.

Using the above assumptions, we prove a generalization bound for the RRR estimator of the resolvent.

Theorem 2. *Let (RC), (SD), and (KE) hold for some $\alpha \in (0, 2]$, $\beta \in (0, 1]$ and $\tau \in [\beta, 1]$, respectively, and let $\text{cl}(\text{Im}(S_\pi)) = \mathcal{L}_\pi^2(\mathcal{X})$. Denoting $\lambda_k^* = \lambda_k(S_\pi^*(\mu I - L)^{-1}S_\pi)$, $k \in \mathbb{N}$, and given $\delta \in (0, 1)$ and $r \in [n]$, if RRR estimator is build from the Dirichlet form and*

$$\text{if } \alpha \geq \tau, \gamma \asymp n^{-\frac{1}{\alpha+\beta}} \text{ and } \varepsilon_n^* = n^{-\frac{\alpha}{2(\alpha+\beta)}}, \text{ or if } \alpha < \tau, \gamma \asymp n^{-\frac{1}{\beta+\tau}} \text{ and } \varepsilon_n^* = n^{-\frac{\alpha}{2(\beta+\tau)}} \quad (22)$$

then there exists a constant $c > 0$, depending only on \mathcal{H} and gap $\lambda_r^* - \lambda_{r+1}^* > 0$, such that for large enough $n \geq r$ with probability at least $1 - \delta$ in the i.i.d. draw of \mathcal{D}_n from π it holds that

$$\mathcal{E}(\widehat{G}_{\mu, \gamma}^r) \leq (\widehat{\sigma}_{r+1} \wedge \sqrt{\lambda_{r+1}^*}) + c\varepsilon_n^* \ln \delta^{-1}. \quad (23)$$

Proof sketch. The regularization bias is bounded by $c_\alpha \gamma^{\alpha/2}$ by Prop. 9 of App. E.2, the rank reduction bias is upper bounded by $\lambda_{r+1}(S_\pi^*(\mu I - L)^{-1}S_\pi)$, while the bounds on the variance terms critically rely on the well-known perturbation result for spectral projectors reported in Prop. 4, App. A. The latter is then chained to Pinelis-Sakhanenko's inequality and Minsker's inequality for self-adjoint HS-operators, Props. 12 and 13 in App. E.3.1, respectively. Combining the bias and variance terms, we obtain the balancing equations for the regularization parameter and then the next result follows. \square

Note that the learning rate (23) implies the \mathcal{L}_π^2 -norm learning rate. Moreover, for $\alpha \geq \tau$, it matches information theoretic lower bounds for transfer operator learning upon replacing parameters α , β and τ related to the space \mathcal{W} with their \mathcal{L}_π^2 analogues [22], see App. E.6. This motivates the development of the first mini-max optimality for the IG learning, for which our results an important first step.

To conclude this section, we address the spectral learning bounds steaming from the Prop. 2. The main task to do so is to control the metric distortions, which we show how in App. E.5. In this context, an additional assumption $\alpha \geq 1$ is needed, since otherwise the metric distortions can blow-up due to eigenfunctions being out of the RKHS space. Importantly, our analysis reveals that

$$\frac{|\lambda_i - \widehat{\lambda}_i|}{|\mu - \lambda_i| |\mu - \widehat{\lambda}_i|} \leq (\widehat{s}_i \wedge 2\sqrt{\lambda_{r+1}^*/\lambda_r^*}) + c\varepsilon_n^* \ln \delta^{-1}, \quad i \in [r], \quad (24)$$

where $\widehat{s}_i = \widehat{\sigma}_i \widehat{\eta}_i$ is the empirical spectral bias that informs how good is the estimation of the particular eigenpair is (see Fig. 1 a)), $\widehat{\sigma}_i$ being given in (20) and $\widehat{\eta}_i = \|\widehat{h}_i\|_{\mathcal{H}} / \|\widehat{W}_\mu^{1/2} \widehat{h}_i\|_{\mathcal{H}}$.

6 Experiments

In this section, we showcase the key features of our method outlined in Table ???. We demonstrate that our approach: (1) avoids the spurious effects noted in other IG methods [15, 1], (2) is more effective than transfer operator methods [21], and (3) validates our bounds in a prediction task for a model with a non-constant diffusion term. Further details are available in Appendix F.

One dimensional four well potential We first investigate the overdamped Langevin dynamics in a potential that presents four different wells, two principal wells and then in each of them two smaller wells, given by $V(x) = 4(x^8 + 0.8 \exp(-80(x^2)) + 0.2 \exp(-80(x-0.5)^2) + 0.5 \exp(-40(x+0.5)^2))$. This leads to three relevant eigenpairs: the slowest mode corresponds to the transition between the two principal wells, while the others two capture transitions between the smaller wells. In Figure 1, we show that the empirical bias $\widehat{s}_1 = \widehat{\sigma}_1 \widehat{\eta}_1$ allows us to choose the hyperparameters of the model: higher

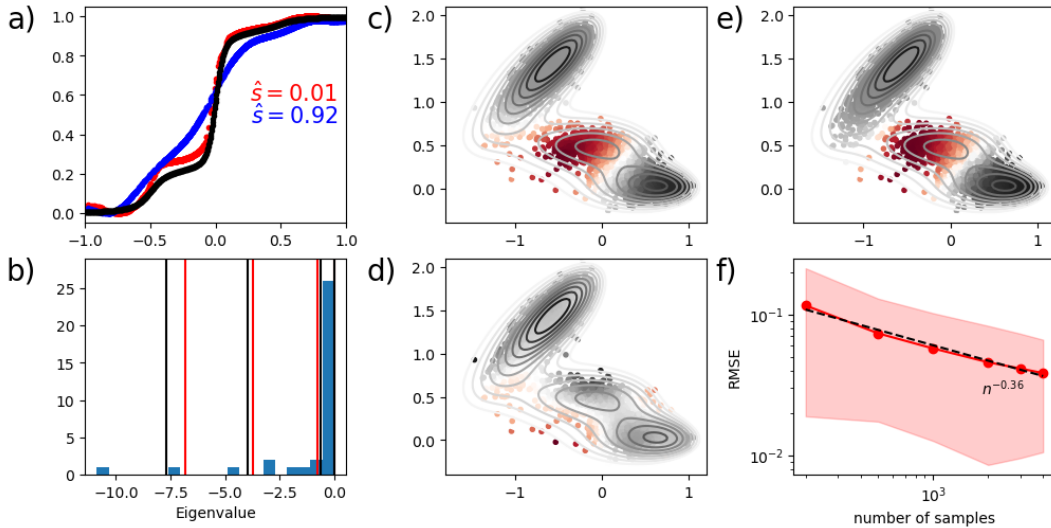


Figure 1: **a)** Empirical biases $\hat{s}_1 = \hat{\sigma}_1 \hat{\eta}_1$ and estimation of the first (nontrivial) eigenfunction of the IG of a Langevin process under a four well potential. Ground truth is black, our method RRR is red and blue for two different kernel lengthscales. **b)** Eigenvalue estimation for the same process compared to the methods in [15, 1], for which eigenvalue histogram in blue shows spuriousness. **c)** Estimation of the second eigenfunction of a Langevin process under Muller brown potential (white level lines) by RRR, Transfer Operator (TO) in **d)** and ground truth in **e)**. Observe that TO fails to recover the metastable state. **f)** Prediction RMSE for the CIR model.

empirical bias leads to wrong operator. Compared to KRR [15, 1], there is no spuriousness in the estimation of our eigenvalues, as shown in panel **b)**.

Muller Brown potential We next study Langevin dynamics under more challenging conditions: the Muller brown potential. Figure 1(c-e) depicts the second eigenfunction obtained by our method compared to the ground truth one and that found by the transfer operator approach, with the same number of samples. Notably, our physics informed approach outperforms transfer operator learning for this task. Note that with different lag times, we were able to recover this second eigenfunction.

CIR model Finally, we show with the CIR model that our method is not limited to Langevin process with constant diffusion. For this process, the conditional expectation of the state X_t is analytically known. We can thus compare the prediction of our model with respect to this expectation using root mean squared error (RMSE) and compute it for different number of samples to validate our bounds. Conditional expectation were computed on 100 different simulations at $t = \ln(2)/a$ which corresponds to the half life of the mean reversion. Results are shown in panel **d)** Figure 1.

7 Conclusion

We developed a novel energy-based framework for learning the Infinitesimal Generator of stochastic diffusion SDEs using kernel methods. Our approach integrates physical priors, achieves fast error rates, and provides the first spectral learning guarantees for generator learning. A limitation is its computational complexity, scaling as $n^2 d^2$. Future work will explore alternative methods to enhance computational efficiency and investigate a broader suite of SDEs beyond stochastic diffusion.

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Supplementary Material

This appendix includes additional background on SDE and RKHS, proofs of the results omitted in the main body and information about the numerical experiments.

A Background

A.1 Basics on operator theory for Markov processes.

We provide here some basics on operator theory for Markov processes. Let $\mathcal{X} \subset \mathbb{R}^d$ ($d \in \mathbb{N}$) and $(X_t)_{t \in \mathbb{R}_+}$ be a \mathcal{X} -valued time-homogeneous Markov process defined on a filtered probability space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \in \mathbb{R}_+}, \mathbb{P})$ where $\mathcal{F}_t = \sigma(X_s, s \leq t)$ is the natural filtration of $(X_t)_{t \in \mathbb{R}_+}$. The dynamics of X can be described through of a family of probability densities $(p_t)_{t \in \mathbb{R}_+}$ such that for all $t \in \mathbb{R}_+$, $E \in \mathcal{B}(\mathcal{X})$,

$$\mathbb{P}(X_t \in E | X_0 = x) = \int_E p_t(x, y) dy.$$

Let \mathcal{G} be a set of real valued and measurable functions on \mathcal{X} . For any $t \in \mathbb{R}_+$ the transfer operator (TO) $A_t : \mathcal{G} \rightarrow \mathcal{G}$ maps any measurable function $f \in \mathcal{G}$ to

$$(A_t f)(x) = \int_{\mathcal{X}} f(y) p_t(x, y) dy. \quad (25)$$

In theory of Markov processes, the family $(A_t)_{t \in \mathbb{R}_+}$ is referred to as the Markov semigroup associated to the process X .

Remark 1. A possible choice is $\mathcal{G} = \mathcal{L}^\infty(\mathcal{X})$. Here, we are interested in another choice of \mathcal{G} related to the existence of an invariant measure for A_t i.e., a σ -finite measure π on $(\mathcal{X}, \mathcal{B}(\mathcal{X}))$ such that $P_t^* \pi = \pi$ for any $t \in \mathbb{R}_+$. In that case, we can choose $\mathcal{G} = \mathcal{L}_\pi^2(\mathcal{X})$ so that, for all $f \in \mathcal{L}_\pi^2(\mathcal{X})$, $P_t f$ converges to f in $\mathcal{L}_\pi^2(\mathcal{X})$ as t goes to 0. Note that $P_0 f = f$ and $P_\infty f = \int f d\mathcal{X}$ for a suitable integrable function $f : \mathcal{X} \rightarrow \mathbb{R}$.

Within the existence of this invariant measure π , the process X is then characterized by the infinitesimal generator (IG) $L : \mathcal{L}_\pi^2(\mathcal{X}) \rightarrow \mathcal{L}_\pi^2(\mathcal{X})$ of the family $(A_t)_{t \in \mathbb{R}_+}$ defined by

$$L = \lim_{t \rightarrow 0^+} \frac{A_t - I}{t}. \quad (26)$$

In other words, L characterizes the linear differential equation $\partial/\partial_t A_t f = L A_t f$ satisfied by the transfer operator. The domain of L denoted $\text{dom}(L)$ coincides with the the Sobolev space $\mathcal{W}_\pi^{1,2}(\mathcal{X})$

$$\mathcal{W}_\pi^{1,2}(\mathcal{X}) = \{f \in \mathcal{L}_\pi^2(\mathcal{X}) \mid \|f\|_{\mathcal{W}}^2 = \|f\|_{\mathcal{L}_\pi^2}^2 + \|\nabla f\|_{\mathcal{L}_\pi^2}^2 < \infty\}.$$

The spectrum of the IG can be difficult to capture due to the potential unboundedness of L . To circumvent this problem, one can focus on an auxiliary operator, the resolvent, which, under certain conditions, shares the same eigenfunctions as L and becomes compact. The following result can be found in Yosida's book ([46], Chap. IX) : For every $\mu > 0$, the operator $(\mu I - L)$ admits an inverse $L_\mu = (\mu I - L)^{-1}$ that is a continuous operator on \mathcal{X} and

$$(\mu I - L)^{-1} = \int_0^\infty e^{-\mu t} A_t dt.$$

The operator L_μ is the *resolvent* of L and the corresponding *resolvent set* of L is defined by

$$\rho(L) = \{\mu \in \mathbb{C} \mid (\mu I - L) \text{ is bijective and } L_\mu \text{ is continuous}\}.$$

In fact, $\rho(L)$ contains all real positive numbers and $(\mu I - L)^{-1}$ is bounded. Here, we assume that L has *compact resolvent*, i.e. $\rho(L) \neq \emptyset$ and there exists $\mu_0 \in \rho(L)$ such that L_{μ_0} is compact. Note that, through the resolvent identity, this implies the compactness of all resolvents L_μ for $\mu \in \rho(L)$. Let then $\mu \in \rho(L)$. As $(L, \text{dom}(L))$ is assumed to be self-adjoint, so does L_μ , so that L_μ is both compact and self-adjoint. Then, its *spectrum* $\text{Sp}(L_\mu) = \mathbb{C} \setminus \rho(L_\mu)$ is purely discrete and consists of isolated eigenvalues $(\lambda_i^\mu)_{i \in \mathbb{N}}$ such that $|\lambda_i^\mu| \rightarrow 0$ associated with an orthonormal basis $(f_i)_{i \in \mathbb{N}}$ (see [46], chapter XI). In other words, the spectral decomposition of the resolvent writes

$$L_\mu = \sum_{i \in \mathbb{N}} \lambda_i^\mu f_i \otimes f_i$$

where the functions $f_i \in \mathcal{L}_\pi^2(\mathcal{X})$ are also eigenfunctions of the operator L we get

$$L = \sum_{i \in \mathbb{N}} \lambda_i f_i \otimes f_i.$$

Example 3 (Langevin). *Let $(k_b T) \in \mathbb{R}$. The overdamped Langevin equation driven by a potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ is given by $dX_t = -\nabla V(X_t)dt + \sqrt{2(k_b T)}dW_t$ and $X_0 = x$. Its invariant measure of the solution process X is the Boltzman distribution $\pi(dx) = z^{-1}e^{-(k_b T)^{-1}V(x)}dx$ where z denotes a normalizing constant. Its infinitesimal generator L is defined by $Lf = -\nabla V^\top \nabla f + (k_b T)\Delta f$, for $f \in \mathcal{W}_\pi^{1,2}(\mathcal{X})$, and if $\nabla V \in \mathcal{L}_\pi^2(\mathcal{X})$ is positive and coercive, it has compact resolvent. Finally, since $\int (-Lf)g d\pi = -\int \left[\nabla \left((k_b T) \nabla f(x) \frac{e^{-(k_b T)^{-1}V(x)}}{z} \right) \right] g(x) dx = (k_b T) \int \nabla f^\top \nabla g d\pi = \int f(-Lg) d\pi$, generator L is self-adjoint and associated to a gradient Dirichlet form with $s(x) = (k_b T)^{1/2}(\delta_{ij})_{i \in [d], j \in [p]}$.*

Example 4 (Cox-Ingersoll-Ross process). *Let $d = 1$, $a, b \in \mathbb{R}$, $\sigma \in \mathbb{R}_+^*$. The Cox-Ingersoll-Ross process is solution of the SDE $dX_t = (a + bX_t)dt + \sigma\sqrt{X_t}dW_t$ and $X_0 = x$. Its invariant measure π is a Gamma distribution with shape parameter a/σ^2 and rate parameter b/σ^2 . Its infinitesimal generator L is defined for $f \in \mathcal{L}_\pi^2(\mathcal{X})$ by $Lf = (a + bx)\nabla f + \frac{\sigma^2 x}{2}\Delta f$. Note that by integration by parts, we can check that the generator L satisfies $\int (-Lf)g d\pi = \int \frac{\sigma^2 x}{2} f'(x)g'(x) \pi(dx) = \int f(-Lg) d\pi$, and it is associated to a gradient Dirichlet form with $s(x) = \sigma\sqrt{x}/\sqrt{2}$.*

A.2 Infinitesimal generator for diffusion processes

After defining the infinitesimal generator for Markov processes (see A.1), we provide its explicit form for solution processes of equations like(1). Given a smooth function $f \in \mathcal{C}^2(\mathcal{X}, \mathbb{R})$, Itô's formula (see for instance [4], B, p.495) provides for $t \in \mathbb{R}_+$,

$$\begin{aligned} f(X_t) - f(X_0) &= \int_0^t \sum_{i=1}^d \partial_i f(X_s) dX_s^i + \frac{1}{2} \int_0^t \sum_{i,j=1}^d \partial_{ij}^2 f(X_s) d\langle X^i, X^j \rangle_s \\ &= \int_0^t \nabla f(X_s)^\top dX_t + \frac{1}{2} \int_0^t \text{Tr}[X_s^\top (\nabla^2 f)(X_s) X_s] ds. \end{aligned}$$

Recalling (1), we get

$$\begin{aligned} f(X_t) &= f(X_0) + \int_0^t \left[\nabla f(X_s)^\top a(X_s) + \frac{1}{2} \text{Tr} [b(X_s)^\top (\nabla^2 f(X_s)) b(X_s)] \right] ds \\ &\quad + \int_0^t \nabla f(X_s)^\top b(X_s) dW_s. \end{aligned} \quad (27)$$

Provided f and b are smooth enough, the expectation of the last stochastic integral vanishes so that we get

$$\mathbb{E}[f(X_t)|X_0 = x] = f(x) + \int_0^t \mathbb{E} \left[\nabla f(X_s)^\top a(X_s) + \frac{1}{2} \text{Tr} [b(X_s)^\top (\nabla^2 f(X_s)) b(X_s)] \middle| X_0 = x \right] ds$$

Recalling that $L = \lim_{t \rightarrow 0^+} (A_t f - f)/t$, we get for every $x \in \mathcal{X}$,

$$\begin{aligned} Lf(x) &= \lim_{t \rightarrow 0} \frac{\mathbb{E}[f(X_t)|X_0 = x] - f(x)}{t} \\ &= \lim_{t \rightarrow 0} \frac{1}{t} \left[\int_0^t \mathbb{E} \left[\nabla f(X_s)^\top a(X_s) + \frac{1}{2} \text{Tr} [(X_s)^\top (\nabla^2 f(X_s)) b(X_s)] \right] ds \middle| X_0 = x \right] \\ &= \nabla f(x)^\top a(x) + \frac{1}{2} \text{Tr} [b(x)^\top (\nabla^2 f(x)) b(x)], \end{aligned} \quad (28)$$

which provides the closed formula for the IG associated with the solution process of (1).

A.3 Spectral perturbation theory

Recalling that for a bounded linear operator A on some Hilbert space \mathcal{H} the resolvent set of the operator A is defined as $\rho(A) = \{\lambda \in \mathbb{C} \mid A - \lambda I \text{ is bijective and } (A - \lambda I)^{-1} \text{ is continuous}\}$, and its spectrum $\text{Sp}(A) = \mathbb{C} \setminus \{\rho(A)\}$, let $\lambda \subseteq \text{Sp}(A)$ be isolated part of spectra, i.e. both λ and $\mu = \text{Sp}(A) \setminus \lambda$ are closed in $\text{Sp}(A)$. Then, the *Riesz spectral projector* $P_\lambda: \mathcal{H} \rightarrow \mathcal{H}$ is defined by

$$P_\lambda = \frac{1}{2\pi} \int_\Gamma (zI - A)^{-1} dz, \quad (29)$$

where Γ is any contour in the resolvent set $\text{Res}(A)$ with λ in its interior and separating λ from μ . Indeed, we have that $P_\lambda^2 = P_\lambda$ and $\mathcal{H} = \text{Im}(P_\lambda) \oplus \text{Ker}(P_\lambda)$ where $\text{Im}(P_\lambda)$ and $\text{Ker}(P_\lambda)$ are both invariant under A and $\text{Sp}(A|_{\text{Im}(P_\lambda)}) = \lambda$, $\text{Sp}(A|_{\text{Ker}(P_\lambda)}) = \mu$. Moreover, $P_\lambda + P_\mu = I$ and $P_\lambda P_\mu = P_\mu P_\lambda = 0$.

Finally if A is compact operator, then the Riesz-Schauder theorem, see e.g. [37], assures that $\text{Sp}(T)$ is a discrete set having no limit points except possibly $\lambda = 0$. Moreover, for any nonzero $\lambda \in \text{Sp}(T)$, then λ is an eigenvalue (i.e. it belongs to the point spectrum) of finite multiplicity, and, hence, we can deduce the spectral decomposition in the form

$$A = \sum_{\lambda \in \text{Sp}(A)} \lambda P_\lambda, \quad (30)$$

where geometric multiplicity of λ , $r_\lambda = \text{rank}(P_\lambda)$, is bounded by the algebraic multiplicity of λ . If additionally A is normal operator, i.e. $AA^* = A^*A$, then $P_\lambda = P_\lambda^*$ is orthogonal projector for each $\lambda \in \text{Sp}(A)$ and $P_\lambda = \sum_{i=1}^{r_\lambda} \psi_i \otimes \psi_i$, where ψ_i are normalized eigenfunctions of A corresponding to λ and r_λ is both algebraic and geometric multiplicity of λ .

We conclude this section with well-known perturbation bounds for eigenfunctions and spectral projectors of self-adjoint compact operators.

Proposition 3 ([10]). *Let A be compact self-adjoint operator on a separable Hilbert space \mathcal{H} . Given a pair $(\widehat{\lambda}, \widehat{f}) \in \mathbb{C} \times \mathcal{H}$ such that $\|\widehat{f}\| = 1$, let λ be the eigenvalue of A that is closest to $\widehat{\lambda}$ and let f be its normalized eigenfunction. If $\widehat{g} = \min\{|\widehat{\lambda} - \lambda| \mid \lambda \in \text{Sp}(A) \setminus \{\lambda\}\} > 0$, then $\sin(\angle(\widehat{f}, f)) \leq \|A\widehat{f} - \widehat{\lambda}\widehat{f}\|/\widehat{g}$.*

Proposition 4 ([50]). *Let A and \widehat{A} be two compact operators on a separable Hilbert space. For nonempty index set $J \subset \mathbb{N}$ let*

$$\text{gap}_J(A) = \min\{|\lambda_i(A) - \lambda_j(A)| \mid i \in \mathbb{N} \setminus J, j \in J\}$$

denote the spectral gap w.r.t J and let P_J and \widehat{P}_J be the corresponding spectral projectors of A and \widehat{A} , respectively. If A is self-adjoint and for some $\|A - \widehat{A}\| < \text{gap}_J(A)$, then

$$\|P_J - \widehat{P}_J\| \leq \frac{\|A - \widehat{A}\|}{\text{gap}_J(A)}.$$

B Representations in the RKHS

In section 2, we have defined the infinitesimal generator of a diffusion process and specified its form when associated with Dirichlet forms. These operators act on $\mathcal{L}^2_\pi(\mathcal{X})$ or specific subsets of it. To develop our learning procedure, we need to understand these operators' actions when embedding into the RKHS, and define their versions for feature maps.

IG and Dirichlet operator in RKHS. As a reminder, we consider \mathcal{H} be an RKHS and let $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be the associated kernel function. The canonical feature map is denoted by $\phi(x) = k(x, \cdot)$ for $x \in \mathcal{X}$ $k(x, x') = \langle \phi(x), \phi(x') \rangle$ for all $x, x' \in \mathcal{X}$. Assuming that k is square-integrable with respect to the measure π , we define the injection operator $S_\pi : \mathcal{H} \hookrightarrow \mathcal{L}^2_\pi(\mathcal{X})$ and its adjoint $S_\pi^* : \mathcal{L}^2_\pi(\mathcal{X}) \rightarrow \mathcal{H}$ by $S_\pi^* f = \int_{\mathcal{X}} f(x) \phi(x) \pi(dx)$. As a preliminary step, we need to define the reproducing partial derivatives in RKHS, which we introduce via Mercer kernels.

Definition 1 (Mercer kernel). *A kernel function $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is called a Mercer kernel if it is a continuous and symmetric function such that for any finite set of points $\{x_1, \dots, x_n\} \subset \mathcal{X}$, the matrix $(k(x_i, x_j))_{i,j=1}^n$ is positive semi-definite.*

Several standard kernels satisfy the Mercer property with $s \geq 1$, including the Gaussian kernel which we will consider subsequently.

For $s \in \mathbb{N}$ and $m \in \mathbb{N}$, we define the index set $I_s^m = \{\alpha \in \mathbb{N}^m : |\alpha| \leq s\}$ where $|\alpha| = \sum_{j=1}^s \alpha_j$, for $\alpha = (\alpha_1, \dots, \alpha_m) \in \mathbb{N}^m$. For a function $f : \mathbb{R}^m \rightarrow \mathbb{R}$ and $x = (x_1, \dots, x_m) \in \mathbb{R}^m$, we denote its partial derivative $d^\alpha f$ at point x (if it exists) as

$$D^\alpha f(x) = \prod_{j=1}^m D_j^{\alpha_j} f(x) = \frac{\partial^{|\alpha|}}{\partial^{\alpha_1} x_1 \dots \partial^{\alpha_m} x_m} f(x).$$

For a function $k \in \mathcal{C}^{2s}(\mathcal{X} \times \mathcal{X})$ with $\mathcal{X} \subset \mathbb{R}^d$ and $\alpha \in I_s^d$, we define

$$D^\alpha k(x, y) = D^{(\alpha, 0)} k(x, y) = \frac{\partial^{|\alpha|}}{\partial^{\alpha_1} x_1 \dots \partial^{\alpha_m} x_m} k(x, y). \quad (31)$$

and

$$D^{(0, \alpha)} k(x, y) = \frac{\partial^{|\alpha|}}{\partial^{\alpha_1} y_1 \dots \partial^{\alpha_m} y_m} k(x, y).$$

Theorem 3 (Theorem 1 in [49]). *Let $s \in \mathbb{N}$, $\mathcal{X} \subseteq \mathbb{R}^m$ and k be a Mercer kernel such that $k \in \mathcal{C}^{2s}(\mathcal{X} \times \mathcal{X})$ with corresponding RKHS \mathcal{H} . Then the following hold:*

i. For any $x \in \mathcal{X}$, $\alpha \in I_s^m$,

$$(D^\alpha k)_x(y) = D^\alpha k(x, y) \in \mathcal{H}. \quad (32)$$

ii. A partial derivative reproducing property holds for $\alpha \in I_s^m$

$$(D^\alpha h)(x) = \langle (D^\alpha k)_x, h \rangle_{\mathcal{H}}, \quad \forall h \in \mathcal{H}. \quad (33)$$

Theorem 3 allows us to introduce the first and second order operators D and D^2 that act on any feature map $\phi(x)$ as

$$D\phi(x) = ((D^{e_i} k)_x)_{i \in [d]} \quad \text{and} \quad D^2\phi(x) = ((D^{e_i+e_j} k)_x)_{i,j \in [d]}$$

where the $(D^{e_i} k)_x$ and $(D^{e_i+e_j} k)_x$ can be defined via (32). Then, we define the operator d that maps any feature map $\phi(x)$ to $d\phi(x) = s(x)^\top D\phi(x)$. Denote $s^\top = [\bar{s}_1 | \dots | \bar{s}_d] : x \in \mathcal{X} \mapsto s^\top(x) = [\bar{s}_1(x) | \dots | \bar{s}_d(x)] \in \mathbb{R}^{p \times d}$. We have

$$s(x)^\top Dh(x) = \sum_{i=1}^d \bar{s}_i(x) \partial_i h(x) = \sum_{i=1}^d \bar{s}_i(x) \langle D^{e_i} \phi(x), h \rangle_{\mathcal{H}} = \langle d\phi(x), h \rangle_{\mathcal{H}},$$

so that we can define the embedding of the Dirichlet operator $B = s^\top \nabla : \mathcal{L}_\pi^2(\mathcal{X}) \rightarrow [\mathcal{L}_\pi^2(\mathcal{X})]^p$ into RKHS $d\phi : \mathcal{X} \rightarrow \mathcal{H}^p$ via the reproducing property as $\langle d\phi(x), h \rangle_{\mathcal{H}} = [BS_\pi h](x) = s(x)^\top Dh(x) \in \mathbb{R}^p$, $h \in \mathcal{H}$. In fact, $d\phi$ is a p -dimensional vector with components $d_k\phi : \mathcal{X} \rightarrow \mathcal{H}$ given via $\langle d_k\phi(x), h \rangle_{\mathcal{H}} = s_k(x)^\top Dh(x)$, $k \in [p]$. Then, we can define

$$T = -\mathbb{E}_{x \sim \pi}[d\phi(x) \otimes d\phi(x)] = -\sum_{k \in [p]} \mathbb{E}_{x \sim \pi}[d_k\phi(x) \otimes d_k\phi(x)].$$

which captures correlations between input and the outputs of the generator in the RKHS. Defining $w\phi : \mathcal{X} \rightarrow \mathcal{H}^{p+1}$ by $w\phi(x) = [\sqrt{\mu}\phi(x), d_1\phi(x), \dots, d_p\phi(x)]^\top \in \mathbb{R}^{d+1}$, we can consider

$$\begin{aligned} W_\mu &= Z_\mu^* Z_\mu = S_\pi^*(\mu I - L) S_\pi \\ &= \mathbb{E}_{x \sim \pi}[\mu\phi(x) \otimes \phi(x) + d\phi(x) \otimes d\phi(x)] = \mathbb{E}_{x \sim \pi}[w\phi(x) \otimes w\phi(x)] \end{aligned}$$

which corresponds to the RKHS covariance operator w.r.t. energy space \mathcal{W} .

Examples. One way to ensure that the essential assumption ((**KE**)) holds is to show that $w\phi$ fulfils the boundedness condition ((**BK**)), i.e. $w\phi \in \mathcal{L}_\pi^\infty(\mathcal{X}, \mathcal{H}^{1+p})$. Let's show that the property holds true for the Damped Langevin (see Example 1) and the CIR process (see Example 2) if we consider the Radial Basis Function (RBF) kernel $k(x, y) = k_x(y) = \exp(-\kappa\|x - y\|^2)$ where $\kappa > 0$ is a free parameter that sets the ‘‘spread’’ of the kernel. As a reminder, for every $x \in \mathcal{X}$, we have

$$\|w\phi(x)\|^2 = \mu\|\phi(x)\|^2 + \sum_{k=1}^p \|d_k\phi(x)\|^2 \quad \text{with} \quad d_k = s_k(x)^\top D\phi(x).$$

Recalling that for the overdamped Langevin process $s(x) = (k_b T)^{1/2} (\delta_{ij})_{i \in [d], j \in [p]}$, ss^\top is diagonal so that $\langle s(x)^\top Dk_x(\cdot), s(x)^\top Dk_x(\cdot) \rangle = 0$ for every $x \in \mathcal{X}$. As $\|\phi(x)\|^2 = 1$, we get that for every $x \in \mathcal{X}$, $\|w\phi(x)\|^2 \leq \mu =: c_{\mathcal{H}}$.

Consider now the CIR process. We have $d = p = 1$ and $s(x) = \sigma\sqrt{x}/\sqrt{2}$ for any $x \in \mathcal{X}$. For the very same reasons, $\langle s(x)^\top Dk_x(\cdot), s(x)^\top Dk_x(\cdot) \rangle = 0$ for every $x \in \mathcal{X}$, so that $\|w\phi(x)\|^2 \leq \mu =: c_{\mathcal{H}}$. In both Langevin and CIR cases, we have $w\phi \in \mathcal{L}_\pi^\infty(\mathcal{X}, \mathcal{H}^{1+p})$ when considering an RBF kernel.

C Statistical learning framework

C.1 Spectral perturbation bounds

In this section, we prove key perturbation result and discuss the properties of the metric distortion. We conclude this section with the approximation bound for arbitrary estimator $G \in \mathcal{B}_r(\mathcal{H})$ that is the basis of the statistical bounds that follow. This result is a direct consequence of [21] and Davis-Khan spectral perturbation result for compact self-adjoint operators, [10].

In the framework of Koopman operator learning [22], spectral bounds are expressed in terms of a distortion metric between the RKHS \mathcal{H} and $\mathcal{L}_\pi^2(\mathcal{X})$, corresponding to the cost incurred from observing the operator's action on the \mathcal{H} rather than on its domain $\mathcal{L}_\pi^2(\mathcal{X})$. Aligned with the risk definition (9), here we measure in a certain way the distortion between the \mathcal{H} and $\mathcal{W}_\pi^\mu(\mathcal{X})$ as given in definitions in (10).

Proposition 2. *Let $\widehat{G} = \sum_{i \in [r]} (\mu - \widehat{\lambda}_i)^{-1} \widehat{h}_i \otimes \widehat{g}_i$ be the spectral decomposition of $\widehat{G}: \mathcal{H} \rightarrow \mathcal{H}$, where $\widehat{\lambda}_i \geq \widehat{\lambda}_{i+1}$ and let $\widehat{f}_i = S_\pi \widehat{h}_i / \|S_\pi \widehat{h}_i\|_{\mathcal{L}_\pi^2}$, for $i \in [r]$. Then for every $\mu > 0$ and $i \in [r]$*

$$\frac{|\lambda_i - \widehat{\lambda}_i|}{|\mu - \lambda_i| |\mu - \widehat{\lambda}_i|} \leq \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i) \quad \text{and} \quad \|\widehat{f}_i - f_i\|_{\mathcal{L}_\pi^2}^2 \leq \frac{2 \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)}{\mu [\text{gap}_i - \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)]_+}, \quad (11)$$

where gap_i is the difference between i -th and $(i+1)$ -th eigenvalue of $(\mu I - L)^{-1}$.

Proof. We first remark that

$$\|((\mu I - L)^{-1} - \widehat{\lambda}_i I_{\mathcal{L}_\pi^2(\mathcal{X})})^{-1}\|_{\mathcal{H} \rightarrow \mathcal{W}}^{-1} \leq \|((\mu I - L)^{-1} Z_\mu - Z_\mu \widehat{G}) \widehat{h}_i\|_{\mathcal{H} \rightarrow \mathcal{W}} / \|Z_\mu \widehat{h}_i\| \leq \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i).$$

Then, from the first inequality, using that $(\mu I - L)^{-1}$ is self-adjoint as operator $\mathcal{W}_\pi^\mu(\mathcal{X}) \rightarrow \mathcal{W}_\pi^\mu(\mathcal{X})$, we obtain the first bound in (11).

So, observing that for every $(\mu - \lambda)^{-1} \in \text{Sp}((\mu I - L)^{-1}) \setminus \{(\mu - \lambda_i)^{-1}\}$,

$$|(\mu - \widehat{\lambda}_i)^{-1} - (\mu - \lambda)^{-1}| \geq |(\mu - \lambda_i)^{-1} - (\mu - \lambda)^{-1}| - |(\mu - \widehat{\lambda}_i)^{-1} - (\mu - \lambda_i)^{-1}|$$

we conclude that $|(\mu - \widehat{\lambda}_i)^{-1} - (\mu - \lambda)^{-1}| \geq |(\mu - \lambda_i)^{-1} - (\mu - \lambda)^{-1}| - \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)$, and

$$\min\{|(\mu - \widehat{\lambda}_i)^{-1} - (\mu - \lambda)^{-1}| \mid (\mu - \lambda)^{-1} \in \text{Sp}((\mu I - L)^{-1}) \setminus \{(\mu - \lambda_i)^{-1}\}\} \geq \text{gap}_i - \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i).$$

So, applying Proposition 3, we obtain

$$\begin{aligned} \sin(\angle(\widehat{f}_i, f_i)) &\leq \frac{\|(\mu I - L)^{-1} \widehat{f}_i - (\mu - \widehat{\lambda}_i)^{-1} \widehat{f}_i\|}{[\text{gap}_i - \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)]_+} \leq \frac{\|((\mu I - L)^{-1} Z_\mu - Z_\mu \widehat{G}) \widehat{h}_i\| / \|Z_\mu \widehat{h}_i\|}{[\text{gap}_i - \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)]_+} \\ &\leq \frac{\mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)}{[\text{gap}_i - \mathcal{E}(\widehat{G}) \eta(\widehat{h}_i)]_+}. \end{aligned}$$

Since, clearly $\|\widehat{f}_i - f_i\|^2 \leq 2(1 - \cos(\angle(\widehat{f}_i, f_i))) \leq 2 \sin(\angle(\widehat{f}_i, f_i))$, the proof of the second bound is completed. \square

Next, we adapt the [22, Proposition 1] to our setting as follows.

Proposition 5. *Let $\widehat{G} \in \mathcal{B}_r(\mathcal{H})$. For all $i \in [r]$ the metric distortion of \widehat{h}_i w.r.t. energy space $\mathcal{W}_\pi^\mu(\mathcal{X})$ can be tightly bounded as*

$$1 / \sqrt{\|W_\mu\|} \leq \eta(\widehat{h}_i) \leq \|\widehat{G}\| / \sigma_{\min}^+(Z_\mu \widehat{G}). \quad (34)$$

D Empirical estimation

The Reduced Rank Regression (RRR) estimator is the exact minimizer of (17) under fixed rank constraint. Specifically, RRR is the minimizer $\widehat{G}_{\mu,\gamma}^r$ of $\widehat{\mathcal{R}}_\gamma(G)$ within the set of bounded operators $\text{HS}_r(\mathcal{H})$ on \mathcal{H} that have rank at most r . The regularization term $\gamma\|G\|_{\text{HS}}^2$ is added to ensure stability. The closed form solution of the empirical RRR estimator is

$$\widehat{G}_{\mu,\gamma}^r = \widehat{H}_\gamma^{-1/2} [\widehat{H}_\gamma^{1/2} C]_r, \quad (35)$$

while its population counterpart is given by $G_{\mu,\gamma}^r = W_{\mu,\gamma}^{-1/2} [W_{\mu,\gamma}^{1/2} C]_r$.

In order to prove Theorem 1, recall kernel matrices in (19) and define

$$F_\mu = \begin{bmatrix} \mu\mathbf{K} & \sqrt{\mu}\mathbf{N} \\ \sqrt{\mu}\mathbf{N}^\top & \mathbf{M} \end{bmatrix} \quad \text{and} \quad F_{\mu,\gamma} = \begin{bmatrix} \mu\mathbf{K}_\gamma & \sqrt{\mu}\mathbf{N} \\ \sqrt{\mu}\mathbf{N}^\top & \mathbf{M} + \gamma\mu\mathbf{I} \end{bmatrix}. \quad (36)$$

Now we provide the explicit forms of the matrices \mathbf{N} and \mathbf{M} in the case of Langevin (see Example 1) and CIR (see Example 2) processes, considering an RBF kernel $k(x, y) = k_x(y) = \exp(-\kappa\|x - y\|^2)$. As a reminder (see (36)), $\mathbf{N} \in \mathbb{R}^{n \times pn}$ and $\mathbf{M} \in \mathbb{R}^{pn \times pn}$ are Gram matrices whose elements, for $k \in [1 + p], i, j \in [n]$ are given by

$$\mathbf{N}_{i,(k-1)n+j} = n^{-1} \langle \phi(x_i), d_k \phi(x_j) \rangle_{\mathcal{H}} \quad \text{and} \quad \mathbf{M}_{(k-1)n+i,(\ell-1)n+j} = n^{-1} \langle d_k \phi(x_i), d_\ell \phi(x_j) \rangle_{\mathcal{H}},$$

where $d_k \phi(x_j) = s_k(x_j)^\top D \phi(x_j)$ and $D \phi(x_j) = Dk(x_j, \cdot)$ is defined by (31). For $k \in [p], i, j \in [n]$, we have

$$\begin{aligned} \langle \phi(x_i), d_k \phi(x_j) \rangle_{\mathcal{H}} &= \langle k_{x_i}, s_k(x_j)^\top Dk_{x_j} \rangle_{\mathcal{H}} \\ &= \left\langle k_{x_i}, s_k(x_j)^\top \left(\lim_{h \rightarrow 0} \frac{k(\cdot, x_j + he_l) - k(\cdot, x_j)}{h} \right)_{l \in [d]} \right\rangle \\ &= \lim_{h \rightarrow 0} \left\langle k_{x_i}, s_k(x_j)^\top \left(\frac{k(\cdot, x_j + he_l) - k(\cdot, x_j)}{h} \right)_{l \in [d]} \right\rangle \\ &= s_k(x_j)^\top \left(\lim_{h \rightarrow 0} \frac{k(x_i, x_j + he_l) - k(x_i, x_j)}{h} \right)_{l \in [d]} \\ &= s_k(x_j)^\top (D^{(0, e_l)} k(x_i, x_j))_{l \in [d]} \\ &= 2\gamma s_k(x_j)^\top ((x_i^{(l)} - x_j^{(l)}) k(x_i, x_j))_{l \in [d]} \end{aligned}$$

where we have used the continuity of the inner product to get the third line and the reproducing property to obtain the following one. Similarly, for $k, \ell \in [p], j \in [n]$, we get

$$\begin{aligned} \langle d_k \phi(x_i), d_\ell \phi(x_j) \rangle_{\mathcal{H}} &= \left\langle s_k(x_i)^\top (D^{(e_{l'}, 0)} k(x_i, \cdot))_{l' \in [d]}, s_\ell(x_j)^\top \left(\lim_{h \rightarrow 0} \frac{k(\cdot, x_j + he_l) - k(\cdot, x_j)}{h} \right)_{l \in [d]} \right\rangle \\ &= \lim_{h \rightarrow 0} \left\langle s_k(x_i)^\top (D^{(e_{l'}, 0)} k(x_i, \cdot))_{l' \in [d]}, s_\ell(x_j)^\top \left(\frac{k(\cdot, x_j + he_l) - k(\cdot, x_j)}{h} \right)_{l \in [d]} \right\rangle \\ &= \lim_{h \rightarrow 0} \left\langle (D^{(e_{l'}, 0)} k(x_i, \cdot))_{l' \in [d]}, s_k(x_j) s_\ell(x_j)^\top \left(\frac{k(\cdot, x_j + he_l) - k(\cdot, x_j)}{h} \right)_{l \in [d]} \right\rangle \\ &= s_k(x_i) s_\ell(x_j)^\top \left(\lim_{h \rightarrow 0} \frac{D^{(e_{l'}, 0)} k(x_i, x_j + he_l) - D^{(e_{l'}, 0)} k(x_i, x_j)}{h} \right)_{l', l \in [d]} \\ &= s_k(x_i) s_\ell(x_j)^\top (\mathfrak{D}_{l', l} k(x_i, x_j))_{l', l \in [d]}, \end{aligned}$$

where we have used the partial derivative reproducing (32) property and where we define for $l' \neq l$,

$$\begin{aligned}\mathfrak{D}_{l',l}k(x_i, x_j) &= \lim_{h \rightarrow 0} \frac{D^{(e_{l'},0)}k(x_i, x_j + he_l) - D^{(e_{l'},0)}k(x_i, x_j)}{h} \\ &= -2\gamma \lim_{h \rightarrow 0} \frac{(x_i^{(l')} - x_j^{(l')})k(x_i, x_j + he_l) - (x_i^{(l')} - x_j^{(l')})k(x_i, x_j)}{h} \\ &= -4\gamma^2(x_i^{(l')} - x_j^{(l')})(x_i^{(l)} - x_j^{(l)})k(x_i, x_j),\end{aligned}\quad (37)$$

and for $l \in [d]$,

$$\begin{aligned}\mathfrak{D}_{l,l}k(x_i, x_j) &= \lim_{h \rightarrow 0} \frac{D^{(e_l,0)}k(x_i, x_j + he_l) - D^{(e_l,0)}k(x_i, x_j)}{h} \\ &= -2\gamma \lim_{h \rightarrow 0} \frac{(x_i^{(l)} - x_j^{(l)} - h)k(x_i, x_j + he_l) - (x_i^{(l)} - x_j^{(l)})k(x_i, x_j)}{h} \\ &= [2\gamma - 4\gamma^2(x_i^{(l)} - x_j^{(l)})^2]k(x_i, x_j) = 2\gamma[1 - 2\gamma(x_i^{(l)} - x_j^{(l)})^2]k(x_i, x_j).\end{aligned}\quad (38)$$

For the overdamped Langevin (see Example 1), for $k \leq d$, $s_k(x_i) = (k_b T)^{1/2} e_k$ and $s_k(x_i) s_\ell(x_j)^\top = (k_b T) I$ so that

$$N_{i,(k-1)n+j} = n^{-1} \langle \phi(x_i), d_k \phi(x_j) \rangle_{\mathcal{H}} = 2\gamma(k_b T)^{1/2} n^{-1} (x_i^{(k)} - x_j^{(k)})k(x_i, x_j)$$

and

$$M_{(k-1)n+i,(\ell-1)n+j} = n^{-1} \langle d_k \phi(x_j), d_\ell \phi(x_j) \rangle_{\mathcal{H}} = (k_b T) n^{-1} (\mathfrak{D}_{l',l}k(x_j, x_j))_{l',l \in [d]},$$

where the elements of \mathfrak{D} are given by (37) and (38). For the CIR process (see Example 2) in dimension $d = 1$, we have $s(x) = \sigma \sqrt{x} / \sqrt{2}$. Then,

$$N_{i,(k-1)n+j} = n^{-1} \langle \phi(x_i), d_k \phi(x_j) \rangle_{\mathcal{H}} = \sqrt{2} \sigma \gamma n^{-1} \sqrt{x_j} (x_i - x_j) \exp(-\gamma |x_i - x_j|^2)$$

and

$$M_{(k-1)n+i,(\ell-1)n+j} = n^{-1} \langle d_k \phi(x_i), d_\ell \phi(x_j) \rangle_{\mathcal{H}} = \sigma^2 \gamma n^{-1} \sqrt{x_i} \sqrt{x_j} \exp(-\gamma |x_i - x_j|^2).$$

Based on the previous formulas, using Theorem 1, which we prove next, one can estimate generator's eigenpairs in practice.

Theorem 1. *Given $\mu > 0$ and $\gamma > 0$, let $J_{\mu,\gamma} = K - N(M + \gamma\mu I)^{-1} N^\top + \gamma I$. Let $(\hat{\sigma}_i^2, v_i)_{i \in [r]}$ be the leading eigenpairs of the following generalized eigenvalue problem*

$$\mu^{-1} (J_{\mu,\gamma} - \gamma I) K v_i = \hat{\sigma}_i^2 J_{\mu,\gamma} v_i, \quad v_i^\top K v_j = \delta_{ij}, \quad i, j \in [r]. \quad (20)$$

Denoting $V_r = [v_1 | \dots | v_r] \in \mathbb{R}^{n \times r}$ and $\Sigma_r = \text{diag}(\hat{\sigma}_1, \dots, \hat{\sigma}_r)$, if $(\nu_i, w_i^\ell, w_i^r)_{i \in [r]}$ are eigentriplets of matrix $V_r^\top V_r \Sigma_r^2 \in \mathbb{R}^{r \times r}$, then the eigenvalue decomposition the RRR estimator $\hat{G}_{\mu,\gamma}^r = \hat{Z}_\mu U_r V_r^\top \hat{S}$ is given by $\hat{G}_{\mu,\gamma}^r = \sum_{i \in [r]} (\mu - \hat{\lambda}_i)^{-1} \hat{h}_i \otimes \hat{g}_i$, where $\hat{\lambda}_i = \mu - 1/\nu_i$, $\hat{g}_i = \nu_i^{-1/2} \hat{S}^* V_r w_i^\ell$ and $\hat{h}_i = \hat{Z}_\mu^* U_r w_i^r$ for $U_r = (\mu\gamma)^{-1} [\mu^{-1/2} I | -N(M + \gamma\mu I)^{-1}]^\top (K V_r - \mu V_r \Sigma_r^2) \in \mathbb{R}^{(1+p)n \times r}$.

Proof. First, note that $\mu J_{\mu,\gamma} \succ 0$ is exactly Schur's complement w.r.t. second diagonal block of $F_{\mu,\gamma} \succ 0$, and that, due to block inversion lemma [14], we have that

$$F_{\mu,\gamma}^{-1} = \begin{bmatrix} \mu^{-1} J_{\mu,\gamma} & \mu^{-1/2} J_{\mu,\gamma}^{-1} N (M + \gamma\mu I)^{-1} \\ \mu^{-1} / (M + \gamma\mu I)^{-1} N^\top J_{\mu,\gamma}^{-1} & A \end{bmatrix}. \quad (39)$$

where A is some $np \times np$ matrix. The first step in computing the RRR estimator lies in computing a truncating SVD of $\widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C}$, that is $\widehat{C}\widehat{W}_{\mu,\gamma}^{-1}\widehat{C}q_i = \widehat{\sigma}_i^2 q_i$, $i \in [r]$. Now, using the low-rank eigenvalue problem formulation [14], we have that $q_i = \widehat{S}^* v_i$ and $\widehat{S}\widehat{W}_{\mu,\gamma}^{-1}\widehat{C}\widehat{S}^* v_i = \widehat{\sigma}_i^2 v_i$. Now, recalling that $\widehat{S} = [\mu^{-1/2} | 0]\widehat{Z}_\mu$ we obtain and that $\widehat{Z}_\mu(\widehat{Z}_\mu^* \widehat{Z}_\mu + \mu\gamma I)^{-1} = (\widehat{Z}_\mu \widehat{Z}_\mu^* + \mu\gamma I)^{-1} \widehat{Z}_\mu$, we obtain

$$[\mu^{-1/2} I | 0] F_{\mu,\gamma}^{-1} F_\mu [\mu^{-1/2} I | 0]^\top K v_i = \widehat{\sigma}_i^2 v_i,$$

which after some algebra, using (39)

$$\mu^{-1}(I - \gamma J_{\mu,\gamma}^{-1}) K v_i = \widehat{\sigma}_i^2 v_i,$$

i.e. $\mu^{-1}(I - \gamma J_{\mu,\gamma}^{-1}) K V_r = V_r \Sigma_r^2$.

By normalizing right singular value functions q_i of $\widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C}$, that is by asking that $\langle q_i, q_i \rangle_{\mathcal{H}} = v_i^\top K v_i = 1$, we obtain that $[\widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C}]_r = \widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C} Q_r Q_r^*$, for $Q_r = [q_1 | \dots | q_r]$. In other words, we have

$$\widehat{G}_{\mu,\gamma} = \widehat{W}_{\mu,\gamma}^{-1} \widehat{Z}_\mu^* [\mu^{-1/2} I | 0]^\top \widehat{S} \widehat{S}^* V_r V_r^\top \widehat{S} = \widehat{Z}_\mu^* F_{\mu,\gamma}^{-1} [\mu^{-1/2} I | 0]^\top K V_r V_r^\top \widehat{S} = \widehat{Z}_\mu^* U_r V_r^\top \widehat{S},$$

where we used that $J_{\mu,\gamma}^{-1} K V_r = \gamma^{-1} [K V_r - \mu V_r \Sigma_r^2]$. Once with this form, we apply [21, Theorem 2] to obtain the result. \square

Finally, next result provides the reasoning for using empirical metric distortion of Theorem 23.

Proposition 6. *Under the assumptions of Theorem 1, for every $i \in [r]$*

$$\widehat{\eta}_i = \frac{\|\widehat{h}_i\|}{\|\widehat{Z}_\mu \widehat{h}_i\|} = \sqrt{\frac{(w_i^r)^* U_r^\top F_\mu U_r w_i^r}{\|F_\mu U_r w_i^r\|^2}}, \quad (40)$$

and

$$\left| \widehat{\eta}_i - \eta(\widehat{h}_i) \right| \leq \left(\eta(\widehat{h}_i) \wedge \widehat{\eta}_i \right) \eta(\widehat{h}_i) \widehat{\eta}_i \|\widehat{W}_\mu - W_\mu\|. \quad (41)$$

Proof. First, note that (40) follows directly from Theorem 1. Next, since for every $i \in [r]$,

$$(\widehat{\eta}_i)^{-2} - (\eta(\widehat{h}_i))^{-2} = \frac{\langle \widehat{h}_i, (\widehat{W}_\mu - W_\mu) \widehat{h}_i \rangle}{\|\widehat{h}_i\|^2} \leq \|\widehat{W}_\mu - W_\mu\|,$$

we obtain

$$\left| \widehat{\eta}_i^{-1} - (\eta(\widehat{h}_i))^{-1} \right| \leq \frac{|\widehat{\eta}_i^{-2} - (\eta(\widehat{h}_i))^{-2}|}{(\eta(\widehat{h}_i))^{-1} \vee \widehat{\eta}_i^{-1}} \leq \left(\eta(\widehat{h}_i) \wedge \widehat{\eta}_i \right) \|\widehat{W}_\mu - W_\mu\|.$$

\square

E Learning bounds

E.1 Main assumptions

We start by observing that due to **(BK)**, we have that operator $Z_\mu \in \text{HS}(\mathcal{H}, \mathcal{W}_\pi^\mu(\mathcal{X}))$, which according to the spectral theorem for positive self-adjoint operators, has an SVD, i.e. there exists at most countable positive sequence $(\sigma_j)_{j \in J}$, where $J = \{1, 2, \dots\} \subseteq \mathbb{N}$, and ortho-normal systems $(z_j)_{j \in J}$

and $(h_j)_{j \in J}$ of $\text{cl}(\text{Im}(Z_\mu))$ and $\text{Ker}(Z_\mu)^\perp$, respectively, such that $Z_\mu h_j = \sigma_j z_j$ and $Z_\mu^* z_j = \sigma_j h_j$, $j \in J$.

Now, given $\alpha \geq 0$, let us define scaled injection operator $Z_{\mu,\alpha}: \mathcal{H} \rightarrow \mathcal{W}_\pi^\mu(\mathcal{X})$ as

$$Z_{\mu,\alpha} = \sum_{j \in J} \sigma_j^\alpha z_j \otimes h_j. \quad (42)$$

Clearly, we have that $Z_\mu = Z_{\mu,1}$, while $\text{Im } Z_{\mu,0} = \text{cl}(\text{Im}(Z_\mu))$. Next, we equip $\text{Im}(Z_{\mu,\alpha})$ with a norm $\|\cdot\|_{\mathcal{H},\alpha}$ to build an interpolation space

$$[\mathcal{H}]_\alpha = \left\{ f \in \text{Im}(Z_{\mu,\alpha}) \mid \|f\|_{\mathcal{H},\alpha}^2 = \sum_{j \in J} \sigma_j^{-2\alpha} \langle f, z_j \rangle_{\mathcal{W}}^2 < \infty \right\},$$

noting that the inner product in $\mathcal{W}_\pi^\mu(\mathcal{X})$ is given by bilinear energy functional

$$\langle f, g \rangle_{\mathcal{W}} = \mu \langle f, g \rangle_{\mathcal{L}_\pi^2} - \langle f, Lg \rangle_{\mathcal{L}_\pi^2}.$$

We remark that for $\alpha = 1$ the space $[\mathcal{H}]_\alpha$ is just an RKHS \mathcal{H} seen as a subspace of $\mathcal{W}_\pi^\mu(\mathcal{X})$. Moreover, we have the following injections

$$[\mathcal{H}]_{\alpha_1} \hookrightarrow [\mathcal{H}]_1 \hookrightarrow [\mathcal{H}]_{\alpha_2} \hookrightarrow [\mathcal{H}]_0 = \mathcal{W}_\pi^\mu(\mathcal{X}),$$

where $\alpha_1 \geq 1 \geq \alpha_2 \geq 0$.

In addition, from **(BK)** we also have that RKHS \mathcal{H} can be embedded into

$$W_\pi^{\mu,\infty}(\mathcal{X}) = \{f \in \mathcal{W}_\pi^\mu(\mathcal{X}) \mid \|f\|_{W_\pi^{\mu,\infty}} = \text{ess sup}_{x \sim \pi} [|f(x)|^2 - f(x)[Lf](x)] < \infty\}$$

that is, for some $\tau \in (0, 1]$

$$[\mathcal{H}]_1 \hookrightarrow [\mathcal{H}]_\tau \hookrightarrow W_\pi^{\mu,\infty}(\mathcal{X}) \hookrightarrow \mathcal{W}_\pi^\mu(\mathcal{X}).$$

Now, according to [12], if $Z_{\mu,\tau,\infty}: [\mathcal{H}]_\tau \hookrightarrow L_\pi^\infty(\mathcal{X})$ denotes the injection operator, its boundedness implies the polynomial decay of the singular values of Z_μ , i.e. $\sigma_j^2(Z_\mu) \lesssim j^{-1/\tau}$, $j \in J$, and the condition **(KE)** is assured.

Assumption **(SD)** allows one to quantify the effective dimension of \mathcal{H} in ambient space $\mathcal{W}_\pi^\mu(\mathcal{X})$, while the kernel embedding property **(KE)** allows one to estimate the norms of whitened feature maps, in our generator setting vector-valued since they define $\text{rank}(1+p)$ operators on \mathcal{H} ,

$$\xi(x) := W_{\mu,\gamma}^{-1/2} w\phi(x) \in \mathcal{H}^{1+p}. \quad (43)$$

This object plays a key role in deriving the learning rates for regression problems, [23] and the following result is bounding it.

Lemma 1. *Let **(KE)** hold for some $\tau \in [\beta, 1]$ and $c_\tau \in (0, \infty)$. Then,*

$$\mathbb{E}_{x \sim \pi} \|\xi(x)\|_{\mathcal{H}^{1+p}}^2 \leq \begin{cases} \frac{c_\beta^\beta}{1-\beta} (\mu\gamma)^{-\beta} & , \beta < 1, \\ c_\tau (\mu\gamma)^{-1} & , \beta = 1. \end{cases} \quad \text{and} \quad \|\xi\|_\infty^2 = \text{ess sup}_{x \sim \pi} \|\xi(x)\|_{\mathcal{H}^{1+p}}^2 \leq c_\tau (\mu\gamma)^{-\tau}. \quad (44)$$

Proof. W.l.o.g. set $\mu = 1$, observing that the only change in the proof is in scaling $\gamma > 0$. We first observe that for every $j \in J$ from definition of $w\phi$ and fact that $h_j(x) = [Z_\mu h_j](x)$ π -a.e., it holds that

$$\sum_{i \in [1+p]} \langle w_i \phi(x), h_j \rangle^2 = \mu |h_j(x)|^2 - h_j(x) [LZ_\mu h_j](x) = \mu |[Z_\mu h_j](x)|^2 - [Z_\mu h_j](x) [LZ_\mu h_j](x), \quad \pi\text{-a.e.},$$

implying that $\sum_{i \in [1+p]} \langle w_i \phi(x), h_j \rangle^2 \leq \sigma_j \mu |z_j(x)|^2 - z_j(x) [Lz_j](x)$. So, for every $\tau > 0$

$$\begin{aligned} \|\xi(x)\|_{\mathcal{H}^{1+p}}^2 &= \sum_{j \in J} \sum_{i \in [1+p]} \langle W_{\mu, \gamma}^{-1/2} w_i \phi(x), h_j \rangle^2 = \sum_{j \in J} \sum_{i \in [1+p]} \frac{1}{\sigma_j^2 + \gamma} \langle w_i \phi(x), h_j \rangle^2 \\ &= \sum_{j \in J} \sum_{i \in [1+p]} \frac{\sigma_j^{2(1-\tau)}}{\sigma_j^2 + \gamma} \frac{\langle w_i \phi(x), h_j \rangle^2}{\sigma_j^2} \sigma_j^{2\tau} = \gamma^{-\tau} \sum_{j \in J} \sum_{i \in [1+p]} \frac{(\sigma_j^2 \gamma^{-1})^{1-\tau}}{\sigma_j^2 \gamma^{-1} + 1} \frac{\langle w_i \phi(x), h_j \rangle^2}{\sigma_j^2} \sigma_j^{2\tau} \\ &\leq \gamma^{-\tau} \sum_{j \in J} \frac{\mu |h_j(x)|^2 - h_j(x) [LZ_\mu h_j](x)}{\sigma_j^2} \sigma_j^{2\tau} = \gamma^{-\tau} \sum_{j \in J} (\mu |z_j(x)|^2 - z_j(x) [Lz_j](x)) \sigma_j^{2\tau}, \end{aligned}$$

and, due to (21), we obtain $\|\xi\|_\infty^2 \leq \gamma^{-\tau} c_\tau$. On the other hand, we also have that

$$\text{tr}(\mathbb{E}_{x \sim \pi}[\xi(x) \otimes \xi(x)]) = \text{tr}(W_{\mu, \gamma}^{-1/2} W_\mu W_{\mu, \gamma}^{-1/2}) = \text{tr}(W_{\mu, \gamma}^{-1} W_\mu),$$

which is an effective dimension of the RKHS \mathcal{H} in $\mathcal{W}_\pi^\mu(\mathcal{X})$. Therefore, following the proof of Fischer and Steinwart [12, Lemma 11] for classical covariances in \mathcal{L}_π^2 , we show that the bound on the effective dimension is

$$\text{tr}(W_{\mu, \gamma}^{-1} W_\mu) = \sum_{j \in N} \frac{\sigma_j^2}{\sigma_j^2 + \gamma} \leq \begin{cases} \frac{c_\beta^\beta}{1-\beta} \gamma^{-\beta} & , \beta < 1, \\ c_\tau \gamma^{-1} & , \beta = 1. \end{cases} \quad (45)$$

For the case $\beta = 1$, it suffices to see that

$$\|z_j\|_{\mathcal{W}} = \mathfrak{E}_\mu[z_j] \leq \|z_j\|_{W_\pi^\mu, \infty} = \text{ess sup}_{x \sim \pi} [|z_j(x)|^2 - z_j(x) [LZ_\mu z_j](x)],$$

and, hence

$$\text{tr}(W_{\mu, \gamma}^{-1} W_\mu) \leq \gamma^{-1} \sum_{j \in N} \sigma_j^2 \|z_j\|_{\mathcal{W}}^2 = \gamma^{-1} \sum_{j \in N} \sigma_j^2 \mathfrak{E}_\mu[z_j] \leq \gamma^{-1} c_\tau.$$

For $\beta < 1$ we can apply the same classical reasoning as in the proof of Proposition 3 of [8]. \square

Proposition 7. *If the eigenfunctions of L belong to $[\mathcal{H}]_\alpha$, then Condition **(RC)** is satisfied.*

Proof. Note first that the resolvent $(\mu I - L)^{-1}$ admits same eigenfunctions as the generator L , meaning that $\text{Im}((\mu I - L)^{-1} Z_\mu) \subseteq \text{cl}(\text{Im}(Z_{\mu, \alpha}))$. But according to [47, Theorem 2.2], this last condition is equivalent to Condition **(RC)**. \square

Finally we prove here Proposition 8

Proposition 8. *Given $\mu > 0$, let $\mathcal{H} \subseteq \mathcal{W}_\pi^\mu(\mathcal{X})$ be the RKHS associated to kernel $k \in \mathcal{C}^2(\mathcal{X} \times \mathcal{X})$ such that $Z_\mu \in \text{HS}(\mathcal{H}, \mathcal{W}_\pi^\mu(\mathcal{X}))$, and let $P_{\mathcal{H}}$ be the orthogonal projector onto the closure of $\text{Im}(Z_\mu) \subseteq \mathcal{W}_\pi^\mu(\mathcal{X})$. Then for every $\varepsilon > 0$ there exists a finite rank operator $G: \mathcal{H} \rightarrow \mathcal{H}$ such that $\mathcal{R}(G) \leq \|(I - P_{\mathcal{H}})(\mu I - L)^{-1} Z_\mu\|_{\text{HS}(\mathcal{H}, \mathcal{W})}^2 + \varepsilon$. Consequently, when k is universal, $\mathcal{R}(G) \leq \varepsilon$.*

Proof. Recall first that since $Z_\mu \in \text{HS}(\mathcal{H}, \mathcal{W}_\pi^\mu(\mathcal{X}))$, according to the spectral theorem for positive self-adjoint operators, Z_μ admits an SVD. Its form is provided in (42) taking $\alpha = 1$.

Now, recalling that $[\cdot]_r$ denotes the r -truncated SVD, i.e. $[[Z_\mu]]_r = \sum_{j \in [r]} \sigma_j z_j \otimes h_j$, since $\|Z_\mu - [[Z_\mu]]_r\|_{\text{HS}}^2 = \sum_{j > r} \sigma_j^2$, for every $\delta > 0$ there exists $r \in \mathbb{N}$ such that $\|Z_\mu - [[Z_\mu]]_r\|_{\text{HS}} < \mu \delta / 3$. Consequently since all the eigenvalues of L are non-positive, $\|(\mu I - L)^{-1}(Z_\mu - [[Z_\mu]]_r)\|_{\text{HS}} \leq \|Z_\mu - [[Z_\mu]]_r\|_{\text{HS}} / \mu \leq \delta / 3$. Next since $\text{Im}(P_{\mathcal{H}}(\mu I - L)^{-1} Z_\mu) \subseteq \text{cl}(\text{Im}(Z_\mu))$, for any $j \in [r]$, there exists

$g_j \in \mathcal{H}$ s.t. $\|P_{\mathcal{H}}(\mu I - L)^{-1}z_j - Z_{\mu}g_j\| \leq \frac{\delta}{3r}$, and, denoting $B_r := \sum_{j \in [r]} \sigma_j g_j \otimes h_j$ we conclude $\|P_{\mathcal{H}}(\mu I - L)^{-1}[[Z_{\mu}]_r - Z_{\mu}B_r]\|_{\text{HS}} \leq \delta/3$. Finally we recall that the set of non-defective matrices is dense in the space of matrices [40], implying that the set of non-defective rank- r linear operators is dense in the space of rank- r linear operators on a Hilbert space. Therefore, there exists a non-defective $G \in B_r(\mathcal{H})$ such that $\|G - B_r\|_{\text{HS}} < \delta/(3\sigma_1(Z_{\mu}))$. So, we conclude

$$\begin{aligned} & \|(\mu I - L)^{-1}Z_{\mu} - Z_{\mu}G\|_{\text{HS}} \\ & \leq \|(I - P_{\mathcal{H}})(\mu I - L)^{-1}Z_{\mu}\|_{\text{HS}} + \|(\mu I - L)^{-1}Z_{\mu} - [(\mu I - L)^{-1}Z_{\mu}]_r\|_{\text{HS}} \\ & \quad + \|[(\mu I - L)^{-1}Z_{\mu}]_r - Z_{\mu}B_r\|_{\text{HS}} + \|Z_{\mu}(G - B_r)\|_{\text{HS}} \\ & \leq \|(I - P_{\mathcal{H}})(\mu I - L)^{-1}Z_{\mu}\|_{\text{HS}} + \delta. \end{aligned}$$

□

Example 5. *These three conditions depend on the process X (through its generator L) as well as the chosen RKHS. They are satisfied, for example, by choosing for k as a Gaussian kernel. Indeed, the sub-linearity conditions on A and B required to ensure the existence and uniqueness of the solution process of (1) ensure that A and B are sufficiently 'nice' to fulfil, notably, condition ((BK)).*

E.2 Bounding the Bias

Recalling the error decomposition and passing to the \mathcal{H} and \mathcal{L}_{π}^2 -norms, we have that

$$\mathcal{E}(\widehat{G}) \leq \underbrace{\|(\mu I - L)^{-1}Z_{\mu} - Z_{\mu}G_{\mu,\gamma}\|_{\mathcal{H} \rightarrow \mathcal{W}}}_{\text{regularization bias}} + \underbrace{\|W_{\mu}^{1/2}(G_{\mu,\gamma} - G_{\mu,\gamma}^r)\|}_{\text{rank reduction bias}} + \underbrace{\|W_{\mu}^{1/2}(G_{\mu,\gamma}^r - \widehat{G}_{\mu,\gamma}^r)\|}_{\text{estimator's variance}}, \quad (46)$$

and continue to prove the bound of the first term. Note that, while this proof technique is standard for operator learning [23, 28], we present it here for the sake of completeness.

Proposition 9. *Let $G_{\mu,\gamma} = W_{\mu,\gamma}^{-1}C$ for $\gamma > 0$, and $P_{\mathcal{H}}: \mathcal{W}_{\pi}^{\mu}(\mathcal{X}) \rightarrow \mathcal{W}_{\pi}^{\mu}(\mathcal{X})$ be the orthogonal projector onto $\text{cl}(\text{Im}(Z_{\mu}))$. If the assumptions (BK), (SD) and (RC) hold, then $\|G_{\mu,\gamma}\| \leq c_{\alpha} c_{\mathcal{W}}^{(\alpha-1)/2}$ for $\alpha \in [1, 2]$, $\|G_{\mu,\gamma}\| \leq c_{\alpha} (\mu\gamma)^{(\alpha-1)/2}$ for $\alpha \in (0, 1]$, and*

$$\|(\mu I - L)^{-1}Z_{\mu} - Z_{\mu}G_{\mu,\gamma}\|_{\mathcal{H} \rightarrow \mathcal{W}} \leq c_{\alpha} (\mu\gamma)^{\frac{\alpha}{2}} + \|(I - P_{\mathcal{H}})(\mu I - L)^{-1}Z_{\mu}\|_{\mathcal{H} \rightarrow \mathcal{W}}. \quad (47)$$

Proof. Recalling that $P_{\mathcal{H}} := \sum_{j \in J} z_j \otimes z_j$, start by denoting the orthogonal projectors on the subspace of k leading left singular functions of Z_{μ} as $P_k := \sum_{j \in [k]} z_j \otimes z_j$, respectively. Next, observe that $C = Z_{\mu}^*(\mu I - L)^{-1}Z_{\mu}$ and $Z_{\mu}^*W_{\mu,\gamma}^{-1} = Z_{\mu}^*(Z_{\mu}^*Z_{\mu} + \mu\gamma I)^{-1} = (Z_{\mu}Z_{\mu}^* + \mu\gamma I)^{-1}Z_{\mu}$. Therefore,

$$\begin{aligned} (\mu I - L)^{-1}Z_{\mu} - Z_{\mu}G_{\mu,\gamma} &= (I - Z_{\mu}W_{\mu,\gamma}^{-1}Z_{\mu}^*)(\mu I - L)^{-1}Z_{\mu} \\ &= (I - (Z_{\mu}Z_{\mu}^* + \mu\gamma I)^{-1}Z_{\mu}Z_{\mu}^*)(\mu I - L)^{-1}Z_{\mu} \\ &= \mu\gamma(Z_{\mu}Z_{\mu}^* + \mu\gamma I)^{-1}(\mu I - L)^{-1}Z_{\mu} \end{aligned}$$

and, hence

$$\begin{aligned}
(\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma} &= \left(\sum_{j \in J} \frac{\mu \gamma}{\sigma_j^2 + \mu \gamma} z_j \otimes z_j \right) (\mu I - L)^{-1} Z_\mu \\
&= \left(\sum_{j \in J} \frac{\mu \gamma}{(\sigma_j^2 + \mu \gamma) \sigma_j} z_j \otimes (Z_\mu h_j) \right) (\mu I - L)^{-1} Z_\mu \\
&= \left(\sum_{j \in J} \frac{\mu \gamma}{(\sigma_j^2 + \mu \gamma) \sigma_j} z_j \otimes h_j \right) C.
\end{aligned}$$

Therefore, for every $k \in J$, $\|P_k((\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma})\|_{\mathcal{H} \rightarrow \mathcal{W}}^2$ becomes

$$\left\| \left(\sum_{j \in [k]} \frac{\mu \gamma}{(\sigma_j^2 + \mu \gamma) \sigma_j} z_j \otimes h_j \right) C^2 \left(\sum_{j \in [k]} \frac{\gamma}{(\sigma_j^2 + \mu \gamma) \sigma_j} h_j \otimes z_j \right) \right\|_{\mathcal{H} \rightarrow \mathcal{W}},$$

which, due to **(RC)**, implies that

$$\|P_k((\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma})\|_{\mathcal{H} \rightarrow \mathcal{W}} \leq c_\alpha \left\| \sum_{j \in [k]} \frac{\mu \gamma \sigma_j^\alpha}{\sigma_j^2 + \mu \gamma} z_j \otimes z_j \right\|_{\mathcal{W} \rightarrow \mathcal{W}}.$$

On the other hand,

$$\sum_{j \in [k]} \frac{\mu \gamma \sigma_j^\alpha}{\sigma_j^2 + \mu \gamma} z_j \otimes z_j = \gamma^{\frac{\alpha}{2}} \sum_{j \in [k]} \frac{(\sigma_j^2 (\mu \gamma)^{-1})^{\frac{\alpha}{2}}}{\sigma_j^2 (\mu \gamma)^{-1} + 1} z_j \otimes z_j \leq (\mu \gamma)^{\frac{\alpha}{2}} \sum_{j \in [k]} z_j \otimes z_j,$$

where the inequality holds due to $x^s \leq x + 1$ for all $x \geq 0$ and $s \in [0, 1]$. Since the norm of the projector equals one, we get $\|P_k((\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma})\| \leq c_\alpha (\mu \gamma)^{\frac{\alpha}{2}}$.

Next, observe that

$$\|(P_{\mathcal{H}} - P_k)((\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma})\|_{\mathcal{H} \rightarrow \mathcal{W}}^2 = \left\| \sum_{j \in J \setminus [k]} \frac{\mu^2 \gamma^2}{(\sigma_j^2 + \mu \gamma)^2} (Z_\mu^* z_j) \otimes (Z_\mu^* z_j) \right\|_{\mathcal{H} \rightarrow \mathcal{H}}$$

which is bounded by

$$\sum_{j \in J \setminus [k]} \frac{\mu^2 \gamma^2}{(\sigma_j^2 + \mu \gamma)^2} \|Z_\mu^* z_j\|^2 \leq \sum_{j \in J \setminus [k]} \frac{\mu^2 \gamma^2 \sigma_j^{2\alpha}}{(\sigma_j^2 + \mu \gamma)^2} \leq \sum_{j \in J \setminus [k]} \sigma_j^{2\alpha}.$$

Using triangular inequality, for every $k \in J$ we have that $\|P_{\mathcal{H}}((\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma})\|_{\mathcal{H} \rightarrow \mathcal{W}}$ is bounded by

$$\|P_k((\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma})\|_{\mathcal{H} \rightarrow \mathcal{W}} + \|(P_{\mathcal{H}} - P_k)((\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma})\|_{\mathcal{H} \rightarrow \mathcal{W}}$$

and, therefore,

$$\|P_{\mathcal{H}}((\mu I - L)^{-1} Z_\mu - Z_\mu G_{\mu, \gamma})\|_{\mathcal{H} \rightarrow \mathcal{W}} \leq c_\alpha (\mu \gamma)^{\frac{\alpha}{2}} + \sum_{j \in J \setminus [k]} (\sigma_j^{2\beta})^{\frac{\alpha}{2}},$$

and, hence, letting $k \rightarrow \infty$ we obtain $\|P_{\mathcal{H}}(\mu I - L)^{-1}Z_{\mu} - Z_{\mu}G_{\mu,\gamma}\| \leq c_{\alpha}(\mu\gamma)^{\frac{\alpha}{2}}$. Hence, (47) follows from triangular inequality.

To estimate the $\|G_{\mu,\gamma}\|$, note that **(RC)** implies $\|G_{\mu,\gamma}\| \leq c_{\alpha} \|W_{\mu,\gamma}^{-1}W_{\mu}^{\frac{1+\alpha}{2}}\|$ and considering two cases. First, if **(RC)** holds for some $\alpha \in [1, 2]$, then, clearly $\|G_{\mu,\gamma}\| \leq c_{\alpha}c_{\mathcal{W}}^{(\alpha-1)/2}$. On the other hand, if $\alpha \in (0, 1]$, then

$$\frac{\sigma_j^{1+\alpha}}{\sigma_j^2 + \mu\gamma} = (\mu\gamma)^{-1} \frac{(\sigma_j^2(\mu\gamma)^{-1})^{\frac{1+\alpha}{2}}}{\sigma_j^2(\mu\gamma)^{-1} + 1} \leq (\mu\gamma)^{\frac{\alpha-1}{2}},$$

and, thus, $\|G_{\mu,\gamma}\| \leq c_{\alpha} \gamma^{(\alpha-1)/2}$. \square

Remark 2. Inequality (47) says that the regularization bias is comprised of a term depending on the choice of γ , and on a term depending on the ‘‘alignment’’ between \mathcal{H} and $\text{Im}((\mu I - L)^{-1}Z_{\mu})$. The term $\|(I - P_{\mathcal{H}})(\mu I - L)^{-1}Z_{\mu}\|$ can be set to zero by two different approaches. One is choose a kernel which in some way minimizes $\|(I - P_{\mathcal{H}})(\mu I - L)^{-1}Z_{\mu}\|$. Another is to choose a universal kernel [38, Chapter 4], for which $\text{Im}((\mu I - L)^{-1}S_{\pi}) \subseteq \text{cl}(\text{Im}(S_{\pi}))$. While we here develop theory for universal kernels, deep learning approaches that leverage on our approach can be developed, which is the direction to pursue in future.

In order to proceed with bounding the bias due to rank reduction for both considered estimators, we first provide auxiliary result.

Proposition 10. Let $B := W_{\mu,\gamma}^{-1/2}C$, let **(RC)** hold for some $\alpha \in (0, 2]$, and for $j \in \mathbb{N}$ denote

$$\lambda_j^* = \sigma_j^2((\mu I - L)^{-1}Z_{\mu}) = \lambda_j(S_{\pi}^*(\mu I - L)^{-1}S_{\pi}) \quad (48)$$

Then for every $j \in \mathbb{N}$

$$\lambda_j^* - c_{\alpha}^2 c_{\mathcal{W}}^{\alpha/2} (\mu\gamma)^{\alpha/2} \leq \sigma_j^2(B) \leq \lambda_j^*. \quad (49)$$

Proof. Start by observing that

$$\begin{aligned} B^*B &= [(\mu I - L)^{-1}Z_{\mu}]^* Z_{\mu} W_{\mu,\gamma}^{-1} Z_{\mu}^* (\mu I - L)^{-1} Z_{\mu} \\ &= [(\mu I - L)^{-1}Z_{\mu}]^* (\mu I - L)^{-1} Z_{\mu} - \mu\gamma [(\mu I - L)^{-1}Z_{\mu}]^* (Z_{\mu} Z_{\mu}^* + \mu\gamma I)^{-1} (\mu I - L)^{-1} Z_{\mu}, \end{aligned}$$

implies that, using $[(\mu I - L)^{-1}Z_{\mu}]^* = S_{\pi}^*$ and $[(\mu I - L)^{-1}Z_{\mu}]^* (\mu I - L)^{-1} Z_{\mu} = S_{\pi}^* (\mu I - L)^{-1} S_{\pi}$,

$$S_{\pi}^* (\mu I - L)^{-1} S_{\pi} - \sum_{j \in J} \frac{\mu\gamma}{\sigma_j^2 + \mu\gamma} (S_{\pi}^* z_j) \otimes (S_{\pi}^* z_j) = B^*B \preceq Z_{\mu}^* Z_{\mu}.$$

Next, similarly to the above, for every $k \in J$, we have

$$\begin{aligned} \left\| \sum_{j \in [k]} \frac{\mu\gamma}{\sigma_j^2 + \mu\gamma} (S_{\pi}^* z_j) \otimes (S_{\pi}^* z_j) \right\| &\leq c_{\alpha}^2 \left\| \sum_{j \in [k]} \frac{\sigma_j^{2\alpha}}{\sigma_j^2(\mu\gamma)^{-1} + 1} z_j \otimes z_j \right\| \\ &= c_{\alpha}^2 \left\| \sum_{j \in [k]} \frac{(\sigma_j^2(\mu\gamma)^{-1})^{\alpha/2} \sigma_j^{\alpha} (\mu\gamma)^{\alpha/2}}{\sigma_j^2(\mu\gamma)^{-1} + 1} z_j \otimes z_j \right\| \leq c_{\alpha}^2 \gamma^{\alpha/2} \|W_{\mu}\|^{\alpha/2}, \end{aligned}$$

and

$$\left\| \sum_{j \in J \setminus [k]} \frac{\gamma}{\sigma_j^2 + \mu\gamma} (S_\pi^* z_j) \otimes (S_\pi^* z_j) \right\| \leq c_\alpha^2 \sum_{j \in J \setminus [k]} \frac{\gamma}{\sigma_j^2 + \mu\gamma} \sigma_j^{2\alpha} \leq c_\alpha^2 \sum_{j \in J \setminus [k]} (\sigma_j^{2\beta})^{\alpha/\beta}.$$

So, as before, letting $k \rightarrow \infty$ we get the result. \square

As a consequence, we obtain the bound for the rank reduction bias of the RRR method.

Proposition 11 (RRR). *Let (RC) hold for some $\alpha \in (0, 2]$. Then the bias of $G_{\mu,\gamma}^r$ due to rank reduction, recalling (48) is bounded as*

$$\sqrt{\lambda_{r+1}^*} - c_\alpha c_{\mathcal{W}}^{\alpha/4} (\mu\gamma)^{\alpha/4} - 2c_\alpha (\mu\gamma)^{(1 \wedge \alpha)/2} \leq \|Z_\mu(G_{\mu,\gamma} - G_{\mu,\gamma}^r)\| \leq \sqrt{\lambda_{r+1}^*}. \quad (50)$$

Proof. Observe that

$$\|Z_\mu(G_{\mu,\gamma} - G_{\mu,\gamma}^r)\| \leq \|W_{\mu,\gamma}^{1/2}(G_{\mu,\gamma} - G_{\mu,\gamma}^r)\| = \|B - \llbracket B \rrbracket_r\| = \sigma_{r+1}(B) \leq \sigma_{r+1}((\mu I - L)^{-1} Z_\mu)$$

while

$$\begin{aligned} \|Z_\mu(G_{\mu,\gamma} - G_{\mu,\gamma}^r)\| &\geq \|W_{\mu,\gamma}^{1/2}(G_{\mu,\gamma} - G_{\mu,\gamma}^r)\| - (\mu\gamma)^{1/2} \|G_{\mu,\gamma} - G_{\mu,\gamma}^r\| \\ &\geq \sigma_{r+1}((\mu I - L)^{-1} Z_\mu) - c_\alpha \|W_\mu\|^{\alpha/4} (\mu\gamma)^{\alpha/4} - 2c_\alpha (\mu\gamma)^{(1 \wedge \alpha)/2}. \end{aligned}$$

\square

E.3 Bounding the Variance

E.3.1 Concentration Inequalities

All the statistical bounds we present will rely on two versions of Bernstein inequality. The first one is Pinelis and Sakhnenko inequality for random variables in a separable Hilbert space, see [8, Proposition 2].

Proposition 12. *Let $A_i, i \in [n]$ be i.i.d copies of a random variable A in a separable Hilbert space with norm $\|\cdot\|$. If there exist constants $\Lambda > 0$ and $\sigma > 0$ such that for every $m \geq 2$ $\mathbb{E}\|A\|^m \leq \frac{1}{2}m!\Lambda^{m-2}\sigma^2$, then with probability at least $1 - \delta$*

$$\left\| \frac{1}{n} \sum_{i \in [n]} A_i - \mathbb{E}A \right\| \leq \frac{4\sqrt{2}}{\sqrt{n}} \log \frac{2}{\delta} \sqrt{\sigma^2 + \frac{\Lambda^2}{n}}. \quad (51)$$

On the other hand, we recall that in [32], a dimension-free version of the non-commutative Bernstein inequality for finite-dimensional symmetric matrices is proposed (see also Theorem 7.3.1 in [41] for an easier to read and slightly improved version) as well as an extension to self-adjoint Hilbert-Schmidt operators on a separable Hilbert spaces.

Proposition 13. *Let $A_i, i \in [n]$ be i.i.d copies of a Hilbert-Schmidt operator A on the separable Hilbert space. Let $\|A\| \leq c$ almost surely, $\mathbb{E}A = 0$ and let $\mathbb{E}[A^2] \preceq V$ for some trace class operator V . Then with probability at least $1 - \delta$*

$$\left\| \frac{1}{n} \sum_{i \in [n]} A_i \right\| \leq \frac{2c}{3n} \mathcal{L}_A(\delta) + \sqrt{\frac{2\|V\|}{n}} \mathcal{L}_A(\delta), \quad (52)$$

where

$$\mathcal{L}_A(\delta) = \log \frac{4}{\delta} + \log \frac{\text{tr}(V)}{\|V\|}.$$

Proposition 14. Given $\delta > 0$, with probability in the i.i.d. draw of $(x_i)_{i=1}^n$ from π , it holds that

$$\mathbb{P}\{\|\widehat{W}_\mu - W_\mu\| \leq \varepsilon_n(\delta)\} \geq 1 - \delta,$$

where

$$\varepsilon_n(\delta) = \frac{2c_{\mathcal{W}}}{3n} \mathcal{L}(\delta) + \sqrt{\frac{2\|W_\mu\|}{n} \mathcal{L}(\delta)} \quad \text{and} \quad \mathcal{L}(\delta) = \log \frac{4 \text{tr}(W_\mu)}{\delta \|W_\mu\|}. \quad (53)$$

Proof. Proof follows directly from Proposition 13 applied to rank- $(1+p)$ operators $w\phi(x_i) \otimes w\phi(x_i)$ using the fact that $W_\mu = \mathbb{E}[w\phi(x_i) \otimes w\phi(x_i)]$. \square

Proposition 15. Let **(KE)** hold for $\tau \in [\beta, 1]$. Given $\delta > 0$, with probability in the i.i.d. draw of $(x_i)_{i=1}^n$ from π , it holds that

$$\mathbb{P}\left\{\|W_{\mu,\gamma}^{-1/2}(\widehat{W}_\mu - W_\mu)W_{\mu,\gamma}^{-1/2}\| \leq \varepsilon_n^1(\gamma, \delta)\right\} \geq 1 - \delta, \quad (54)$$

where

$$\varepsilon_n^1(\gamma, \delta) = \frac{2c_\tau \mu^{-\tau}}{3n\gamma^\tau} \mathcal{L}^1(\gamma, \delta) + \sqrt{\frac{2c_\tau \mu^{-\tau}}{n\gamma^\tau} \mathcal{L}^1(\gamma, \delta)}, \quad (55)$$

and

$$\mathcal{L}^1(\gamma, \delta) = \ln \frac{4}{\delta} + \ln \frac{\text{tr}(W_{\mu,\gamma}^{-1}W_\mu)}{\|W_{\mu,\gamma}^{-1}W_\mu\|}.$$

Moreover,

$$\mathbb{P}\left\{\|W_{\mu,\gamma}^{1/2}\widehat{W}_{\mu,\gamma}^{-1}W_{\mu,\gamma}^{1/2}\| \leq \frac{1}{1 - \varepsilon_n^1(\gamma, \delta)}\right\} \geq 1 - \delta. \quad (56)$$

Proof. The idea is to apply Proposition 13 for operator $\xi(x) \otimes \xi(x)$, where $\xi(x)$ is defined in (43). Due to (1), we have that $\|A\| \leq \|\xi\|_\infty^2 \leq (\mu\gamma)^{-\tau} c_\tau$. On the other hand, we have that

$$\mathbb{E}_{x \sim \pi} [\xi(x) \otimes \xi(x)]^2 \preceq \|\xi\|_\infty^2 \mathbb{E}_{x \sim \pi} [\xi(x) \otimes \xi(x)] = \|\xi\|_\infty^2 W_{\mu,\gamma}^{-1/2} W_\mu W_{\mu,\gamma}^{-1/2},$$

and, hence (54) follows. To complete the proof, observe that

$$\|I_{\mathcal{H}} - W_{\mu,\gamma}^{-1/2}\widehat{W}_{\mu,\gamma}W_{\mu,\gamma}^{-1/2}\| = \|W_{\mu,\gamma}^{-1/2}(W_\mu - \widehat{W}_\mu)W_{\mu,\gamma}^{-1/2}\| \leq \varepsilon_n^1(\gamma, \delta),$$

and, hence for $\varepsilon_n^1(\gamma, \delta)$ smaller than one we obtain

$$\|W_{\mu,\gamma}^{1/2}\widehat{W}_{\mu,\gamma}^{-1}W_{\mu,\gamma}^{1/2}\| = \|(W_{\mu,\gamma}^{-1/2}\widehat{W}_{\mu,\gamma}W_{\mu,\gamma}^{-1/2})^{-1}\| \leq \frac{1}{1 - \|I_{\mathcal{H}} - W_{\mu,\gamma}^{-1/2}\widehat{W}_{\mu,\gamma}W_{\mu,\gamma}^{-1/2}\|}.$$

\square

Proposition 16. Let **(RC)**, **(SD)** and **(KE)** hold for some $\alpha \in (0, 2]$, $\beta \in (0, 1]$ and $\tau \in [\beta, 1]$. Given $\delta > 0$, with probability in the i.i.d. draw of $(x_i)_{i=1}^n$ from π , it holds

$$\mathbb{P}\left\{\|W_{\mu,\gamma}^{-1/2}(\widehat{W}_\mu - W_\mu)W_{\mu,\gamma}^{-1}C\|_{\text{HS}} \leq \varepsilon_n^2(\gamma, \delta)\right\} \geq 1 - \delta,$$

where

$$\varepsilon_n^2(\gamma, \delta) = 4\sqrt{2}c_\alpha c_\tau \ln \frac{2}{\delta} \sqrt{\frac{c_\beta \mu^{-\beta}}{n\gamma^\beta} + \frac{c_\tau \mu^{-\tau}}{n^2\gamma^\tau}} \begin{cases} (\mu\gamma)^{-(\tau-\alpha)/2} & , \alpha \leq \tau, \\ c_{\mathcal{W}}^{(\alpha-\tau)/2} & , \alpha \geq \tau. \end{cases} \quad (57)$$

Proof. As before, w.l.o.g. set $\mu = 1$. First, recall that $\text{HS}(\mathcal{H})$ equipped with $\|\cdot\|_{\text{HS}}$ is separable Hilbert space. Hence, we will apply Proposition 12 for $A = \xi(x) \otimes \psi(x)$, where $\psi(x) = CW_{\mu,\gamma}^{-1}w\phi(x) \in \mathcal{H}^{1+p}$. To that end, observe that $\mathbb{E}\|A\|_{\text{HS}}^m = \mathbb{E}[\|\xi(x)\|_{\mathcal{H}^{1+p}}^m \|\psi(x)\|_{\mathcal{H}^{1+p}}^m]$, and that

$$\mathbb{E}[\|\xi(x)\|_{\mathcal{H}^{1+p}}^m] \leq \frac{1}{2}m! \left(\gamma^{-\tau/2} \sqrt{c_\tau}\right)^{m-2} \left(\sqrt{\text{tr}(W_{\mu,\gamma}^{-1}W_\mu)}\right)^2.$$

Recalling Lemma 1, the task is to bound $\|\psi(x)\|_{\mathcal{H}^{1+p}}^2 = \sum_{i \in [1+p]} \|CW_{\mu,\gamma}^{-1}w_i\phi(x)\|_{\mathcal{H}}^2$. Using **(RC)**, we have that

$$\|\psi(x)\|_{\mathcal{H}^{1+p}}^2 \leq c_\alpha \sum_{i \in [1+p]} \|W_\mu^{(1+\alpha)/2} W_{\mu,\gamma}^{-1} w_i \phi(x)\|_{\mathcal{H}}^2 = c_\alpha \sum_{j \in J} \sum_{i \in [1+p]} \langle W_\mu^{(1+\alpha)/2} W_{\mu,\gamma}^{-1} w_i \phi(x), h_j \rangle_{\mathcal{H}}^2.$$

But, since

$$\langle W_\mu^{(1+\alpha)/2} W_{\mu,\gamma}^{-1} w_i \phi(x), h_j \rangle_{\mathcal{H}} = \frac{\sigma_j^{1+\alpha}}{\sigma_j^2 + \gamma} \langle w_i \phi(x), h_j \rangle_{\mathcal{H}},$$

expanding as in proof of Lemma 1 and using **(KE)**, we have that

$$\|\psi(x)\|_{\mathcal{H}^{1+p}}^2 \leq c_\alpha \sum_{j \in J} \sum_{i \in [1+p]} \left[\frac{\sigma_j^{(2+\alpha-\tau)}}{\sigma_j^2 + \gamma} \right]^2 \frac{\langle w_i \phi(x), h_j \rangle_{\mathcal{H}}^2}{\sigma_j^2} \sigma_j^{2\tau} \leq \begin{cases} \gamma^{-(\tau-\alpha)} & , \alpha \leq \tau, \\ c_{\mathcal{W}}^{(\alpha-\tau)} & , \alpha \geq \tau. \end{cases}$$

Therefore, we can set

$$\Lambda^2 = c_\alpha c_\tau^2 \begin{cases} \gamma^{-(2\tau-\alpha)} & , \alpha \leq \tau, \\ c_{\mathcal{W}}^{(\alpha-\tau)} \gamma^{-\tau} & , \alpha \geq \tau. \end{cases} \quad \text{and} \quad \sigma^2 = c_\alpha c_\tau c_\beta \begin{cases} \gamma^{-(\beta+\tau-\alpha)} & , \alpha \leq \tau, \\ c_{\mathcal{W}}^{(\alpha-\tau)} \gamma^{-\beta} & , \alpha \geq \tau. \end{cases}$$

in Proposition 12 to obtain the bound □

Proposition 17. *Let **(KE)** hold for $\tau \in [\beta, 1]$. Given $\delta > 0$, with probability in the i.i.d. draw of $(x_i)_{i=1}^n$ from π , it holds*

$$\mathbb{P} \left\{ \|W_{\mu,\gamma}^{-1/2}(\widehat{C} - C)\|_{\text{HS}} \leq \varepsilon_n^3(\gamma, \delta) \right\} \geq 1 - \delta,$$

where

$$\varepsilon_n^3(\gamma, \delta) = \frac{4\sqrt{2}c_{\mathcal{W}}}{\mu} \ln \frac{2}{\delta} \sqrt{\frac{c_\beta \mu^{-\beta}}{n\gamma^\beta} + \frac{c_\tau \mu^{-\tau}}{n^2\gamma^\tau}}. \quad (58)$$

Proof. First, note that since $\|\phi(x)\|_{\mathcal{H}}^2 \leq \mu^{-1}\|w\phi(x)\|_{\mathcal{H}^{1+p}}^2$ and $C \preceq \mu^{-1}W_\mu$, **(KE)** and **(SD)** for W_μ imply analogous assumptions for C . Hence, we can apply Proposition 13 from [23], which using the observation that $\|W_{\mu,\gamma}^{-1/2}C_\gamma^{1/2}\|^2 = \|C_\gamma^{1/2}(\mu C_\gamma - T)^{-1}C_\gamma^{1/2}\|^2 \leq \mu^{-1}\|C_\gamma C_\gamma^{-1}\| = \mu^{-1}$, completes the proof. □

Next, we develop concentration bounds of some key quantities used to build RRR empirical estimator.

E.3.2 Variance and Norm of KRR Estimator

Proposition 18. *Let (RC), (SD) and (KE) hold for some $\alpha \in (0, 2]$, $\beta \in (0, 1]$ and $\tau \in [\beta, 1]$. Given $\delta > 0$ if $\varepsilon_n^1(\gamma, \delta) < 1$, then with probability at least $1 - \delta$ in the i.i.d. draw of $(x_i, y_i)_{i=1}^n$ from ρ*

$$\mathbb{P} \left\{ \|W_{\mu, \gamma}^{1/2}(\widehat{G}_{\mu, \gamma} - G_{\mu, \gamma})\| \leq \frac{\varepsilon_n^2(\gamma, \delta/3) + \varepsilon_n^3(\gamma, \delta/3)}{1 - \varepsilon_n^1(\gamma, \delta/3)} \right\} \geq 1 - \delta.$$

Proof. Note that $W_{\mu, \gamma}^{1/2}(\widehat{G}_{\mu, \gamma} - G_{\mu, \gamma}) = W_{\mu, \gamma}^{1/2}(\widehat{W}_{\mu, \gamma}^{-1}\widehat{C} - W_{\mu, \gamma}^{-1}C)$, and, hence,

$$\begin{aligned} W_{\mu, \gamma}^{1/2}(\widehat{G}_{\mu, \gamma} - G_{\mu, \gamma}) &= W_{\mu, \gamma}^{1/2}\widehat{W}_{\mu, \gamma}^{-1}(\widehat{C} - \widehat{W}_{\mu, \gamma}W_{\mu, \gamma}^{-1}C \pm C) \\ &= W_{\mu, \gamma}^{1/2}\widehat{W}_{\mu, \gamma}^{-1}W_{\mu, \gamma}^{1/2} \left(W_{\mu, \gamma}^{-1/2}(\widehat{C} - C) - W_{\mu, \gamma}^{-1/2}(\widehat{W}_{\mu, \gamma} - W_{\mu, \gamma})W_{\mu, \gamma}^{-1}C \right). \end{aligned} \quad (59)$$

Thus, taking the norm and using $\|C_{\gamma}^{-1}T\| \leq c_{\alpha}\sigma_1^{\alpha-1}(S_{\pi})$ with the Propositions 16 and 15 we prove the first bound. \square

E.3.3 Variance of Singular Values

In this section we prove concentration of singular values computed in Theorem 1, a necessary step to derive learning rates for RRR estimator.

Proposition 19. *Let (RC), (SD) and (KE) hold for some $\alpha \in (0, 2]$, $\beta \in (0, 1]$ and $\tau \in [\beta, 1]$. Let $B = W_{\mu, \gamma}^{-1/2}C$ and $\widehat{B} = \widehat{W}_{\mu, \gamma}^{-1/2}\widehat{C}$. Given $\delta > 0$ if $\varepsilon_n^1(\gamma, \delta/5) < 1$, then with probability at least $1 - \delta$ in the i.i.d. draw of $(x_i)_{i=1}^n$ from π*

$$|\sigma_i^2(\widehat{B}) - \sigma_i^2(B)| \leq \|\widehat{B}^*\widehat{B} - B^*B\| \leq \varepsilon_n^4(\gamma, \delta/3), \quad (60)$$

where

$$\varepsilon_n^4(\gamma, \delta/3) = (\varepsilon_n^2(\gamma, \delta/3) + \varepsilon_n^3(\gamma, \delta/3)) \left(\frac{1}{\mu} + \frac{\varepsilon_n^2(\gamma, \delta/3) + \varepsilon_n^3(\gamma, \delta/3)}{1 - \varepsilon_n^1(\gamma, \delta/3)} \right). \quad (61)$$

Proof. We start from the Weyl's inequalities for the square of singular values

$$|\sigma_i^2(\widehat{B}) - \sigma_i^2(B)| \leq \|\widehat{B}^*\widehat{B} - B^*B\|, \quad i \in [n].$$

But, since,

$$\widehat{B}^*\widehat{B} - B^*B = \widehat{C}^*\widehat{W}_{\mu, \gamma}^{-1}\widehat{C} - C^*W_{\mu, \gamma}^{-1}C = (\widehat{C} - C)^*\widehat{W}_{\mu, \gamma}^{-1}\widehat{C} + C^*W_{\mu, \gamma}^{-1}(\widehat{C} - C) + C^*(\widehat{W}_{\mu, \gamma}^{-1} - W_{\mu, \gamma}^{-1})\widehat{C}$$

denoting $M = W_{\mu, \gamma}^{-1/2}(\widehat{C} - C)$, $N = W_{\mu, \gamma}^{-1/2}(\widehat{W}_{\mu, \gamma} - W_{\mu, \gamma})$ and $R = W_{\mu, \gamma}^{1/2}(\widehat{G}_{\mu, \gamma} - G_{\mu, \gamma})$, we have

$$\begin{aligned} \widehat{B}^*\widehat{B} - B^*B &= B^*M + M^*C_{\gamma}^{1/2}\widehat{G}_{\mu, \gamma} - B^*N\widehat{G}_{\mu, \gamma} = B^*M + (M^*C_{\gamma}^{1/2} - B^*N)(\widehat{G}_{\mu, \gamma} \pm G_{\mu, \gamma}) \\ &= B^*M + M^*B - B^*NG_{\mu, \gamma} + (M^* - B^*NW_{\mu, \gamma}^{-1/2})R \\ &= (G_{\mu, \gamma})^*(\widehat{C} - C) + (\widehat{C} - C)G_{\mu, \gamma} - (G_{\mu, \gamma})^*(\widehat{W}_{\mu, \gamma} - W_{\mu, \gamma})G_{\mu, \gamma} + (M^* + (G_{\mu, \gamma})^*N^*)R. \end{aligned}$$

Therefore, recalling that, due to (59), $R = W_{\mu, \gamma}^{1/2}\widehat{W}_{\mu, \gamma}^{-1}W_{\mu, \gamma}^{1/2}(M - NG_{\mu, \gamma})$, we conclude

$$\begin{aligned} \widehat{B}^*\widehat{B} - B^*B &= (G_{\mu, \gamma})^*(\widehat{C} - C) + (\widehat{C} - C)G_{\mu, \gamma} - (G_{\mu, \gamma})^*(\widehat{W}_{\mu, \gamma} - W_{\mu, \gamma})G_{\mu, \gamma} \\ &\quad + (M - NG_{\mu, \gamma})^*W_{\mu, \gamma}^{1/2}\widehat{W}_{\mu, \gamma}^{-1}W_{\mu, \gamma}^{1/2}(M - NG_{\mu, \gamma}). \end{aligned} \quad (62)$$

Next, observe that

- $\|(\widehat{C}-C)G_{\mu,\gamma}\| \leq \|(\widehat{C}-C)W_{\mu,\gamma}^{1/2}\| \|W_{\mu,\gamma}^{1/2}C\| \leq \mu^{-1} \|W_{\mu,\gamma}^{1/2}(\widehat{C}-C)\|$ is bounded by Proposition 17
- $\|M-NG_{\mu,\gamma}\| \leq \|W_{\mu,\gamma}^{-1/2}(\widehat{C}-C)\| + \|W_{\mu,\gamma}^{-1/2}(\widehat{W}_\mu - W_\mu)W_{\mu,\gamma}^{-1}C\|$ is bounded by Propositions 16 and 17,
- $\|G_{\mu,\gamma}^*(\widehat{W}_\mu - W_\mu)G_{\mu,\gamma}\| \leq \mu^{-1} \|W_{\mu,\gamma}^{-1/2}(\widehat{W}_\mu - W_\mu)W_{\mu,\gamma}^{-1}C\|$ is bounded by Proposition 16.

Therefore, using additionally Proposition 15 result follows. \square

Remark that to bound singular values we can rely on the fact

$$|\sigma_i(\widehat{B}) - \sigma_i(B)| = \frac{|\sigma_i^2(\widehat{B}) - \sigma_i^2(B)|}{\sigma_i(\widehat{B}) + \sigma_i(B)} \leq \frac{|\sigma_i^2(\widehat{B}) - \sigma_i^2(B)|}{\sigma_i(\widehat{B}) \vee \sigma_i(B)}.$$

E.3.4 Variance of RRR Estimator

Recalling the notation $B := W_{\mu,\gamma}^{-1/2}C$ and $\widehat{B} := \widehat{W}_{\mu,\gamma}^{-1/2}\widehat{C}$, let denote P_r and \widehat{P}_r denote the orthogonal projector onto the subspace of leading r right singular vectors of B and \widehat{B} , respectively. Then we have $\llbracket B \rrbracket_r = BP_r$ and $\llbracket \widehat{B} \rrbracket_r = \widehat{B}\widehat{P}_r$, and, hence $G_{\mu,\gamma}^r = G_{\mu,\gamma}P_r$ and $\widehat{G}_{\mu,\gamma}^r = \widehat{G}_{\mu,\gamma}\widehat{P}_r$.

Proposition 20. *Let (RC), (SD) and (KE) hold for some $\alpha \in (0, 2]$, $\beta \in (0, 1]$ and $\tau \in [\beta, 1]$. Given $\delta > 0$ and $\gamma > 0$, if $\varepsilon_n^1(\gamma, \delta) < 1$, then with probability at least $1 - \delta$ in the i.i.d. draw of $(x_i)_{i=1}^n$ from π ,*

$$\|Z_\mu(G_{\mu,\gamma}^r - \widehat{G}_{\mu,\gamma}^r)\| \leq \frac{\varepsilon_n^2(\gamma, \delta/3) + \varepsilon_n^3(\gamma, \delta/3)}{1 - \varepsilon_n^1(\gamma, \delta/3)} + \frac{\sigma_1(B)}{\sigma_r^2(B) - \sigma_{r+1}^2(B)} \varepsilon_n^4(\gamma, \delta/3). \quad (63)$$

Proof. Start by observing that $\|Z_\mu(G_{\mu,\gamma}^r - \widehat{G}_{\mu,\gamma}^r)\| \leq \|W_{\mu,\gamma}^{1/2}(G_{\mu,\gamma}^r - \widehat{G}_{\mu,\gamma}^r)\|$ and

$$\begin{aligned} W_{\mu,\gamma}^{1/2}(G_{\mu,\gamma}^r - \widehat{G}_{\mu,\gamma}^r) &= (W_{\mu,\gamma}^{1/2}\widehat{W}_{\mu,\gamma}^{-1}W_{\mu,\gamma}^{1/2}) \\ &\quad \left(W_{\mu,\gamma}^{-1/2}(\widehat{W}_\mu - W_\mu)G_{\mu,\gamma}P_r + W_{\mu,\gamma}^{-1/2}(\widehat{C} - C)\widehat{P}_r + B(\widehat{P}_r - P_r) \right). \end{aligned}$$

Using that the norm of orthogonal projector \widehat{P} is bounded by one and applying Propositions 15 and 16 together with Propositions 4 and 19 completes the proof. \square

E.4 Proof of Theorem 2

E.4.1 Operator Norm Error Bounds

Summarising previous sections, in order to prove Theorem 2, we just need to analyse the bounds ε_n^1 , ε_n^2 and ε_n^3 . Note that we fix the hyperparameter $\mu > 0$, which affects the constants, but need to chose the decay rate of Tikhonov regularization parameter $\gamma > 0$ to obtain balancing of bias and variance in the generalization bounds.

Let us first assume regime $\alpha \geq \tau$, which covers "well-specified learning" when non-trivial eigenfunctions of L are inside \mathcal{H} . Since $\alpha \geq \tau$ and $\beta \leq \tau$, we have that for large enough n one has

$$\varepsilon_n^1(\gamma, \delta) \lesssim \frac{n^{-1/2}}{\gamma^{\tau/2}} \ln \delta^{-1} \quad \text{and} \quad \varepsilon_n^i(\gamma, \delta) \lesssim \left(\frac{n^{-1/2}}{\gamma^{\beta/2}} \vee \frac{n^{-1}}{\gamma^{\tau/2}} \right) \ln \delta^{-1}, \quad i = 2, 3, 4. \quad (64)$$

But, since the bias term is $\lesssim \gamma^{\alpha/2}$ and the slow term from Proposition 20 is $1/\sqrt{n\gamma^\beta}$, we can set $\gamma_n = n^{-\frac{1}{\alpha+\beta}}$ and obtain

$$\gamma_n^{\alpha/2} = \frac{n^{-1/2}}{\gamma_n^{\beta/2}} = n^{-\frac{\alpha}{2(\alpha+\beta)}}, \quad \text{and} \quad \frac{n^{-1/2}}{\gamma_n^{\tau/2}} = n^{-\frac{\alpha+\beta-\tau}{2(\alpha+\beta)}},$$

which, due to $\alpha \geq \tau$, implies

$$\lim_{n \rightarrow \infty} \varepsilon_n^1(\gamma_n, \delta/3) = \lim_{n \rightarrow \infty} \varepsilon_n^2(\gamma_n, \delta/3) = \lim_{n \rightarrow \infty} \varepsilon_n^3(\gamma, \delta/3) = \lim_{n \rightarrow \infty} \varepsilon_n^4(\gamma, \delta/3) = 0.$$

Therefore, for this choice of regularization parameter Equation (46) with Propositions 9, 11 and 20 assure that

$$\mathcal{E}(\widehat{G}_{\mu, \gamma}^r) - \sigma_{r+1}(B) \leq \mathcal{E}(\widehat{G}_{\mu, \gamma}^r) - \sqrt{\lambda_{r+1}^*} \lesssim n^{-\frac{\alpha}{2(\alpha+\beta)}}. \quad (65)$$

Now, let us consider the more difficult to learn case $\alpha < \tau$ when eigenfunctions of the generator have only weaker norms than the RKHS one. Then, for large enough n bounds in (64) hold for $i = 3$, but

$$\varepsilon_n^2(\gamma, \delta) \vee \varepsilon_n^4(\gamma, \delta) \lesssim \left(\frac{n^{-1/2}}{\gamma^{(\beta+\tau-\alpha)/2}} \vee \frac{n^{-1}}{\gamma^{(2\tau-\alpha)/2}} \right) \ln \delta^{-1}. \quad (66)$$

Then, by balancing the slow terms with bias $\gamma^{\alpha/2}$, we set $\gamma_n = n^{-\frac{1}{\tau+\beta}}$ and obtain

$$\gamma_n^{\alpha/2} = \frac{n^{-1/2}}{\gamma_n^{(\tau+\beta-\alpha)/2}} = n^{-\frac{\alpha}{2(\tau+\beta)}}, \quad \text{and} \quad \frac{n^{-1/2}}{\gamma_n^{\tau/2}} = n^{-\frac{\beta}{2(\tau+\beta)}},$$

which, since $\tau \geq \beta$, implies

$$\lim_{n \rightarrow \infty} \varepsilon_n^1(\gamma_n, \delta/3) = \lim_{n \rightarrow \infty} \varepsilon_n^2(\gamma_n, \delta/3) = \lim_{n \rightarrow \infty} \varepsilon_n^3(\gamma, \delta/3) = \lim_{n \rightarrow \infty} \varepsilon_n^4(\gamma, \delta/3) = 0,$$

and we obtain

$$\mathcal{E}(\widehat{G}_{\mu, \gamma}^r) - \sigma_{r+1}(B) \leq \mathcal{E}(\widehat{G}_{\mu, \gamma}^r) - \lambda_{r+1}^* \lesssim n^{-\frac{\alpha}{2(\tau+\beta)}}. \quad (67)$$

Therefore, denoting

$$\gamma_n \asymp \begin{cases} n^{-\frac{1}{\tau+\beta}} & , \alpha \leq \tau, \\ n^{-\frac{1}{\alpha+\beta}} & , \alpha \geq \tau, \end{cases} \quad \text{and} \quad \varepsilon_n^* = \begin{cases} n^{-\frac{\alpha}{2(\tau+\beta)}} & , \alpha \leq \tau, \\ n^{-\frac{\alpha}{2(\alpha+\beta)}} & , \alpha \geq \tau. \end{cases} \quad (68)$$

as a consequence the operator norm error bound in Theorem 2 holds, and we have the following result on the estimation of singular values of $(\mu I - L)^{-1} Z_\mu$, that is λ_i^* s by singular values of \widehat{B} , that is $\widehat{\sigma}_i$ s from Theorem 1.

Proposition 21. *Let (RC), (SD) and (KE) hold for some $\alpha \in (0, 2]$ and $\beta \in (0, 1]$ and $\tau \in [\beta, 1]$, and define (68). Then, there exists a constant $c > 0$ such that for every given $\delta \in (0, 1)$, large enough $n > r$ and with probability at least $1 - \delta$ in the i.i.d. draw of $(x_i)_{i=1}^n$ from π for all $i \in [r]$*

$$|\widehat{\sigma}_i^2 - \lambda_i^*| \lesssim \varepsilon_n^* \ln \delta^{-1} \quad (69)$$

Proof. The proof is direct consequence of Propositions 10 and 19 using (64)-(66). \square

E.5 Spectral Learning Rates

Finally, we conclude the proof of Theorem 2 showing the concentration of eigenpairs. Recalling Proposition 2, we need to combine the operator norm bound and metric distortion. Since, as indicated in Proposition 9, the population KRR estimator can grow in the operator norm whenever the regularity condition is violated $\alpha < 1$, leading to possibly unbounded metric distortions w.r.t. increasing sample size, we restrict to the case $\alpha \geq 1$.

First, combining (65)-(67) and Proposition 21, we have that

$$\mathcal{E}(\widehat{G}_{\mu,\gamma}^r) \leq (\widehat{\sigma}_{r+1} \wedge \lambda_{r+1}^*) + c \varepsilon_n^* \ln \delta^{-1}.$$

On the other hand, from Propositions 40 and 14, we have that with failure probability δ

$$(\widehat{\eta}_i)^2 - (\eta(\widehat{h}_i))^{-2} \leq \varepsilon_n(\delta),$$

which, if we can prove that $\widehat{\eta}_i$ and $\eta(\widehat{h}_i)$ are bounded, concludes the proof for empirical spectral biases. To that end, recall that, c.f. Proposition 5, for RRR estimator we have

$$\begin{aligned} \eta(\widehat{h}_i) &\leq \frac{\|\widehat{G}_{\mu,\gamma}^r\|}{\sigma_r(Z_\mu \widehat{G}_{\mu,\gamma}^r)} \leq \frac{\|\widehat{G}_{\mu,\gamma}\|}{\sigma_r((\mu I - L)^{-1} Z_\mu) - \mathcal{E}(\widehat{G}_{\mu,\gamma}^r)} \leq \frac{\|G_{\mu,\gamma}\| + \|\widehat{G}_{\mu,\gamma} - G_{\mu,\gamma}\|}{\sqrt{\lambda_r^*} - \mathcal{E}(\widehat{G}_{\mu,\gamma}^r)} \\ &\leq \frac{\|G_{\mu,\gamma}\| + (\mu\gamma)^{-1/2} \|W_{\mu,\gamma}^{1/2}(\widehat{G}_{\mu,\gamma} - G_{\mu,\gamma})\|}{\sqrt{\lambda_r^*} - \mathcal{E}(\widehat{G}_{\mu,\gamma}^r)} \lesssim \frac{1 + n^{-1/2} \gamma^{-(\beta+1)/2}}{\sqrt{\lambda_r^*} - n^{-1/2} \gamma^{-\beta/2}} = \frac{1 + n^{-\frac{\alpha-1}{\alpha+\beta}}}{\sqrt{\lambda_r^*} - n^{-\frac{\alpha}{\alpha+\beta}}} \end{aligned}$$

where in the last inequality we have applied Propositions 9 and 18. Thus, using Proposition 40, the proof of Theorem 2 is concluded.

E.6 Discussion of the learning rates

In this section, we discuss the learning rates reported in Table ?? . Notice that although the papers we compare to employ a different risk, our comparison remains meaningful because our energy-based risk measure provides an upper bound on their risk measure. This ensures that any upper bound derived with our risk also applies to theirs.

- The learning bound for IG obtained in [1] covers only pure diffusion processes (Laplacian with constant weights). Their learning rate is non-parametric and depends on the state space dimension d in a counter-intuitive way $O(n^{-\frac{d}{2(d+1)}})$ in [1, Theorem 3], highlighting a potential limitation of their approach. In comparison, when we specify our RRR method with an RBF kernel (i.e. $\beta = 0$), we achieve a much faster parametric learning rate $O(n^{-1/2})$.
- The recent work of [36] covers Langevin processes via a kernel approach, but they derive a sub-optimal learning bound for IG of order $O(n^{-1/4})$ in [36, Theorem 4.4]. For Langevin diffusions, our RRR method with an RBF kernel achieves a faster parametric rate $O(n^{-1/2})$. Moreover, the computational complexity of their method is $O(n^3 d^3)$, which limits its application in realistic molecular dynamics scenarios.
- As for [15, Theorem 7], although they considered general diffusions, they only derived a suboptimal bound for the variance component of their risk, with an explicit dependence on the dimension of the state space.

Finally, we note that the mentioned works lack learning guarantees for eigenfunctions and eigenvalues. Notably, their methods are prone to the spurious eigenvalue phenomenon, requiring expert manual review of each eigenpair to select plausible ones.

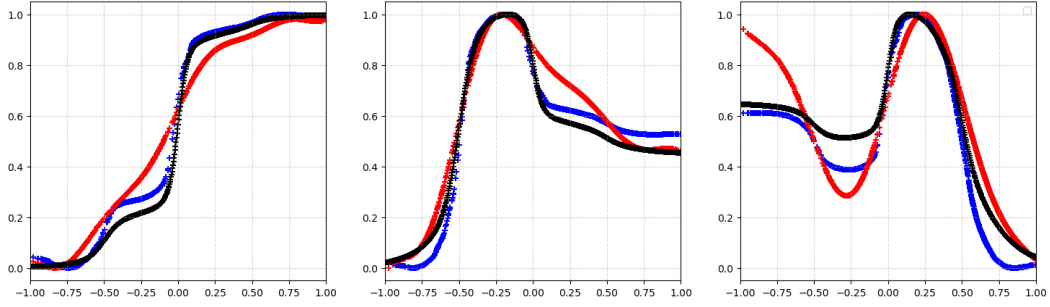


Figure 2: Results of the RRR given by our method for two different length scales (blue and red) compared with ground truth (black) for the Langevin dynamics driven by a four well one dimensional potential.

F Experiments

Four well potential For this experiment, we used an in-house code to simulate the system. The equations of motions were discretized using the Euler-Maruyama scheme with a timestep of 10^{-4} . RRR was fitted using 1000 points, $\mu = 5$ and $\gamma = 10^{-5}$. The length scales used were 0.05 and 0.5. This experiment was reproduced 100 times leading to very small change in the estimation of the eigenfunctions. Here we report the result of one of them.

Muller Brown For this experiment, we used an in-house code to simulate the system. The equations of motions were discretized using the Euler-Maruyama scheme with a timestep of 10^{-3} and a temperature of 2 (arbitrary units). RRR was fitted using 2000 points, $\mu = 1$ and $\gamma = 10^{-5}$. The length scale used was 0.6.

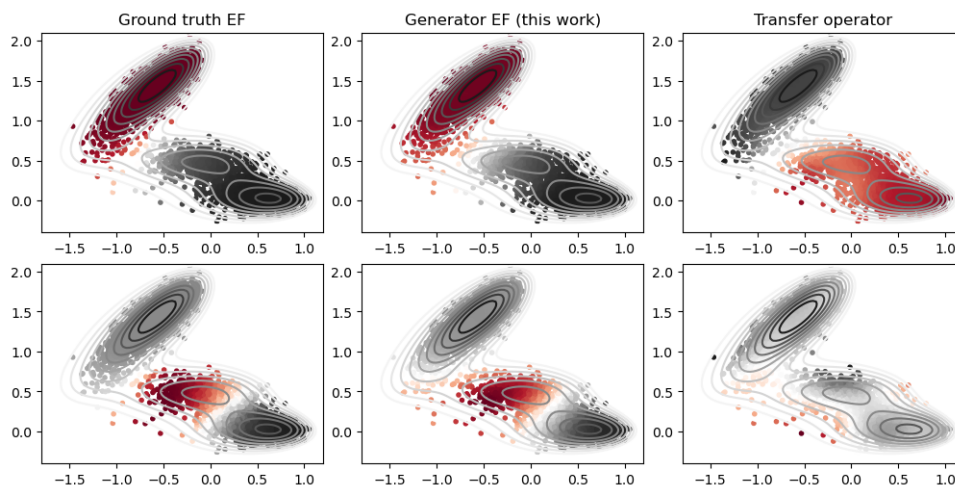


Figure 3: Results of the RRR given by our method for two different length scales (blue and red) compared with ground truth for the Langevin dynamics driven by a four well one dimensional potential.

notation	meaning	notation	meaning
\wedge	minimum	\vee	maximum
$\llbracket \cdot \rrbracket_r$	r -truncated SVD of an operator	I	identity operator
$\text{HS}(\mathcal{H}, \mathcal{G})$	space of Hilbert-Schmidt operators $\mathcal{H} \rightarrow \mathcal{G}$	$B_r(\mathcal{H})$	set of rank- r Hilbert-Schmidt operators on \mathcal{H}
$\ A\ $	operator norm of an operator A	$\ A\ _{\text{HS}}$	Hilbert-Schmidt norm of operator A
$\sigma_i(\cdot)$	i -th singular value of an operator	$\lambda_i(\cdot)$	i -th eigenvalue of an operator
\mathcal{X}	state space of the Markov process	$(X_t)_{t \geq 0}$	time-homogeneous Markov process
p	transition kernel of the Markov process	π	invariant measure of the Markov process
a	drift of the Itô process	b	diffusion of the Itô process
$\mathcal{L}_\pi^2(\mathcal{X})$	L2 space of functions on \mathcal{X} w.r.t. measure π	A	Transfer operator on $\mathcal{L}_\pi^2(\mathcal{X})$
$\mathcal{W}_\pi^{1,2}(\mathcal{X})$	Sobolev space w.r.t. measure π on \mathcal{X}	L	Generator of the semigroup on $\mathcal{W}_\pi^{1,2}(\mathcal{X})$
s	Dirichlet form diffusion	B	Dirichlet form operator on $\mathcal{W}_\pi^{1,2}(\mathcal{X})$
μ	shift parameter	$\mathcal{W}_\pi^\mu(\mathcal{X})$	regularized energy space
$k(x, y)$	kernel	ϕ	canonical feature map
\mathcal{H}	reproducing kernel Hilbert space	S_π	canonical injection $\mathcal{H} \hookrightarrow \mathcal{L}_\pi^2(\mathcal{X})$
$\ell\phi$	generator embedding	Z_μ	canonical injection $\mathcal{H} \hookrightarrow \mathcal{W}_\pi^\mu(\mathcal{X})$
D^v	v -directional derivative	D	derivative
$D^v\phi$	embedding of the v -directional derivative	$D\phi$	derivative embedding
$w_k\phi$	k -th component of Dirichlet operator embedding	$w\phi$	Dirichlet operator embedding
σ_j	j -th singular value of Z_μ	J	countable index set of singular values of Z_μ
z_j	j -th left singular function of Z_μ	h_j	j -th right singular function of Z_μ
$\mathbb{1}$	function in $\mathcal{L}_\pi^2(\mathcal{X})$ with the constant output 1	γ	regularization parameter
\mathcal{R}	true risk	\mathcal{E}	operator norm error
\mathcal{E}_{HS}	excess risk, i.e. HS norm error	\mathcal{R}_0	irreducible risk
\mathcal{D}_n	dataset $(x_i)_{i \in [n]}$	$\widehat{\mathcal{R}}$	empirical risk
\widehat{S}	sampling operator w.r.t. $\mathcal{L}_\pi^2(\mathcal{X})$	\widehat{Z}_μ	sampling operator w.r.t. $\mathcal{W}_\pi^\mu(\mathcal{X})$
C	covariance operator w.r.t. $\mathcal{L}_\pi^2(\mathcal{X})$	\widehat{C}	empirical covariance operator w.r.t. $\mathcal{L}_\pi^2(\mathcal{X})$
C_γ	regularized covariance operator w.r.t. $\mathcal{L}_\pi^2(\mathcal{X})$	\widehat{C}_γ	regularized empirical covariance operator w.r.t. $\mathcal{L}_\pi^2(\mathcal{X})$
W_μ	covariance operator w.r.t. $\mathcal{W}_\pi^\mu(\mathcal{X})$	\widehat{W}_μ	empirical covariance operator w.r.t. $\mathcal{W}_\pi^\mu(\mathcal{X})$
$W_{\mu,\gamma}$	regularized covariance operator w.r.t. $\mathcal{W}_\pi^\mu(\mathcal{X})$	$\widehat{W}_{\mu,\gamma}$	regularized empirical covariance operator w.r.t. $\mathcal{W}_\pi^\mu(\mathcal{X})$
T	derivative-covariance operator	\widehat{T}	empirical derivative-covariance operator
K	kernel Gram matrix w.r.t. $\mathcal{L}_\pi^2(\mathcal{X})$	K_γ	regularized kernel Gram matrix w.r.t. $\mathcal{L}_\pi^2(\mathcal{X})$
F_μ	kernel Gram matrix w.r.t. $\mathcal{W}_\pi^\mu(\mathcal{X})$	$F_{\mu,\gamma}$	regularized kernel Gram matrix w.r.t. $\mathcal{W}_\pi^\mu(\mathcal{X})$
M	derivative-derivative kernel Gram matrix	N	feature-derivative kernel Gram matrix
G	population estimator of $(\mu I - L)^{-1}$ on \mathcal{H}	\widehat{G}	empirical estimator of $(\mu I - L)^{-1}$ on \mathcal{H}
$G_{\mu,\gamma}$	population KRR estimator	$\widehat{G}_{\mu,\gamma}$	empirical KRR estimator
$G_{\mu,\gamma}^r$	population RRR estimator	$\widehat{G}_{\mu,\gamma}^r$	empirical RRR estimator
P	spectral projector	\widehat{P}	empirical spectral projector
η	metric distortion	$\widehat{\eta}$	empirical metric distortion
λ	generator eigenvalue	$\widehat{\lambda}$	eigenvalue of the empirical estimator
f	generator eigenfunction in $\mathcal{L}_\pi^2(\mathcal{X})$	\widehat{f}	empirical eigenfunction in $\mathcal{L}_\pi^2(\mathcal{X})$
\widehat{h}	right empirical eigenfunction	\widehat{g}	left empirical eigenfunction
$c_{\mathcal{W}}$	boundness constant	$P_{\mathcal{H}}$	orthogonal projector in $\mathcal{W}_\pi^\mu(\mathcal{X})$ onto $\text{Im}(Z_\mu)$
α	regularity parameter	c_α	regularity constant
β	spectral decay parameter	c_β	spectral decay constant
τ	embedding parameter	c_τ	embedding constant

Table 1: Summary of used notations.