

KERNEL AUTOCOVARIANCE OPERATORS OF STATIONARY PROCESSES: ESTIMATION AND CONVERGENCE

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ABSTRACT. We consider autocovariance operators of a stationary stochastic process on a Polish space that is embedded into a reproducing kernel Hilbert space. We investigate how empirical estimates of these operators converge along realizations of the process under various conditions. In particular, we examine ergodic and strongly mixing processes and prove several asymptotic results as well as finite sample error bounds with a detailed analysis for the Gaussian kernel. We provide applications of our theory in terms of consistency results for *kernel PCA* with dependent data and the *conditional mean embedding* of transition probabilities. Finally, we use our approach to examine the nonparametric estimation of Markov transition operators and highlight how our theory can give a consistency analysis for a large family of spectral analysis methods including kernel-based *dynamic mode decomposition*.

1. INTRODUCTION

The *kernel mean embedding* (i.e., the embedding of a probability distribution into a reproducing kernel Hilbert space, see [Berlinet and Thomas-Agnan 2004](#); [Smola et al. 2007](#)) and the theory of *kernel (cross-)covariance operators* have spawned a vast variety of nonparametric models and statistical tests over the last years (for an overview of the kernel embedding theory, we refer the reader to the survey by [Muandet et al. 2017](#) and references therein). However, consistency results for empirical kernel mean embedding methods are almost exclusively based on the assumption that the underlying data is independent and identically distributed.

Kernel covariance operators serve as the theoretical foundation of several spectral analysis and component decomposition techniques including *kernel principal component analysis*, *kernel independent component analysis* and *kernel canonical correlation analysis*. Consistency results and the statistical analysis of these methods can therefore be directly based on the estimation of kernel covariance operators ([Zwald and Blanchard, 2006](#); [Fukumizu et al., 2007](#); [Rosasco et al., 2010](#)). Moreover, kernel covariance operators and their connection to L^p -space integral operators and random matrices are a fundamental concept used to formalize statistical learning ([Smale and Zhou, 2007](#); [Rosasco et al., 2010](#)).

In this paper, we extend the statistical theory of kernel covariance operators from the independent scenario to *kernel autocovariance operators* of a stochastic process (that is, kernel cross-covariance operators with respect to a time-lagged version of the process). Recently, several applications for dependent data, sequence modeling, and time series analysis based on kernel mean embeddings have emerged. Popular approaches include state space models ([Song et al., 2009](#)), filtering ([Fukumizu](#)

et al., 2013; Gebhardt et al., 2019), transition models (Sun et al., 2019; Grünewälder et al., 2012b) and reinforcement learning (van Hoof et al., 2015; Lever et al., 2016; van Hoof et al., 2017; Stafford and Shawe-Taylor, 2018; Gebhardt et al., 2018). A theoretical tool to understand these concepts is the kernel autocovariance operator, as it plays a role in the RKHS-based approximation of transition probabilities. This concept has been introduced in an operator-theoretic sense under the name *conditional mean embedding* by Song et al. (2009) under strong technical requirements (see also Klebanov et al., 2019). These requirements have later been relaxed by developing the theory in a vector-valued regression scenario (Grünewälder et al., 2012a; Park and Muandet, 2020). Although time series are one of the primary fields of application, consistency results for the conditional mean embedding have been limited to the case of independent data until now. As an application of the results of this paper, we prove standard consistency statements for dependent data.

Recent results (Klus et al., 2018a, 2019) show that eigenfunctions of Markov transition operators can be approximated based on conditional mean embeddings and corresponding autocovariance operators. Moreover, it was also discovered in this work that a large family of kernel-based spectral analysis and model order reduction techniques for stochastic processes and dynamical systems (see Kutz et al., 2016; Klus et al., 2018b; Wu and Noé, 2019, for an overview) implicitly approximates the spectral decomposition of an RKHS Markov transition operator which is expressed in terms of kernel autocovariance operators. Different versions of these methods are popular in fluid dynamics (Schmid, 2010; Tu et al., 2014; Williams et al., 2015a,b), signal processing (Molgedey and Schuster, 1994), machine learning (Harmeling et al., 2003; Kawahara, 2016; Hua et al., 2017), and molecular dynamics (Pérez-Hernández et al., 2013; Schwantes and Pande, 2015) under the names *dynamic mode decomposition* and *time-lagged independent component analysis*. Until now, a full statistical convergence analysis of these techniques has not been conducted to the best of our knowledge. A theoretical examination of kernel autocovariance operators contributes significantly to the understanding of kernel-based versions of the aforementioned approaches.

The theory of weakly dependent random processes taking values in infinite-dimensional Banach or Hilbert spaces has become increasingly important especially due to applications in the field of *functional data analysis* (Hörmann and Kokoszka, 2010; Horváth and Kokoszka, 2012; Hsing and Eubank, 2015). In infinite-dimensional statistics, the estimation of covariance and cross-covariance operators (Baker, 1970, 1973) is a fundamental concept. Under parametric model assumptions about the process, the estimation of covariance and autocovariance operators has been examined in various scenarios. For autoregressive (AR) processes in Banach and Hilbert spaces, weak convergence and asymptotic normality has been established (Bosq, 2000, 2002; Mas, 2002; Dehling and Sharipov, 2005; Mas, 2006). Soltani and Hashemi (2011) add the assumption of periodic correlation for AR processes in Hilbert spaces. Allam and Mourid (2014, 2019) provide rates for almost sure convergence of covariance operators in Hilbert–Schmidt norm for an AR process with random coefficients.

For processes in an L^2 function space, the weak convergence of covariance operators has been examined by Kokoszka and Reimherr (2013) under the assumption

of L^4 - m *approximability* (a concept generalizing m -dependence which includes certain autoregressive and nonlinear models, see Hörmann and Kokoszka, 2010) in the context of functional principal component analysis. The importance of autocovariance operators of stationary processes in the L^2 space context is underlined by the concepts of *spectral density operators* (Panaretos and Tavakoli, 2013b,a) as well as *dynamic functional principal components analysis* (Hörmann et al., 2015).

In contrast to the previously mentioned work on processes taking values in Banach and Hilbert spaces, we will consider a stationary process $(X_t)_{t \in \mathbb{Z}}$ taking values in a Polish space E . We consider autocovariance operators of the corresponding embedded Hilbert space process

$$(\varphi(X_t))_{t \in \mathbb{Z}},$$

where $\varphi: E \rightarrow \mathcal{H}$ is the feature map of a reproducing kernel Hilbert space (RKHS) \mathcal{H} (see Section 2.2 for details). This scenario directly falls in line with the classic setting in learning theory, which has led to celebrated results and numerous applications in case of independent and identically distributed data (see for example Cucker and Smale, 2002; Steinwart and Christmann, 2008).

To show consistency of any empirical statistic of the process $(\varphi(X_t))_{t \in \mathbb{Z}}$, we face the challenge that properties of the E -valued process $(X_t)_{t \in \mathbb{Z}}$ must transfer accordingly to the embedded version of the process in the Hilbert space. In this situation, it is unlikely that we can transfer parametric properties of $(X_t)_{t \in \mathbb{Z}}$ to the nonlinearly embedded process $(\varphi(X_t))_{t \in \mathbb{Z}}$ without additional assumptions about the feature map φ . In contrast to the previously mentioned literature, we will consider a more general setting without a parametric model assumption about the underlying process $(X_t)_{t \in \mathbb{Z}}$.

Recently, Blanchard and Zadorozhnyi (2019) derived a Bernstein-type inequality for Hilbert space processes for a class of mixing properties called \mathcal{C} -mixing (Maume-Deschamps, 2006). As a special case, the authors show that under restrictive Lipschitz conditions on the feature map φ , this mixing property is preserved under the RKHS embedding of a so-called τ -mixing process. The derived inequality is then used to obtain concentration bounds for the context of RKHS learning theory, including covariance operator estimation without a time lag. To the best of our knowledge, this is the first time that RKHS covariance operator estimation is addressed in the context of weakly dependent data. As described for example by Hang and Steinwart (2017), the class of \mathcal{C} -mixing coefficients is only partly related to the classical strong mixing coefficients found in the literature (Doukhan, 1994; Bradley, 2005), which we will consider in this paper, in particular the concept of α -mixing.

The contributions of this paper are:

- (1) A mathematical framework for kernel autocovariance operators of a stationary discrete-time process $(X_t)_{t \in \mathbb{Z}}$ taking values in an abstract Polish space.
- (2) An investigation of ergodicity and strong mixing in the context of the RKHS-embedded process $(\varphi(X_t))_{t \in \mathbb{Z}}$ under minimal requirements on the RKHS feature map φ . In particular, our assumptions are easily justifiable for further application in work on RKHS time series.

- (3) An asymptotic and nonasymptotic estimation error analysis for empirical kernel autocovariance operators based on single trajectories of the process $(X_t)_{t \in \mathbb{Z}}$ in a form that is accessible for work on related topics.
- (4) Applications of our results to
 - (a) consistency of kernel PCA with dependent data;
 - (b) consistency of the conditional mean embedding of transition probabilities under the typical technical assumptions; and
 - (c) the estimation of Markov transition operators and their role in a family of spectral analysis methods for dynamical systems.

This paper is structured as follows. In Section 2 we recall the required preliminaries from spectral theory, Bochner integration, and reproducing kernel Hilbert spaces and formulate our working assumptions. Section 3 addresses the strong law of large numbers of empirical kernel autocovariance operators under an ergodicity hypothesis. We introduce strong mixing and derive standard probabilistic limit results including the central limit theorem in Section 4. General concentration bounds for the estimation error with mixing processes can be found in Section 5, while an extension of these results to the special case of Gaussian kernels is given in Section 6. Based on these results, we highlight applications to kernel PCA from dependent data (Section 7), the conditional mean embedding (Section 8) and the approximation of Markov transition operators (Section 9). We conclude our work in Section 10.

2. PRELIMINARIES

2.1. General notation. We give an overview of our notation and collect well-known facts from operator theory and probability theory. For details, we refer the reader to [Reed and Simon \(1980\)](#) and [Kallenberg \(2002\)](#). In what follows, we write B for a separable real Banach space with norm $\|\cdot\|_B$, and H for a separable real Hilbert space with inner product $\langle \cdot, \cdot \rangle_H$. $L(B)$ stands for the Banach space of bounded linear operators on B equipped with the operator norm $\|\cdot\|$. The expression $H \otimes H$ denotes the tensor product space: $H \otimes H$ is the Hilbert space completion of the algebraic tensor product with respect to the inner product $\langle x_2 \otimes x_1, x'_2 \otimes x'_1 \rangle_{H \otimes H} = \langle x_1, x'_1 \rangle_H \langle x_2, x'_2 \rangle_H$. For $x_1, x_2 \in H$, we interpret the element $x_2 \otimes x_1 \in H \otimes H$ as the linear rank-one operator $x_2 \otimes x_1 : H \rightarrow H$ defined by $x \mapsto \langle x, x_1 \rangle_H x_2$. Whenever $(e_i)_{i \in I}$ is a complete orthonormal system (CONS) in H , $(e_i \otimes e_j)_{i, j \in I}$ is a CONS in $H \otimes H$. Thus, when H is separable, $H \otimes H$ is separable.

Every compact operator A on H admits a *singular value decomposition*, that is, there exist orthonormal systems $\{u_i\}_{i \in J}$ and $\{v_i\}_{i \in J}$ in H such that

$$(2.1) \quad A = \sum_{i \in J} \sigma_i(A) u_i \otimes v_i,$$

where $(\sigma_i(A))_{i \in J}$ are the strictly positive and nonincreasingly ordered (including multiplicities) singular values of A with an appropriate (either countably infinite or

finite) index set J . The convergence in (2.1) is meant with respect to the operator norm. The *rank* of A is defined as the cardinality of J .

For $1 \leq p \leq \infty$, the p -Schatten class $S_p(H)$ consists of all compact operators A on H such that the norm $\|A\|_{S_p(H)} := \|(\sigma_i(A))_{i \in J}\|_{\ell_p}$ is finite. Here $\|(\sigma_i(A))_{i \in J}\|_{\ell_p}$ denotes the ℓ_p sequence space norm of the sequence of singular values. The spaces $S_p(H)$ are two-sided ideals in $L(H)$. Moreover $\|A\| \leq \|A\|_{S_q(H)} \leq \|A\|_{S_p(H)}$ holds for $p \leq q$, i.e., $S_p(H) \subseteq S_q(H)$. For $p = 2$, we obtain the Hilbert space of *Hilbert–Schmidt operators* on H equipped with the inner product $\langle A_1, A_2 \rangle_{S_2(H)} = \text{Tr}(A_1^* A_2)$. For $p = 1$, we obtain the Banach algebra of *trace class operators*. For $p = \infty$, we obtain the Banach algebra of compact operators equipped with the operator norm $\|A\| = \|A\|_{S_\infty(H)}$. The Schatten classes are the completion of finite-rank operators (i.e., operators in $\text{span}\{x \otimes x' \mid x, x' \in H\}$) with respect to the corresponding norm.

We will make frequent use of the fact that the tensor product space $H \otimes H$ can be isometrically identified with the space of Hilbert–Schmidt operators on H , i.e., we have $S_2(H) \simeq H \otimes H$. For elements $x_1, x'_1, x_2, x'_2 \in H$, we have the relation $\langle x_2 \otimes x_1, x'_2 \otimes x'_1 \rangle_{H \otimes H} = \langle x_2 \otimes x_1, x'_2 \otimes x'_1 \rangle_{S_2(H)}$, where the tensors are interpreted as rank-one operators as described above. This property extends to $\text{span}\{x \otimes x' \mid x, x' \in H\}$ by linearity and defines a linear isometric isomorphism between $H \otimes H$ and $S_2(H)$, which can be seen by considering Hilbert–Schmidt operators in terms of their singular value decompositions.

For any topological space E , we will write $\mathcal{F}_E = \mathcal{B}(E)$ for its associated Borel field. For any collection of sets \mathcal{M} , $\sigma(\mathcal{M})$ denotes the intersection of all σ -fields containing \mathcal{M} . For any σ -field \mathcal{F} and countable index set I , we write $\mathcal{F}^{\otimes I}$ as the product σ -field (i.e., the smallest σ -field with respect to which all coordinate projections on E^I are measurable). Note that when E is Polish (i.e., separable and completely metrizable), we have $\mathcal{B}(E^I) = \mathcal{B}(E)^{\otimes I}$, i.e. the Borel field on the product space generated by the product topology and the product of the individual Borel fields are equal. Put differently, the Borel field operator and the product field operator are compatible with respect to product spaces (Dudley, 2002, Proposition 4.1.17). Moreover, E^I equipped with the product topology is Polish.

In this paper, we will consider a stochastic process $(X_t)_{t \in \mathbb{Z}}$ on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with values in the observation space (E, \mathcal{F}_E) , which we assume to be Polish. We will also assume without loss of generality that $(\Omega, \mathcal{F}, \mathbb{P})$ is rich enough to support all performed operations in this paper. For a finite number of random variables ξ_1, \dots, ξ_n defined on $(\Omega, \mathcal{F}, \mathbb{P})$ with values in E , we write $\mathcal{L}(\xi_1, \dots, \xi_n)$ for the *finite-dimensional law*, i.e., *pushforward measure* on $(E^n, \mathcal{B}(E^n))$ induced by ξ_1, \dots, ξ_n .

Assumption 1 (Stationarity). *We assume that the process $(X_t)_{t \in \mathbb{Z}}$ is stationary in the sense that all finite-dimensional laws are identical, that is, $\mathcal{L}(X_{t_1}, \dots, X_{t_r}) = \mathcal{L}(X_{t_1+\eta}, \dots, X_{t_r+\eta})$ for all $t_1, \dots, t_r \in \mathbb{Z}$, $r \in \mathbb{N}$, and time lags $\eta \in \mathbb{N}$.*

For any separable Banach space B , let $L^p(\Omega, \mathcal{F}, \mathbb{P}; B)$ denote the space of strongly $\mathcal{F} - \mathcal{F}_B$ measurable and Bochner p -integrable functions $f: \Omega \rightarrow B$ for $1 \leq p \leq \infty$ (see for example Diestel and Uhl, 1977). In the case of $B = \mathbb{R}$, we simply write

$L^p(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}) = L^p(\mathbb{P})$ for the standard space of real-valued Lebesgue p -integrable functions.

2.2. Reproducing kernel Hilbert spaces. We will briefly introduce the concept of reproducing kernel Hilbert spaces. For a detailed discussion of this topic, we refer the reader to [Berlinet and Thomas-Agnan \(2004\)](#), [Steinwart and Christmann \(2008\)](#) and [Saitoh and Sawano \(2016\)](#). To distinguish standard Hilbert spaces from reproducing kernel Hilbert spaces, we will use the script letter \mathcal{H} for the latter.

Definition 2.1 (Reproducing kernel Hilbert space). *Let E be a set and \mathcal{H} a space of functions from E to \mathbb{R} . Then \mathcal{H} is called a reproducing kernel Hilbert space (RKHS) with corresponding inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ if there exists function $k: E \times E \rightarrow \mathbb{R}$ such that*

- (i) $\langle f, k(x, \cdot) \rangle_{\mathcal{H}} = f(x)$ for all $f \in \mathcal{H}$ (reproducing property), and
- (ii) $\mathcal{H} = \overline{\text{span}\{k(x, \cdot) \mid x \in E\}}$, where the completion is with respect to the RKHS norm.

We call k the reproducing kernel of \mathcal{H} .

It follows in particular that $k(x, x') = \langle k(x, \cdot), k(x', \cdot) \rangle_{\mathcal{H}}$. The canonical feature map $\varphi: E \rightarrow \mathcal{H}$ is given by $\varphi(x) := k(x, \cdot)$. Thus, we obtain $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathcal{H}}$. Every RKHS has a unique symmetric and positive semi-definite kernel k with the reproducing property. Conversely, every symmetric positive semi-definite kernel k induces a unique RKHS with k as its reproducing kernel. In what follows, we will use the term *kernel* synonymously for reproducing kernel/symmetric positive semi-definite kernel for brevity.

We now impose a few restrictions on the considered RKHS, which we assume to be fulfilled for the remainder of this paper.

Assumption 2 (Separability). *The RKHS \mathcal{H} is separable. Note that for a Polish space E , the RKHSs induced by a continuous kernel $k: E \times E \rightarrow \mathbb{R}$ is always separable (see [Steinwart and Christmann, 2008](#), Lemma 4.33). For a more general treatment of conditions implying separability, see [Owhadi and Scovel \(2017\)](#).*

Assumption 3 (Measurability). *The canonical feature map $\varphi: E \rightarrow \mathcal{H}$ is $\mathcal{F}_E - \mathcal{F}_{\mathcal{H}}$ measurable. This is the case when $k(x, \cdot): E \rightarrow \mathbb{R}$ is $\mathcal{F}_E - \mathcal{F}_{\mathbb{R}}$ measurable for all $x \in E$. If this condition holds, then additionally all functions $f \in \mathcal{H}$ are $\mathcal{F}_E - \mathcal{F}_{\mathbb{R}}$ measurable and $k: E \times E \rightarrow \mathbb{R}$ is $\mathcal{F}_E^{\otimes 2} - \mathcal{F}_{\mathbb{R}}$ measurable (see [Steinwart and Christmann, 2008](#), Lemmas 4.24 and 4.25).*

Assumption 4 (Existence of second moments). *We have $\varphi(X_0) \in L^2(\Omega, \mathcal{F}, \mathbb{P}, \mathcal{H})$. Note that this is trivially the case whenever $\sup_{x \in E} k(x, x) < \infty$.*

2.3. Kernel mean embeddings & kernel covariance operators. We now introduce kernel mean embeddings and kernel covariance operators, which are simply the Bochner expectations and covariance operators of RKHS-embedded random variables.

For a random variable X on E satisfying $\varphi(X) \in L^1(\Omega, \mathcal{F}, \mathbb{P}; \mathcal{H})$, we call

$$\mu_X := \mu_{\mathcal{L}(X)} := \mathbb{E}[\varphi(X)] \in \mathcal{H}$$

the *kernel mean embedding* or simply *mean embedding* (Berlinet and Thomas-Agnan, 2004; Smola et al., 2007; Muandet et al., 2017) of X . For every $f \in \mathcal{H}$, the mean embedding satisfies $\mathbb{E}[f(X)] = \langle f, \mu_X \rangle_{\mathcal{H}}$.

Definition 2.2 (Kernel (cross-)covariance operator). *For two random variables X, Y on E satisfying $\varphi(X), \varphi(Y) \in L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathcal{H})$, we call the trace class operator $C_{YX}: \mathcal{H} \rightarrow \mathcal{H}$ defined by*

$$C_{YX} = \mathbb{E}[(\varphi(Y) - \mu_Y) \otimes (\varphi(X) - \mu_X)]$$

the kernel cross-covariance operator of X and Y . We call C_{XX} the kernel covariance operator of X .

For all $f, g \in \mathcal{H}$, we have $\text{Cov}[f(X), g(Y)] = \langle g, C_{YX}f \rangle_{\mathcal{H}}$ as well as $C_{YX} = C_{XY}^*$. As a consequence, C_{XX} is self-adjoint, positive semi-definite and trace class. For additional information about (cross-)covariance operators of Hilbertian random variables, see for example Parthasarathy (1967), Baker (1970), and Baker (1973).

In the literature, the covariance operator is sometimes used as a generalization of the uncentered second moment and therefore defined without centering of the random variables $\varphi(X)$ and $\varphi(Y)$ (Prokhorov, 1956; Parthasarathy, 1967; Bharucha-Reid, 1972; Fukumizu et al., 2013).

Definition 2.3 (Kernel autocovariance operator). *Let $(X_t)_{t \in \mathbb{Z}}$ be a stationary stochastic process with values on E such that $\varphi(X_0) \in L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathcal{H})$. Let $\eta \in \mathbb{N}$. We call $C(\eta) := C_{X_\eta X_0} = C_{X_{t+\eta} X_t} \forall t \in \mathbb{Z}$ the kernel autocovariance operator of the process $(X_t)_{t \in \mathbb{Z}}$ with respect to the time lag η .*

2.4. Product kernels and Hilbert–Schmidt operators. The tensor product space $\mathcal{H} \otimes \mathcal{H} \simeq S_2(\mathcal{H})$ is itself an RKHS with the corresponding canonical feature map $\varphi \otimes \varphi: E \times E \rightarrow \mathcal{H} \otimes \mathcal{H}$ given by $\varphi \otimes \varphi(x_1, x_2) := \varphi(x_1) \otimes \varphi(x_2)$ (Steinwart and Christmann, 2008, Lemma 4.6). The corresponding kernel of $\mathcal{H} \otimes \mathcal{H}$ is the product kernel $k \cdot k: E^2 \times E^2 \rightarrow \mathbb{R}$.

The estimation of the uncentered kernel autocovariance operator can therefore be interpreted as the estimation of a kernel mean on the product RKHS $\mathcal{H} \otimes \mathcal{H}$. In particular, we can write $C(\eta)$ as the kernel mean embedding of the joint distribution $\mathcal{L}(X_\eta, X_0)$ on the measurable space $(E \times E, \mathcal{F}_E \otimes \mathcal{F}_E)$ using the product feature map $\varphi \otimes \varphi$. That is, we have

$$\mu_{\mathcal{L}(X_\eta, X_0)} = \mathbb{E}[\varphi(X_\eta) \otimes \varphi(X_0)],$$

which is exactly the uncentered kernel autocovariance operator of X .

Thus, the analysis of the estimation of the uncentered autocovariance operator covers the problem of estimating the kernel mean $\mu_{\mathcal{L}(X_0)}$ of the marginal $\mathcal{L}(X_0)$. In fact, by considering kernels on the product space $E \times E$ instead of E , we need to account for the challenge that appropriate statistical properties of the process $(X_t)_{t \in \mathbb{Z}}$ (such as ergodicity, mixing, or decay of correlations) have to transfer to the product process $(X_{t+\eta}, X_t)_{t \in \mathbb{Z}}$ on $E \times E$ in order to provide results. We may

therefore concentrate directly on the estimation of uncentered autocovariance operators based on $E \times E$ instead on the estimation of kernel mean embeddings on E . We emphasize that all of our results directly transfer to the much simpler case of estimating the kernel mean $\mu_{\mathcal{L}(X_0)}$ from dependent data by simply replacing the product space $E \times E$ with E and the product feature map $\varphi \otimes \varphi$ with φ in what follows.

Based on this consideration, we make a centering assumption.

Assumption 5 (Centered process). *Without loss of generality, we assume that the embedded process is centered, i.e., $\mu_X = \mathbb{E}[\varphi(X_0)] = 0$. In this case, the centered and the uncentered autocovariance operator coincide:*

$$C(\eta) = \mathbb{E}[\varphi(X_\eta) \otimes \varphi(X_0)].$$

Whenever $\varphi(X_0)$ is not centered, the centered autocovariance operator can be computed by using the centered feature map $\varphi(\cdot) - \mu_{\mathcal{L}(X_0)}$, which is usually replaced with an empirical centering in practical applications.

In what follows, we will repeatedly use the shorthand

$$C_n(\eta) := \frac{1}{n} \sum_{t=1}^n \varphi(X_{t+\eta}) \otimes \varphi(X_t)$$

for the empirical estimate of $C(\eta)$ based on $n + \eta$ consecutive time steps of the process $(X_t)_{t \in \mathbb{Z}}$.

3. STRONG LAW OF LARGE NUMBERS

We now address the strong law of large numbers for the estimator $C_n(\eta)$. To this end, we briefly introduce the concept of measure-preserving dynamical systems and ergodicity. For details, the reader may refer for example to [Petersen \(1983\)](#). We assume without loss of generality that the underlying probability space $(\Omega, \mathcal{F}, \mathbb{P})$ describing $(X_t)_{t \in \mathbb{Z}}$ is the *canonical probability space*, i.e., $\Omega = E^{\mathbb{Z}}$ and $\mathcal{F} = \mathcal{F}_E^{\otimes \mathbb{Z}}$. In this case, we express the process as the family of *coordinate projections* on Ω : for $\omega = (\omega_t)_{t \in \mathbb{Z}} \in \Omega$, we can write $X_t(\omega) = \omega_t = X_0(T^t \omega)$ for all $t \in \mathbb{Z}$, where T is the left-shift operator on Ω defined by $(T\omega)_i = \omega_{i+1}$ for all $i \in \mathbb{Z}$. Note that by stationarity of $(X_t)_{t \in \mathbb{Z}}$, the shift T is measure preserving in the sense that $\mathbb{P}[T^{-1}M] = \mathbb{P}[M]$ for all $M \in \mathcal{F}_E^{\otimes \mathbb{Z}}$. We call $(X_t)_{t \in \mathbb{Z}}$ *ergodic* whenever T is *ergodic in the measure theoretical sense* i.e., for all sets $M \in \mathcal{F}_E^{\otimes \mathbb{Z}}$, we have that $T^{-1}M = M$ implies either $\mathbb{P}[M] = 0$ or $\mathbb{P}[M] = 1$.

We show that for any fixed time lag $\eta \in \mathbb{N}$, the kernel autocovariance operator $C(\eta)$ can be estimated almost surely from realizations of $(X_t)_{t \in \mathbb{Z}}$ whenever the process is ergodic on $(\Omega, \mathcal{F}, \mathbb{P})$ as a consequence of the following generalized version of Birkhoff's ergodic theorem.

Theorem 3.1 ([Beck and Schwartz \(1957\)](#), Theorem 6.). *Let B be a reflexive Banach space and T an ergodic measure-preserving transformation on $(\Omega, \mathcal{F}, \mathbb{P})$. Then for each $f \in L^1(\Omega, \mathcal{F}, \mathbb{P}; B)$,*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n f(T^i \omega) = \mathbb{E}[f],$$

where the convergence holds \mathbb{P} -a.e. with respect to $\|\cdot\|_B$.

We can directly apply this result to obtain almost sure convergence of the empirical estimate of $C(\eta)$ in the case that $(X_t)_{t \in \mathbb{Z}}$ is ergodic.

Corollary 3.2 (Strong consistency). *Let $(X_t)_{t \in \mathbb{Z}}$ be a stationary and ergodic process defined on $(\Omega, \mathcal{F}, \mathbb{P})$ with values in a Polish space E . Then*

$$\lim_{n \rightarrow \infty} C_n(\eta) = C(\eta),$$

where the convergence is \mathbb{P} -a.e. with respect to $\|\cdot\|_{S_2(\mathcal{H})}$.

Proof. The time-lagged product process $(X_t, X_{t+\eta})_{t \in \mathbb{Z}}$ on $E \times E$ can be expressed via the projection tuple $(X_t, X_{t+\eta})(\omega) = (X_0, X_\eta)(T^t \omega)$. By construction, (X_0, X_η) is $\mathbb{P} - \mathcal{F}_E \otimes \mathcal{F}_E$ measurable. Note that because of Assumption 3 and Assumption 4 the product feature map $\varphi \otimes \varphi$ given by $(x, y) \mapsto \varphi(y) \otimes \varphi(x)$ is an element of $L^1(E \times E, \mathcal{F}_E \otimes \mathcal{F}_E, \mathcal{L}(X_0, X_\eta); S_2(\mathcal{H}))$, where $S_2(\mathcal{H})$ is clearly reflexive. Therefore, it holds that the composition $\varphi \otimes \varphi \circ (X_0, X_\eta): \Omega \rightarrow S_2(\mathcal{H})$ given by $\omega \mapsto (X_0, X_\eta)(\omega) \mapsto \varphi(X_\eta) \otimes \varphi(X_0)(\omega)$ is an element of $L^1(\Omega, \mathcal{F}, \mathbb{P}; S_2(\mathcal{H}))$.

The statement follows immediately from the fact that we choose $\varphi \otimes \varphi \circ (X_0, X_\eta)$ as the observable f in Theorem 3.1 and obtain

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{t=1}^n \varphi \otimes \varphi \circ (X_0, X_\eta) \circ T^t = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{t=1}^n \varphi(X_{t+\eta}) \otimes \varphi(X_t) = C(\eta),$$

where the convergence is \mathbb{P} -a.e. in $S_2(\mathcal{H})$. ■

Remark 3.3 (Convergence in Schatten norms). Corollary 3.2 also yields \mathbb{P} -a.e. convergence $C_n(\eta) \rightarrow C(\eta)$ in $S_p(\mathcal{H})$ for all $p \geq 2$. Note that $S_1(\mathcal{H})$ is reflexive if and only if \mathcal{H} is finite-dimensional (see for example Simon, 2005, Theorem 3.2). However, in the finite-dimensional case, all Schatten classes coincide and the question for convergence in Schatten norms becomes trivial. In the general case, it is not clear whether the reflexivity assumption in Theorem 3.1 is not only sufficient but also necessary for a convergence to hold. To the best of our knowledge, no stronger generalization results of Birkhoff's ergodic theorem for Banach-valued random variables exist.

4. ASYMPTOTIC ERROR BEHAVIOR

In order to prove standard results for the asymptotic statistical behavior of $C_n(\eta)$, we first recall the basic notions of strong mixing in statistics (see for example Bradley, 2005). Note that we directly formulate the definition below for stationary processes, while mixing can also be defined for nonstationary processes.

Definition 4.1 (α -mixing). *For σ -fields $\mathcal{F}_1, \mathcal{F}_2 \subseteq \mathcal{F}$, we define*

$$\alpha(\mathcal{F}_1, \mathcal{F}_2) := \sup_{A \in \mathcal{F}_1, B \in \mathcal{F}_2} |\mathbb{P}[A \cap B] - \mathbb{P}[A]\mathbb{P}[B]|.$$

For a stationary process $(X_t)_{t \in \mathbb{Z}}$, we furthermore define

$$\alpha(n) := \alpha((X_t)_{t \in \mathbb{Z}}, n) := \alpha(\mathcal{F}_{-\infty}^0, \mathcal{F}_n^\infty) \quad n \in \mathbb{Z},$$

where $\mathcal{F}_l^m := \sigma(X_t, l \leq t \leq m)$ denotes the σ -field generated by the process $(X_t)_{t \in \mathbb{Z}}$ for time horizons $-\infty \leq l \leq m \leq \infty$.

The process is called α -mixing or *strongly mixing*, when $\alpha(n) \rightarrow 0$ as $n \rightarrow \infty$. In this case, the convergence rate of $\alpha(n)$ is called the *mixing rate* of the associated process. In this paper, we will not focus on the various alternative strong mixing coefficients which are frequently used in statistics (Doukhan, 1994; Bradley, 2005), since α -mixing is the weakest concept among the strong mixing coefficients and covers a wide range of processes in practice.

Remark 4.2 (Terminology). The concept of *strong mixing coefficients* is typically much stronger than the *strong mixing* considered in ergodic theory (Petersen, 1983). Also note that we define the α -mixing coefficient for stationary processes. It can also be defined for nonstationary processes, while mixing in the ergodic theoretical sense typically arises from dynamical systems induced by measure-preserving transformations and is therefore primarily used in the context of stationary stochastic processes.

Example 4.3 (Mixing processes). A wide range of mixing processes can be found in Doukhan (1994) and Bradley (2005). We list some important examples here.

- (1) Irreducible and aperiodic stationary Markov processes are α -mixing (in fact, a stronger mixing property called β -mixing or *absolute regularity* holds, see for example Bradley (2005, Corollary 2.6)).
- (2) Stationary Markov processes satisfying *geometric ergodicity* (for details see Meyn and Tweedie, 2012, Chapter 15) are α -mixing with $\alpha(n) = O(\exp(-cn))$ for some $c > 0$, see Bradley (2005, Theorem 2.7).
- (3) Some stochastically perturbed dynamical systems can be written as stationary Markov processes (Kallenberg, 2002, Proposition 7.6). Therefore (1) and (2) apply in this case. Conditions on the dynamical system under which the induced Markov process is geometrically ergodic (i.e., geometrically α -mixing in the sense of (2)) are given by Doukhan (1994, Section 2.4)
- (4) One can show that a time-discretized version of a diffusion process expressed as a stochastic differential equation results in a geometrically ergodic Markov process (Lacour, 2008).
- (5) Under some requirements, commonly used linear and nonlinear process models on finite-dimensional vector spaces including AR, ARMA, ARCH, and GARCH are α -mixing with $\alpha(n) = O(\exp(-cn))$ for some $c > 0$, see Doukhan (1994, Section 2.4) and Fan and Yao (2003, Section 2.6.1).

We make use of the following classical lemma which we prove for completeness. It ensures that measurable transformations of a finite number of components of a mixing process preserve mixing rates. It is of crucial importance to us since it guarantees that RKHS-embedded versions of mixing processes are again mixing with the same rates.

Lemma 4.4 (Transformed processes are mixing). *Let $(X_t)_{t \in \mathbb{Z}}$ defined on $(\Omega, \mathcal{F}, \mathbb{P})$ be a stationary process with values in a Polish space E equipped with its Borel σ -field*

\mathcal{F}_E . Let F be another Polish space equipped with its Borel σ -field \mathcal{F}_F . Let $k \in \mathbb{N}$ and $h: E^k \rightarrow F$ be $\mathcal{F}_E^{\otimes k} - \mathcal{F}_F$ measurable. Then for the process $(H_t)_{t \in \mathbb{Z}}$ given by

$$H_t := h(X_{t-k+1}, X_{t-k+2}, \dots, X_t)$$

for all $t \in \mathbb{Z}$, we have

$$(4.1) \quad \alpha((H_t)_{t \in \mathbb{Z}}, n) \leq \alpha((X_t)_{t \in \mathbb{Z}}, n - k + 1)$$

for all $n \in \mathbb{Z}$. In particular, if $(X_t)_{t \in \mathbb{Z}}$ is α -mixing, then $(H_t)_{t \in \mathbb{Z}}$ is α -mixing with the same mixing rate as $(X_t)_{t \in \mathbb{Z}}$.

Proof. Let $\mathcal{H}_t^m := \sigma(H_t, l \leq t \leq m) \subseteq \mathcal{F}$ be the σ -field generated by $(H_t)_{t \in \mathbb{Z}}$. By construction, we have $\mathcal{H}_{-\infty}^0 \subseteq \mathcal{F}_{-\infty}^0$ as well as $\mathcal{H}_n^\infty \subseteq \mathcal{F}_{n-k+1}^\infty$ for all $n \in \mathbb{N}$. The assertion (4.1) follows from Definition 4.1. \blacksquare

Corollary 4.5 (Mixing process in product RKHS).

- (a) Let $(X_t)_{t \in \mathbb{Z}}$ be a stationary α -mixing process with values in a Polish space E equipped with Borel σ -field \mathcal{F}_E . Let $\eta \in \mathbb{N}$ be a fixed time lag. Then the $E \times E$ -valued time-lagged product process $(X_t, X_{t+\eta})_{t \in \mathbb{Z}}$ is α -mixing.
- (b) Under Assumptions 2 and 3, the $S_2(\mathcal{H})$ -valued embedded process $(\varphi(X_{t+\eta}) \otimes \varphi(X_t))_{t \in \mathbb{Z}}$ is also α -mixing.

In both cases, the convergence rates of the corresponding mixing coefficients are preserved.

Proof. We use the preceding Lemma 4.4 and set $h: E^k \rightarrow E^2$ to be the map

$$(X_{t-k+1}, X_{t-k+2}, \dots, X_t) \mapsto (X_{t-\eta}, X_t),$$

where $\eta := k-1$. Note that this map is $\mathcal{F}_E^{\otimes k} - \mathcal{F}_E^{\otimes 2}$ measurable by construction, thus (a) follows. For (b), we set h to be the product feature map $\varphi \otimes \varphi: E \times E \rightarrow \mathcal{H} \otimes \mathcal{H}$ and apply (a). \blacksquare

We can now justify the embedded RKHS process $(\varphi(X_{t+\eta}) \otimes \varphi(X_t))_{t \in \mathbb{Z}}$ as an α -mixing process and apply the asymptotic theory of mixing processes to show how kernel autocovariance operators can be estimated from realizations of $(X_t)_{t \in \mathbb{Z}}$.

For brevity, we will introduce the shorthand

$$(4.2) \quad \xi_t := (\varphi(X_{t+\eta}) \otimes \varphi(X_t)) - C(\eta)$$

for $t \in \mathbb{Z}$ and fixed $\eta \in \mathbb{N}$. Then $(\xi_t)_{t \in \mathbb{Z}}$ is a stationary and centered $S_2(\mathcal{H})$ -valued process which is mixing with the same rates as $(X_t)_{t \in \mathbb{Z}}$ by Corollary 4.5. Note that with this notation, we have $C_n(\eta) - C(\eta) = \frac{1}{n} \sum_{t=1}^n \xi_t$.

We will frequently make use of the fact that whenever $\sup_{x \in E} k(x, x) = c < \infty$, then we have \mathbb{P} -a.e.

$$(4.3) \quad \begin{aligned} \|\xi_t\|_{S_2(\mathcal{H})} &\leq 2 \sup_{x_1, x_2 \in E} \|\varphi(x_1)\|_{\mathcal{H}} \|\varphi(x_2)\|_{\mathcal{H}} \\ &= 2 \sup_{x_1, x_2 \in E} k(x_1, x_1)^{1/2} k(x_2, x_2)^{1/2} \\ &= 2c \end{aligned}$$

for all $t \in \mathbb{Z}$. Several properties of the estimation error $C_n(\eta) - C(\eta)$ can be proven by applying results from the asymptotic theory of weakly dependent Banach- and Hilbert space valued processes. We begin with one of the strongest results of this type which is an approximation of $n(C_n(\eta) - C(\eta))$ by a Gaussian process. To this end, let $L(n) := \max(\log n, 1)$ for $n \in \mathbb{N}$.

Theorem 4.6 (Almost sure invariance principle). *Let $(X_t)_{t \in \mathbb{Z}}$ be stationary and α -mixing s.t. $\sum_{t \in \mathbb{Z}} \alpha(t) < \infty$ and let $\sup_{x \in E} k(x, x) < \infty$. Then the operator $T: \mathbb{S}_2(\mathcal{H}) \rightarrow \mathbb{S}_2(\mathcal{H})$ defined by*

$$(4.4) \quad T := \mathbb{E}[\xi_0 \otimes \xi_0] + \sum_{t=1}^{\infty} \mathbb{E}[\xi_0 \otimes \xi_t] + \sum_{t=1}^{\infty} \mathbb{E}[\xi_t \otimes \xi_0]$$

is trace class. Furthermore, there exists a Gaussian measure $\mathcal{N}(0, T)$ on $\mathbb{S}_2(\mathcal{H})$ and a sequence of i.i.d. $\mathbb{S}_2(\mathcal{H})$ -valued Gaussian random variables $(Z_t)_{t \in \mathbb{Z}} \sim \mathcal{N}(0, T)$ defined on $(\Omega, \mathcal{F}, \mathbb{P})$ such that we have \mathbb{P} -a.e.

$$\left\| n(C_n(\eta) - C(\eta)) - \sum_{i=1}^n Z_i \right\|_{\mathbb{S}_2(\mathcal{H})} = o\left(\sqrt{nL(L(n))}\right).$$

Proof. The assumptions ensure that $(\xi_t)_{t \in \mathbb{Z}}$ is \mathbb{P} -a.e. bounded and has summable mixing coefficients by Corollary 4.5. We can directly apply the almost sure invariance principle from [Dedecker and Merlevède \(2010, Corollary 1\)](#) to $(\xi_t)_{t \in \mathbb{Z}}$, which yields the assertion. \blacksquare

A strongly related statement is a standard central limit theorem for weakly dependent sequences which ensures asymptotic normality in the space $\mathbb{S}_2(\mathcal{H})$.

Theorem 4.7 (Central limit theorem). *Under the assumptions of Theorem 4.6, the laws of the sequence $\sqrt{n}(C_n(\eta) - C(\eta))$ converge weakly to a Gaussian measure $\mathcal{N}(0, T)$ on $\mathbb{S}_2(\mathcal{H})$ with covariance operator T defined by (4.4).*

Proof. By our previous analysis, the process $(\xi_t)_{t \in \mathbb{Z}}$ satisfies all assumptions of the central limit theorem by [Merlevède et al. \(1997, Corollary 1\)](#). The above assertions follow directly. \blacksquare

The next result is a compact law of the iterated logarithm. It ensures that an appropriately rescaled version of the estimation error approximates a compact limiting set almost surely. Additionally, it characterizes this set as the accumulation points of the estimation error sequence and gives a norm bound in $\mathbb{S}_2(\mathcal{H})$ depending on the mixing rate. We define the shorthand $a_n := \sqrt{2L(L(n))}$. Let furthermore $\text{acc}(x_n) \in X$ denote the set of all accumulation points of a sequence $(x_n)_{n \in \mathbb{N}}$ in a topological space X .

Theorem 4.8 (Compact law of the iterated logarithm). *Let $(X_t)_{t \in \mathbb{Z}}$ be stationary and α -mixing s.t. $\sum_{t \in \mathbb{Z}} \alpha(t) < \infty$ and let $\sup_{x \in E} k(x, x) = c < \infty$. Then there exists a compact, convex and symmetric set $K \subseteq \mathbb{S}_2(\mathcal{H})$, such that \mathbb{P} -a.e.*

$$(4.5) \quad \lim_{n \rightarrow \infty} \text{dist} \left(\frac{\sqrt{n}(C_n(\eta) - C(\eta))}{a_n}, K \right) = 0$$

as well as \mathbb{P} -a.e.

$$(4.6) \quad \text{acc} \left(\frac{\sqrt{n}(C_n(\eta) - C(\eta))}{a_n} \right) = K.$$

Moreover, whenever $\sum_{t=1}^{\infty} \alpha(t - \eta) = M < \infty$, we have

$$(4.7) \quad \sup_{A \in K} \|A\|_{S_2(\mathcal{H})} = (4c^2 + 32c^2M)^{1/2}.$$

For the proof Theorem 4.8, see Appendix A.

Remark 4.9 (Optimality of mixing rate assumptions). Slightly more general quantile function conditions under which the original results for the derivation of our Theorem 4.7 were shown by (Merlevède et al., 1997, Theorem 4) are known to be necessary for a central limit theorem to hold. For additional information about the special case of real-valued random variables, see Doukhan et al. (1994, Section 4). For bounded random variables, the summability of the mixing coefficients is equivalent to the quantile condition used by Merlevède et al. (1997), see (Rio, 1995, Application 1). From this, similar optimality results can be derived for the law of the iterated logarithm in the real case (see also Rio, 1995).

5. CONCENTRATION BOUNDS

In addition to the previous asymptotic results, concentration properties for the estimation error can be derived by using concentration properties of mixing Hilbertian processes.

Theorem 5.1 (Error bound). *Let $(X_t)_{t \in \mathbb{Z}}$ be stationary and α -mixing with coefficient $(\alpha(t))_{t \in \mathbb{Z}}$. Let $\sup_{x \in E} k(x, x) = c < \infty$. Then for every $\epsilon > 0$, $\nu \in \mathbb{N}$, $n \leq 2$ and $q = 1, \dots, \lfloor n/2 \rfloor$ and $\delta \in (0, 1)$, we have*

$$\begin{aligned} \mathbb{P} \left[\|C_n(\eta) - C(\eta)\|_{S_2(\mathcal{H})} > \epsilon \right] &\leq 4\nu \exp \left(-\frac{(1-\delta)\epsilon^2 q}{32\nu c^2} \right) \\ &\quad + 22\nu q \left(1 + \frac{8c}{\epsilon(1-\delta)^{1/2}} \right)^{1/2} \alpha(\lfloor n/2q \rfloor) \\ &\quad + \frac{1}{\delta\epsilon^2} \sum_{j>\nu} \lambda_j, \end{aligned}$$

where $\lambda_j \in \mathbb{R}$ are the eigenvalues of the covariance operator $\Gamma: S_2(\mathcal{H}) \rightarrow S_2(\mathcal{H})$ defined by

$$(5.1) \quad \Gamma := \mathbb{E} \left[\left((\varphi(X_\eta) \otimes \varphi(X_0)) - C(\eta) \right) \otimes \left((\varphi(X_\eta) \otimes \varphi(X_0)) - C(\eta) \right) \right],$$

which we assume to be ordered nonincreasingly with their multiplicities.

Proof. As previously noted, the process $(\xi_t)_{t \in \mathbb{Z}}$ as given by (4.2) is stationary, centered, and α -mixing in $S_2(\mathcal{H})$. We can therefore apply the concentration bound given by Bosq (2000, Theorem 2.12) to the process $(\xi_t)_{t \in \mathbb{Z}}$. \blacksquare

The above bound requires an optimal trade-off between ν , q , and δ . Note that $\sum_{j>\nu} \lambda_j < \infty$ for every $\nu \in \mathbb{N}$, since Γ is trace class. Knowledge of the mixing rate $(\alpha(t))_{t \geq 1}$ and the decay of the eigenvalues $(\lambda_j)_{j \geq 1}$ of Γ allow to drastically simplify the bound and derive \mathbb{P} -a.e. convergence rates. Whenever $(\lambda_j)_{j \geq 1}$ and $(\alpha(t))_{t \geq 1}$ decay exponentially, a straightforward application of [Bosq \(2000, Corollary 2.4\)](#) can be used to obtain a sharper bound and \mathbb{P} -a.e. convergence rates. We will state this result here for completeness and show how the decay of $(\lambda_j)_{j \geq 1}$ can be precisely bounded for the special case of the Gaussian kernel in the next section.

Theorem 5.2 (Error bound & \mathbb{P} -a.e. convergence rate). *Let $(X_t)_{t \in \mathbb{Z}}$ be stationary and α -mixing with coefficient $(\alpha(t))_{t \in \mathbb{Z}}$. Let $\sup_{x \in E} k(x, x) = c < \infty$. Additionally, let $(\lambda_j)_{j \geq 0}$ be the nonincreasingly ordered eigenvalues (counted with multiplicities) of the covariance operator $\Gamma: \mathcal{S}_2(\mathcal{H}) \rightarrow \mathcal{S}_2(\mathcal{H})$ defined by [\(5.1\)](#).*

If there exist constants $r \in (0, 1)$ and $a > 0$ such that

$$\alpha(t) \leq ar^t \text{ and } \lambda_j < ar^j$$

for all $t, j \in \mathbb{N}$, then for every $\epsilon > 0$, there exist positive constants k_1 and k_2 independent from n , such that

$$\mathbb{P} \left[\|C_n(\eta) - C(\eta)\|_{\mathcal{S}_2(\mathcal{H})} > \epsilon \right] \leq k_1 \exp(-k_2 n^{1/3}).$$

In addition we have the convergence rate

$$\|C_n(\eta) - C(\eta)\|_{\mathcal{S}_2(\mathcal{H})} = O \left(\frac{(\log n)^{3/2}}{n^{1/2}} \right) \quad \mathbb{P}\text{-a.e.}$$

6. CONVERGENCE FOR THE GAUSSIAN KERNEL

[Theorem 5.1](#) and [Theorem 5.2](#) show that the two main quantities of fundamental interest for a bound of the estimation error $\|C_n(\eta) - C(\eta)\|_{\mathcal{S}_2(\mathcal{H})}$ are the mixing rate of $(X_t)_{t \in \mathbb{Z}}$ as well as the covariance of the law $\mathcal{L}(\varphi(X_\eta) \otimes \varphi(X_0))$ on the product RKHS $\mathcal{S}_2(\mathcal{H})$, which is given in terms of the eigenvalues of the covariance operator Γ acting on $\mathcal{S}_2(\mathcal{H})$ defined by [\(5.1\)](#).

While mixing rates can be assessed by imposing structural assumptions on $(X_t)_{t \in \mathbb{Z}}$, the analysis of Γ seems to be more intricate. We will now show that for the case that \mathcal{H} is induced by a Gaussian kernel, decay rates of the eigenvalues of Γ can be obtained.

Theorem 6.1. (Eigenvalue decay of Γ) *Let $E \subseteq \mathbb{R}^d$ and \mathcal{H} be the RKHS induced by the Gaussian kernel*

$$k(x, x') = \exp \left(\frac{-\|x - x'\|_{\mathbb{R}^d}^2}{2\sigma^2} \right)$$

for some bandwidth $\sigma > 0$. Let $(\lambda_j)_{j \geq 1}$ be the nonincreasingly ordered eigenvalues (counted with multiplicities) of the covariance operator Γ on $\mathcal{S}_2(\mathcal{H})$ defined by [\(5.1\)](#). Then the following decay rates hold.

- (1) *When E is compact, then $(\lambda_j)_{j \geq 1} = O(\exp(-cj \log j))$ for some constant $c > 0$.*

- (2) For arbitrary E , if $\mathcal{L}(X_0, X_\eta)$ is absolutely continuous with respect to the Lebesgue measure on $E \times E$ with joint density $p(x, y): E \times E \rightarrow \mathbb{R}$ satisfying $p(x, y) < B \exp(-\|(x, y)\|_{\mathbb{R}^{2d}}^2)$ for some constant $B > 0$, then $(\lambda_j)_{j \geq 1} = O(\exp(-cj))$ for some constant $c > 0$.
- (3) In any case, without additional assumptions about E and $\mathcal{L}(X_0, X_\eta)$ it holds $(\lambda_j)_{j \geq 1} = O(\exp(-cj^{1/(2d)}))$ for some constant $c > 0$.

For the proof of Theorem 6.1, see Appendix A. In total, our previous argumentation shows that we can assess the eigenvalue decay of Γ when we consider the case that k is the Gaussian kernel. We can now obtain \mathbb{P} -a.e. convergence rates and error bounds for the estimator $C_n(\eta)$ when properties of $(X_t)_{t \in \mathbb{Z}}$ are known. In combination with knowledge about mixing rates (see Example 4.3), statements like the following are the immediate consequence.

Example 6.2 (Markov process on compact domain in \mathbb{R}^d). Let $E \subseteq \mathbb{R}^d$ be compact and \mathcal{H} be the RKHS induced by the Gaussian kernel on $E \times E$ for some bandwidth $\sigma > 0$. Let $(X_t)_{t \in \mathbb{Z}}$ be a stationary, geometrically ergodic Markov process on E , then the conclusions of Theorem 5.2 hold.

7. CONSISTENCY OF WEAKLY DEPENDENT KERNEL PCA

By considering the kernel covariance operator $C := C(0)$, we can easily obtain consistency results for kernel PCA (Schölkopf et al., 1998) for the case that the data is dependent. It is well known that kernel PCA approximates the spectral decomposition of C (see for example Blanchard et al., 2007), as we will briefly explain in Section 7.2. Consistency results for kernel PCA from independent data have been obtained by considering the spectral perturbation of covariance operators of Hilbertian random variables (Mas and Menneveau, 2003; Blanchard et al., 2007; Mas and Ruymgaart, 2015; Koltchinskii and Lounici, 2016, 2017; Reiß and Wahl, 2020). Various approaches exist in this context and we do not aim to provide a full overview here. Instead, we will show how our previous results lead to some elementary consistency statements for dependent data. By applying techniques from the previously mentioned literature, these results may be refined and extended accordingly.

We note that convergence in measure and weak convergence of standard linear Hilbertian PCA for $L^2([0, 1])$ -valued stochastic processes was previously investigated by Kokoszka and Reimherr (2013) under the assumption of L^4 - m approximability.

7.1. Notation. For a compact self-adjoint positive-semidefinite operator C on \mathcal{H} , let $(\lambda_i(C))_{i \in I}$ denote the nonzero eigenvalues of C ordered nonincreasingly repeated with their multiplicities for the index set $I = \{1, 2, \dots\}$. Then C admits the spectral decomposition

$$(7.1) \quad C = \sum_{i \in I} \lambda_i(C) v_i \otimes v_i$$

where the v_i are the orthonormal eigenfunctions of C . In addition, let $(\mu_j(C))_{j \in J}$ denote the *distinct* eigenvalues of C for $J = \{1, 2, \dots\}$ with $\Delta_j(C) := \{i \in I \mid$

$\lambda_i(C) = \mu_j\}$ as well as the multiplicity $m_j(C) := |\Delta_j(C)|$. Note that C can also be written as

$$(7.2) \quad C = \sum_{j \in J} \mu_j(C) P_j(C),$$

where $P_j(C)$ is the orthogonal spectral projector onto the eigenspace corresponding to $\mu_j(C)$ and the convergence is with respect to the operator norm. We will additionally consider the *spectral gap*

$$(7.3) \quad g_j(C) := \begin{cases} \mu_1(C) - \mu_2(C), & j = 1, \\ \min\{\mu_{j-1}(C) - \mu_j(C), \mu_j(C) - \mu_{j+1}(C)\}, & j \geq 2. \end{cases}$$

Note that $g_j(C) \neq 0$ by construction.

7.2. Operator interpretation of Kernel PCA. Kernel PCA approximates a finite-rank truncation of the *Karhunen–Loève transformation* of the embedded random variable $\varphi(X_0)$ by approximating the spectral decomposition of the kernel covariance operator $C = \mathbb{E}[\varphi(X_0) \otimes \varphi(X_0)]$ (see for example [Blanchard et al., 2007](#)).

Consider the spectral decomposition (7.1) of C . Let $\{\tilde{v}_i\}_{i \geq 1}$ be an extension of the eigenfunctions $\{v_i\}_{i \in I}$ of C to a complete orthonormal system in \mathcal{H} (that is, the addition of an appropriate ONS spanning the null space of C) By expanding the random variable $\varphi(X_0)$ in terms of $\{\tilde{v}_i\}_{i \geq 1}$, we get the Karhunen–Loève transformation

$$(7.4) \quad \varphi(X_0) = \sum_{i \in I} \langle \varphi(X_0), \tilde{v}_i \rangle_{\mathcal{H}} \tilde{v}_i = \sum_{i \in I} Z_i \tilde{v}_i,$$

where $Z_i := \langle \varphi(X_0), \tilde{v}_i \rangle_{\mathcal{H}} = \tilde{v}_i(X_0)$ are real-valued random variables and convergence in (7.4) is with respect to the norm of \mathcal{H} . Note that we have

$$\text{Cov}[Z_i, Z_j] = \text{Cov}[\tilde{v}_i(X_0), \tilde{v}_j(X_0)] = \langle \tilde{v}_i, C \tilde{v}_j \rangle_{\mathcal{H}} = \lambda_i(C) \delta_{ij},$$

where we extend the set of eigenvalues to the null space, e.g., we set $\lambda_i(C) := 0$ for $i \neq I$. In practice, the data is usually projected onto the first r dominant eigenfunctions in order to obtain an optimal low-dimensional approximation of $\varphi(X_0)$. In particular, for all $r \in I$, the projector $P_{\leq r} := \sum_{i=1}^r v_i \otimes v_i$ minimizes the reconstruction error

$$(7.5) \quad R(T) := \mathbb{E} \left[\|\varphi(X_0) - T\varphi(X_0)\|_{\mathcal{H}}^2 \right]$$

over all operators T in the set of r -dimensional orthogonal projectors on \mathcal{H} . By performing a spectral decomposition of the empirical kernel covariance operator

$$C_n = \frac{1}{n} \sum_{t=1}^n \varphi(X_t) \otimes \varphi(X_t),$$

kernel PCA aims to approximate (7.4) (or $P_{\leq r}$ respectively). We are therefore interested in how well the spectral decomposition of the empirical operator C_n approximates the spectral decomposition of C .

7.3. Consistency results. We can now combine typical results from spectral perturbation theory with our previous error analysis for C_n to obtain consistency statements. Note that we do not aim to provide a full analysis but rather illustrate how our results can be used to assess the error of kernel PCA with weakly dependent data. In the independent case, stronger results have been obtained for example by [Koltchinskii and Lounici \(2016, 2017\)](#), [Milbradt and Wahl \(2020\)](#) and [Reiß and Wahl \(2020\)](#) by directly considering (7.5).

Remark 7.1 (Measurability of spectral properties). As for example shown by [Dauxois et al. \(1982\)](#), the eigenvalues and corresponding eigenprojection operators of C and C_n are measurable and therefore random variables on $(\Omega, \mathcal{F}, \mathbb{P})$.

Theorem 7.2 (Spectral perturbation bounds). *With the notation of Section 7.1, it holds that*

$$(7.6) \quad \sup_{i \geq 1} |\lambda_i(C) - \lambda_i(C_n)| \leq \|C - C_n\| \quad \mathbb{P}\text{-a.e.}$$

as well as

$$(7.7) \quad \|P_j(C) - P_j(C_n)\| \leq \frac{4 \|C - C_n\|}{g_j(C)} \quad \mathbb{P}\text{-a.e.}$$

for all $j \in J$.

See [Gohberg and Krein \(1969, Corollary 2.3\)](#) and [Koltchinskii and Lounici \(2016, Lemma 1\)](#) for proofs of these statements.

The above bounds combined with the strong law of large numbers from Corollary 3.2 for $\|C - C_n\|$ yield consistency results of kernel PCA with weakly dependent data.

Corollary 7.3 (Spectral consistency & convergence rate). *Let $(X_t)_{t \in \mathbb{Z}}$ be stationary and ergodic. Then we have $\sup_{i \geq 1} |\lambda_i(C) - \lambda_i(C_n)| \rightarrow 0$ \mathbb{P} -a.e. as well as $\|P_j(C_n) - P_j(C)\| \rightarrow 0$ \mathbb{P} -a.e. for all $j \geq 1$. In both cases, convergence takes place with the same rate as the convergence $C_n \rightarrow C$ in operator norm.*

Remark 7.4. The preservation of convergence rates in Corollary 7.3 is particularly relevant whenever the assumptions of Theorem 5.1 hold, as is the case in Example 6.2. In this situation, the spectral convergence rate is given by Corollary 7.3. We note that these results are by no means optimal, as they do not consider the full reconstruction error of a finite-rank truncation of (7.4), like for example [Reiß and Wahl \(2020\)](#) in the independent case. Stronger results can be obtained by accessing deeper perturbation results (see for example [Jirak and Wahl, 2020](#)) and are not in the scope of this work.

Whenever the estimation error $\|C - C_n\|$ can be bounded in probability (for example by applying Theorems 5.1 & 5.2), corresponding statements hold for the eigenvalues and spectral projectors as a result of Theorem 7.2.

Corollary 7.5 (Spectral concentration). *Let $\mathbb{P}[\|C_n(0) - C(0)\| \geq \epsilon] \leq f(\epsilon, n)$ for some function $f : \mathbb{R}_{>0} \times \mathbb{N} \rightarrow \mathbb{R}_{\geq 0}$. Then we have*

- (1) $\mathbb{P}[\sup_{i \geq 1} |\lambda_i(C) - \lambda_i(C_n)| \geq \epsilon] \leq f(\epsilon, n)$ and
- (2) $\mathbb{P}[\|P_j(C) - P_j(C_n)\| \geq \epsilon] \leq f(\frac{g_j(C)}{4}\epsilon, n)$ for all j .

Remark 7.6. We note that in the case of weakly dependent data, the representation (7.4) might not always be a desirable model since time-related information in the realization of the process $(\varphi(X_t)_{t \in \mathbb{Z}})$ is discarded. As such, kernel PCA decomposes the RKHS only with respect to the covariance of $\mathcal{L}(\varphi(X_0))$ instead of using autocovariance information from $\mathcal{L}(\varphi(X_{t_1}), \varphi(X_{t_2}), \varphi(X_{t_3}), \dots)$. If one is interested in performing a decomposition that captures the *dynamic behavior* instead of only the *asymptotic spatial behavior*, different approaches are needed. In the context of *functional data analysis*, the concept of *harmonic PCA* or *dynamic PCA* (Panaretos and Tavakoli, 2013a; Hörmann et al., 2015) yields optimal filter functions to reduce the dimensionality of a (weakly) stationary stochastic process. We will address alternative time-based decomposition approaches in Section 9.

8. CONDITIONAL MEAN EMBEDDING OF STATIONARY TIME SERIES

We will now show how the previous theoretical results can be used to obtain consistency results for a large family of nonparametric time series models. A wide variety of kernel techniques for sequential data rely on the RKHS embedding of the conditional η -time step transition probability

$$(8.1) \quad \mathbb{P}[X_{t+\eta} \in \mathcal{A} \mid X_t], \quad \mathcal{A} \in \mathcal{F}_E,$$

which is modeled in terms of the *conditional mean embedding* (Song et al., 2009). In what follows, we will briefly outline the different derivations of the conditional mean embedding.

Applications of the conditional mean embedding in the context of sequential data include, among others, state-space models and filtering (Song et al., 2009; Fukumizu et al., 2013; Gebhardt et al., 2019), the embedding of transition probability models (Song et al., 2010; Grünewälder et al., 2012b; Nishiyama et al., 2012; Sun et al., 2019), predictive state representations (Boots et al., 2013), and reinforcement learning models (van Hoof et al., 2015, 2017; Stafford and Shawe-Taylor, 2018; Gebhardt et al., 2018).

8.1. Operator-theoretic conditional mean embedding. In order to express the transition probability (8.1) in terms of the RKHS \mathcal{H} , one is interested in a conditional mean operator $U: \mathcal{H} \supseteq \text{dom}(U) \rightarrow \mathcal{H}$ which satisfies

$$(8.2) \quad \langle f, U\varphi(x) \rangle_{\mathcal{H}} = \mathbb{E}[f(X_{t+\eta}) \mid X_t = x], \quad f \in \mathcal{H}.$$

Note that the action of U on $\varphi(x) \in \mathcal{H}$ is interpreted as conditioning on the event $\{X_t = x\}$, while evaluations of functions $f \in \mathcal{H}$ with $U\varphi(x)$ under the inner product can be interpreted as a conditional expectation operator in a weak sense. It is important to note that such an operator U does not exist in general. By using properties of the kernel covariance operators, it can be shown that $U := C(\eta)C(0)^\dagger$ satisfies (8.2) under strong technical assumptions, see Klebanov et al. (2019) for details.¹ We call U the *conditional mean operator* and $U\varphi(x)$ the

¹ Klebanov et al. (2019) also propose the operator $\tilde{U} := (C(0)^\dagger C(\eta)^*)^*$, which does not coincide with U in general. However, we will work with the operator $U = C(\eta)C(0)^\dagger$ as given in the main text, since this is the originally proposed version by Song et al. (2009). Additionally, empirical estimates have only been derived for U and therefore this is the version which is commonly used in practical applications.

conditional mean embedding of the transition probability $\mathbb{P}[X_{t+\eta} \in \mathcal{A} \mid X_t = x]$. Here, $C(0)^\dagger: \text{range}(C(0)) \oplus \text{range}(C(0))^\perp \rightarrow \mathcal{H}$ is the Moore–Penrose pseudoinverse of the operator $C(0)$ (see for example Engl et al., 1996). Note that U is in general not globally defined and bounded, i.e., $\text{range}(C(0)) \oplus \text{range}(C(0))^\perp \neq \mathcal{H}$, since $\text{range}(C(0))$ is generally not closed. Song et al. (2009) propose the regularized conditional mean operator

$$(8.3) \quad U^{(\gamma)} := C(\eta) (C(0) + \gamma I_{\mathcal{H}})^{-1},$$

with empirical estimate $U_n^{(\gamma)} := C_n(\eta) (C_n(0) + \gamma I_{\mathcal{H}})^{-1}$. Here, $I_{\mathcal{H}}$ denotes the identity operator on \mathcal{H} and $\gamma > 0$ is a regularization parameter. Note that $U^{(\gamma)}$ as well as $U_n^{(\gamma)}$ are always well-defined as Hilbert–Schmidt operators on \mathcal{H} . Song et al. (2009), Fukumizu et al. (2013), and Fukumizu (2017) examine convergence of this estimate for the case of independent data pairs from the joint distribution of X_t and $X_{t+\eta}$ and show weak consistency with different rates under various technical assumptions. We extend these results to the case of dependent data.

Since the assumptions for this operator-theoretic framework and especially the analytical existence of U are hard to verify, different interpretations have emerged. In settings where (8.2) does not have an analytical solution, the regularized estimate $U_n^{(\gamma)}$ minimizes an empirical risk functional, which we will briefly outline below (Grünwälder et al., 2012a; Park and Muandet, 2020).

8.2. Least-squares conditional mean embedding. In cases when U is not globally defined and bounded, it is natural to approximate a smooth solution to (8.2) by minimizing the risk functional $R'_\gamma: S_2(\mathcal{H}) \rightarrow \mathbb{R}$ given by

$$(8.4) \quad R'_\gamma(A) := \sup_{\substack{f \in \mathcal{H} \\ \|f\|_{\mathcal{H}}=1}} \mathbb{E} [(\mathbb{E}[f(X_{t+\eta}) \mid X_t] - \langle f, A\varphi(X_t) \rangle_{\mathcal{H}})^2] + \gamma \|A\|_{S_2(\mathcal{H})}^2,$$

where $\gamma > 0$ is a regularization parameter. As shown by Grünwälder et al. (2012a), $R'_\gamma(A)$ can be bounded from above by the surrogate risk

$$(8.5) \quad R_\gamma(A) := \mathbb{E}[\|\varphi(X_{t+\eta}) - A\varphi(X_t)\|_{\mathcal{H}}^2] + \gamma \|A\|_{S_2(\mathcal{H})}^2.$$

The corresponding empirical surrogate risk

$$(8.6) \quad R_\gamma^n(A) := \frac{1}{n} \sum_{t=1}^n \|\varphi(X_{t+\eta}) - A\varphi(X_t)\|_{\mathcal{H}}^2 + \gamma \|A\|_{S_2(\mathcal{H})}^2$$

has the minimizer $U_n^{(\gamma)}$, which is a result of vector-valued regression theory (Caponetto and De Vito, 2007). For the case of a finite-dimensional RKHS \mathcal{H} , Grünwälder et al. (2012a) use this setting to provide risk-based consistency results that do not rely on the fact that U is generally not well-defined as an element in the hypothesis space $S_2(\mathcal{H})$. A modified approach by Park and Muandet (2020) avoids the operator-based formulation, but derives a similar empirical surrogate risk from a measure-theoretic perspective. Interestingly, both Grünwälder et al. (2012a) and Park and Muandet (2020) do not derive a closed form solution to the risk (8.5). In particular, the object (8.3) is not considered in their analysis and consistency results are formulated in terms of risk bounds without an analytical regularized solution.

Remark 8.1 (Operator CME versus least-squares CME). From a statistical learning point of view, the operator-theoretic setting describes the *well-specified* case that the conditional mean operator exists in the hypothesis space $S_2(\mathcal{H})$, which is tied to strong assumptions. In this case, only a *sample error* needs to be considered and a *model error* does not exist. The regression viewpoint of Grünewälder et al. (2012a) allows to consider the *misspecified* case that U does not exist in the hypothesis space. An *approximation* error between the best approximation of U in the hypothesis space $S_2(\mathcal{H})$ and U needs to be considered in this case. However, Grünewälder et al. (2012a) do not provide a closed form for the analytical solution of the minimizer of the risk (8.5) – only a solution for the empirical risk (8.6). Moreover, the derived rates are severely limited by the assumption that \mathcal{H} is finite-dimensional. The more general version by Park and Muandet (2020) gives superior convergence results without an analytical operator interpretation. However, even in the operator-free interpretation by Park and Muandet (2020), the operator $U_n^{(\gamma)}$ is implicitly learned (see also Carmeli et al., 2010, Example 3.3(i)). We note that although the operator-based interpretation of the CME is inferior to the regression standpoint by Park and Muandet (2020) from a theoretical perspective, its connection to Markov transition operators highlighted in Section 9 is of great interest in the scenario of dependent data. We expect that additional results based on the derivation of Grünewälder et al. (2012a) could fill this gap and provide a missing analytical solution to the operator-regression problem. We will focus on the well-specified case for simplicity and postpone the approximation analysis in the misspecified case with dependent data to future work. We refer the reader to Klebanov et al. (2019) and Park and Muandet (2020) for a comparison of both cases.

8.3. Kernel sum rule. In the well-specified operator-theoretic setting, Fukumizu et al. (2013, Theorem 2) show that the conditional mean operator U satisfies the more general so-called *kernel sum rule*, which is widely used in nonparametric Bayesian models, especially time series filtering. That is, for a *prior* measure z on (E, \mathcal{F}_E) satisfying the integrability $\int_E \|\varphi(Z)\|_{\mathcal{H}} dz(Z) < \infty$ with a kernel mean embedding $\mu_z = \int \varphi(Z) dz(Z)$ such that $\mu_z \in \text{dom}(C(0)^\dagger)$, we have

$$(8.7) \quad \langle f, U\mu_z \rangle_{\mathcal{H}} = \int_E \mathbb{E}[f(X_{t+\eta}) \mid X_t = x] dz(x), \quad f \in \mathcal{H}.$$

Note that the conditional mean property (8.2) is in fact a special case of the kernel sum rule when z is the Dirac measure at x , i.e., $\mu_z = \varphi(x)$. In applications, the embedded prior μ_z is usually estimated empirically by sampling from z . When $\hat{\mu}_z$ is any kind of consistent estimate of μ_z , we obtain the plug-in estimator $U_n^{(\gamma)} \hat{\mu}_z$ for $U\mu_z$.

8.4. Consistency results. We now outline how our previous results allow to formulate consistency results for the kernel sum rule for dependent data. Prior consistency results for the operator-based setting of the conditional mean embedding and the kernel sum rule are limited to independent data pairs. Note again that a drawback of our approach is the typical assumption that the analytic expression $U\mu_z$ (and in particular $U\varphi(x)$) exists in \mathcal{H} (see Klebanov et al., 2019), while a focus on the minimization properties allows to relax this assumption and consider

convergence to a best approximation under the corresponding risk. We start by giving a generic error decomposition for the kernel sum rule in a form that admits the immediate application of our previous results.

Theorem 8.2 (Kernel sum rule error). *Let z be a prior finite measure on (E, \mathcal{F}_E) and a kernel $k: E \times E \rightarrow \mathbb{R}$ with $\sup_{x \in E} k(x, x) = c < \infty$ such that the kernel sum rule (8.7) applies (in particular, $\mu_z \in \text{dom}(C(0)^\dagger)$). Then the empirical estimate $U_n^{(\gamma)} \hat{\mu}_z$ admits the total error bound*

$$(8.8) \quad \left\| U_n^{(\gamma)} \hat{\mu}_z - U \mu_z \right\|_{\mathcal{H}} \leq e_s(\mu_z, \hat{\mu}_z, n, \gamma) + e_r(\mu_z, \gamma) \quad \mathbb{P}\text{-a. e.}$$

with the worst-case stochastic estimation error

$$e_s(\mu_z, \hat{\mu}_z, n, \gamma) := \frac{c}{\gamma} \|\hat{\mu}_z - \mu_z\|_{\mathcal{H}} + \frac{c^{3/2}}{\gamma^2} \|C_n(0) - C(0)\| + \frac{c^{1/2}}{\gamma} \|C_n(\eta) - C(\eta)\|$$

and the deterministic regularization error

$$e_r(\mu_z, \gamma) := c \|(C(0) + \gamma \mathcal{I}_{\mathcal{H}})^{-1} \mu_z - C(0)^\dagger \mu_z\|_{\mathcal{H}}.$$

The proof for Theorem 8.2 can be found in Appendix A.

Remark 8.3 (Kernel sum rule error). The error decomposition (8.8) leads to the following insights:

- (1) The deterministic regularization error $e_r(\mu_z, \gamma)$ captures the analytic nature of the inverse problem described by $C(0)u = \mu_z$ for $u \in \mathcal{H}$. As such, it is not affected by any estimation. Note that as $\gamma \rightarrow 0$, it holds that $e_r(\mu_z, \gamma) \rightarrow 0$ for every $\mu_z \in \text{dom}(C(0)^\dagger)$. For details, we refer the reader to Engl et al. (1996). In practice, regularization is needed since for estimated right-hand sides $\hat{\mu}_z$, the condition $\hat{\mu}_z \in \text{dom}(C(0)^\dagger)$ is in general not true – even if $\mu_z \in \text{dom}(C(0)^\dagger)$. The convergence rate of $e_r(\mu_z, \gamma)$ depends on the eigendecomposition of $C(0)$ and can be assessed under additional assumptions about the decay rate of the eigenvalues. However, in general the convergence of the regularization error can be arbitrarily slow without additional assumptions, see Schock (1984).
- (2) When $\mu_z = \varphi(x)$, we obtain an error decomposition for the standard conditional mean embedding. In this case, we do not need the empirical estimate $\hat{\mu}_z$ as a proxy for μ_z , since μ_z can be evaluated directly. In this case, we can drop the term $\frac{c}{\gamma} \|\hat{\mu}_z - \mu_z\|_{\mathcal{H}}$ from the estimation error and obtain $e_s(n, \gamma) := \frac{c^{3/2}}{\gamma^2} \|C_n(0) - C(0)\| + \frac{c^{1/2}}{\gamma} \|C_n(\eta) - C(\eta)\|$ instead.
- (3) For convergence of the total error (8.8), we need the two simultaneous conditions $e_s(\mu_z, \hat{\mu}_z, n, \gamma) \rightarrow 0$ and $e_r(\mu_z, \gamma) \rightarrow 0$ as $n \rightarrow \infty$, $\gamma \rightarrow 0$ and $\hat{\mu}_z \rightarrow \mu_z$. The typical trade-off between regularization error and estimation error is reflected in this fact.

Our previous convergence results for the individual estimation errors of $C_n(0)$ and $C_n(\eta)$ allow to bound $e_s(\mu_z, \hat{\mu}_z, n, \gamma)$ and derive regularization schemes $\gamma := \gamma(n, \mu_z, \hat{\mu}_z)$ depending on the trajectory length n and the quality of the prior estimate $\hat{\mu}_z$. Informally speaking, the individual estimation errors must tend to 0 faster than the regularization term, so γ

should not be allowed to converge “too fast” with respect to the rate of increasing sample size n – this is the typical setting in the theory of inverse problems and regularization.

By incorporating additional knowledge about the convergence behavior of $C_n(0)$ and $C_n(\eta)$ from our previous results, Theorem 8.2 yields convergence rates of the estimation error e_s as well as admissible regularization schemes. We give an example below. For simplicity, we assume that $C_n(0)$ and $C_n(\eta)$ are estimated independently, which would of course require two realizations of length n of $(X_t)_{t \in \mathbb{Z}}$. In addition, we require $\hat{\mu}_z$ to converge with standard rate of $-n^{1/2}$, which we tie to the number of samples available for the estimation of $C_n(0)$ and $C_n(\eta)$ in order to avoid additional symbols for different samples.

Example 8.4 (Kernel sum rule consistency). Let $C_n(0)$ and $C(\eta)$ be estimated independently from X_1, \dots, X_n . Assume that \mathbb{P} -a.e., we have the prior convergence rate $\|\mu_z - \hat{\mu}_z\|_{\mathcal{H}} = O(-n^{1/2})$. Under the conditions of Theorem 5.2 (for instance when $(X_t)_{t \in \mathbb{Z}}$ is the Markov process from Example 6.2), we have \mathbb{P} -a.e.

$$e_s(\mu_z, \hat{\mu}_z, n, \gamma) = O\left(\frac{(\log n)^{3/2}}{n^{1/2}\gamma^2}\right).$$

In particular, for every regularization scheme $\gamma = \gamma(n)$ such that

$$\gamma(n) \rightarrow 0 \text{ as well as } \frac{(\log n)^{3/2}}{n^{1/2}\gamma(n)^2} \rightarrow 0$$

for $n \rightarrow \infty$, we have overall strong consistency $U_n^{(\gamma(n))}\hat{\mu}_z \rightarrow U\mu_z$ in the norm of \mathcal{H} .

9. NONPARAMETRIC ESTIMATION OF MARKOV TRANSITION OPERATORS

As the last application of our theory, we will briefly show how the risk functional (8.4) yields a nonparametric model for the estimation of Markov transition operators. Moreover, we elaborate on the recent discovery that this model is actually the theoretical foundation of a well-known family of several data-driven methods for the analysis of dynamical systems (Klus et al., 2019). We only highlight immediate consequences of this approach and emphasize that several theoretical questions need to be answered separately in the vector-valued learning context of Grünewälder et al. (2012a), Grünewälder et al. (2013) and Park and Muandet (2020). The aim of this section is to draw attention to the fact that statistical tools like strong mixing coefficients can be used to show consistency for a range of numerical methods used in other scientific disciplines.

In what follows, we assume that $(X_t)_{t \in \mathbb{Z}}$ is a Markov process, i.e., it holds that $\mathbb{E}[f(X_s) | \mathcal{F}_{-\infty}^t] = \mathbb{E}[f(X_s) | \sigma(X_t)]$ for all bounded measurable functions $f: E \rightarrow \mathbb{R}$ and times $s \geq t$.

For a fixed time lag $\eta \in \mathbb{N}_{>0}$, the *transition operator*, (*backward transfer operator*² or (*stochastic*) *Koopman operator* \mathcal{K} is defined by the relation

$$(9.1) \quad (\mathcal{K}f)(x) = \mathbb{E}[f(X_{t+\eta}) \mid X_t = x]$$

for all functions f in some set F consisting of real (or complex) valued functions defined on the state space E . The Koopman operator describes the propagation of observable functions in F by the time step η .

By simply switching to the adjoint of A in the expression for $R'_\gamma(A)$ defined in (8.4) and using the reproducing property of \mathcal{H} , we have

$$(9.2) \quad R'_\gamma(A) := \sup_{\substack{f \in \mathcal{H} \\ \|f\|_{\mathcal{H}}=1}} \mathbb{E} [(\mathbb{E}[f(X_{t+\eta}) \mid X_t] - (A^*f)(X_t))^2] + \gamma \|A^*\|_{S_2(\mathcal{H})}^2.$$

As a result, we can immediately interpret the adjoint of the conditional mean operator

$$U^{(\gamma)*} = (C(0) + \gamma I_{\mathcal{H}})^{-1} C(\eta)^*$$

as a smooth approximation of the transition operator \mathcal{K} on the class of RKHS functions $F = \mathcal{H}$ with empirical estimate

$$U_n^{(\gamma)*} = (C_n(0) + \gamma I_{\mathcal{H}})^{-1} C_n(\eta)^*.$$

Note that all of our consistency results for kernel autocovariance operators and the conditional mean embedding transfer directly to this setting, as operator norm error bounds for the estimate of $U^{(\gamma)}$ are also valid for its adjoint.

We will now briefly show the connection of the conditional mean operator and its adjoint to a range of data-driven analysis techniques developed in the dynamical systems community.

9.1. Dynamic mode decomposition. The idea of approximating the Markov transition operator \mathcal{K} via $U^{(\gamma)*}$ can be connected to data-driven spectral analysis and model reduction techniques used in engineering, fluid dynamics, molecular dynamics, and atmospheric sciences. Data-driven approximations of the Koopman operator are frequently used to perform analysis, forecasting, model reduction, and control of dynamical systems in various scientific disciplines (Rowley et al., 2009; Brunton et al., 2016; Giannakis, 2019). For an overview of numerical Koopman approximation methods in the context of spectral analysis, see Klus et al. (2016, 2018b). One of the most widely used Koopman spectral analysis and model reduction methods is *extended dynamic mode decomposition (EDMD)* (Williams et al., 2015a). EDMD computes an approximation of the Koopman operator eigendecomposition via a Galerkin-approximation based on a finite set of basis functions in F . When F is chosen to be the RKHS \mathcal{H} , one obtains so-called *kernel EDMD* (Williams et al., 2015b) as a special nonparametric version of EDMD. It was shown by Klus et al. (2019) that (regularized) kernel EDMD actually computes the eigendecomposition of $U_n^{(\gamma)*}$. This new nonparametric asymptotic perspective of kernel EDMD allows to formulate new convergence results of kernel EDMD based on previous results. In contrast to previous results that rely on ergodicity of the underlying system (Klus et al., 2016; Korda and Mezić, 2018; Giannakis et al., 2018),

²The name *backward transfer operator* is classically used in the context of continuous-time processes, where it is used to describe the solution to the *backwards Kolmogorov equation*. In the theory of dynamical systems, the term *Koopman operator* is commonly used.

we are able to give a refined convergence analysis by using mixing properties of the underlying system. However, we note that the operator $U^{(\gamma)*}$ is in general not self-adjoint and a dedicated analysis of spectral properties and convergence is subject to future work.

9.2. Time-based independent component analysis. It is known that the the Koopman operator and its adjoint, the *Perron–Frobenius* operator, can be connected to the solution of the so-called *blind source separation problem* (Klus et al., 2018b, 2019) In fact, eigenfunctions of compositions of empirical autocovariance operators (and their pseudoinverses) are used as projection coordinates in a kernel-based variant of *independent component analysis* (Harmeling et al., 2003; Schwantes and Pande, 2015). As such, consistency results for the Koopman operator can be used to prove convergence for these approaches.

To the best of our knowledge, prior consistency results for EDMD only cover convergence in strong operator topology (i.e., pointwise convergence) for parametric models, i.e. on fixed finite-dimensional subspaces spanned by a dictionary of basis functions. Furthermore, they mostly aim towards deterministic dynamical systems (Korda and Mezić, 2018).

Remark 9.1 (Model error). Note that analytically, $\mathcal{K}f$ is not necessarily an element of \mathcal{H} for all $f \in \mathcal{H}$, hence the kernel Koopman operator needs to be considered on the domain $\text{dom}(\mathcal{K}) := \{f \in \mathcal{H} \mid \mathbb{E}[f(X_{t+\eta}) \mid X_t = \cdot] \in \mathcal{H}\} \subseteq \mathcal{H}$. Therefore, the kernel Koopman operator is in general not a globally defined and bounded operator, which is also reflected in the theory of the conditional mean embedding (see Song et al., 2009). The *model error*, i.e., how well the kernel Koopman operator \mathcal{K} approximates the original Koopman operator in (9.1) for some other function class F is not in the scope of this paper. Klus et al. (2019) investigate this problem for $F = L^\infty(E, \mathcal{F}_E, m; \mathbb{R})$. It is likely that this problem can be tackled from a vector-valued statistical learning standpoint (Park and Muandet, 2020) by introducing suitable *source conditions* and exploiting the approximation theory of *universal* vector-valued kernels (Carmeli et al., 2010).

10. CONCLUSION

In this paper, we provided a mathematically rigorous analysis of kernel autocovariance operators and established classical limit theorems as well as nonasymptotic error bounds under classical ergodic and mixing assumptions. The results were mostly derived from theoretical work on discrete-time processes in Banach and Hilbert spaces and are presented in a form such that they can be easily applied in the context of RKHS-based time series models and frequency domain analysis. We highlighted high-level applications for kernel PCA, the conditional mean embedding, and the nonparametric estimation of Markov transition operators. The theory of vector-valued statistical learning from dependent data may be connected to our considerations in future work. In the context of learning Markov transition operators, the kernel autocovariance operator may lead to an inverse problem that describes the analytical minimizer of an autoregression risk in an operator space.

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APPENDIX A. PROOFS

Proof of Theorem 4.8. We apply Merlève (2008, Theorem 2) to the process $(\xi)_{t \in \mathbb{Z}}$ and immediately obtain the existence of a compact set K with the desired properties such that both (4.5) and (4.6) hold. It now remains to show the norm bound (4.7) for K . The set K is the unit ball of the Hilbert space \mathbb{H} , which is given by the completion of the range of $T^{1/2}$ (where T is given by (4.4) and $T^{1/2}$ denotes its operator square root) with respect to the inner product, defined by

$$(A.1) \quad \left\langle T^{1/2}A, T^{1/2}B \right\rangle_{\mathbb{H}} := \langle A, B \rangle_{S_2(\mathcal{H})}, \quad A, B \in S_2(\mathcal{H}),$$

also called *Cameron–Martin space* or *abstract Wiener space* (for details, we refer the reader to Bogachev, 1998, Chapter 2). For a technical construction of \mathbb{H} and the limit set K in the law of the iterated logarithm in Banach spaces, we refer the reader to Kuelbs (1976, Section 2) as well as Goodman et al. (1981, Section 2). Note that these references elaborate on the i.i.d. case. However, for the construction of \mathbb{H} and K only an abstract limiting probability measure is needed, which is given by the Gaussian measure obtained from Theorem 4.7 and its covariance operator T defined by (4.4), just as shown in the proof of Merlève (2008, Theorem 2). We can therefore analyze properties of K by considering the Cameron–Martin space of the centered Gaussian measure induced by T , which is examined in the previously mentioned literature. The identity (A.1) can be verified by translating the abstract Banach space definition of (Kuelbs, 1976, Equation (2.3)) to our scenario of the separable Hilbert space $S_2(\mathcal{H})$ as, for example, described by Bogachev (1998, Remark 2.3.3).

From (A.1), we obtain

$$(A.2) \quad \|A\|_{S_2(\mathcal{H})} \leq \|T^{1/2}\| \|A\|_{\mathbb{H}}, \quad A \in \mathbb{H}.$$

Since $K = \{A \in \mathbb{H} \mid \|A\|_{\mathbb{H}} \leq 1\}$, a bound for $\|T^{1/2}\| = \|T\|^{1/2}$ depending on the mixing rate of $(\xi_t)_{t \in \mathbb{Z}}$ is sufficient in order to provide a bound for elements of K in the norm of $S_2(\mathcal{H})$.

We now give a norm bound for $T = \mathbb{E}[\xi_0 \otimes \xi_0] + \sum_{t=1}^{\infty} \mathbb{E}[\xi_0 \otimes \xi_t] + \sum_{t=1}^{\infty} \mathbb{E}[\xi_t \otimes \xi_0]$. We clearly have

$$\|\mathbb{E}[\xi_0 \otimes \xi_0]\| \leq 4c^2,$$

since ξ_0 is almost surely bounded by $2c$ by (4.3).

Let $\alpha(n)$ be the mixing coefficients of $(X_t)_{t \in \mathbb{Z}}$. We now note that by (4.1), we have $\alpha((\xi_t)_{t \in \mathbb{Z}}, n) \leq \alpha(n - \eta)$ for all $n \in \mathbb{N}$. This allows to give a bound for the two remaining summands of T :

$$\begin{aligned}
\left\| \sum_{t=1}^{\infty} \mathbb{E}[\xi_t \otimes \xi_0] \right\| &\leq \sum_{t=1}^{\infty} \|\mathbb{E}[\xi_t \otimes \xi_0]\| \\
&= \sum_{t=1}^{\infty} \sup_{\substack{\|A\|_{S_2(\mathcal{H})}=1 \\ \|B\|_{S_2(\mathcal{H})}=1}} |\mathbb{E}[\langle \xi_t, B \rangle \langle \xi_0, A \rangle]| \\
&\leq \sum_{t=1}^{\infty} \sup_{\substack{\|A\|_{S_2(\mathcal{H})}=1 \\ \|B\|_{S_2(\mathcal{H})}=1}} 4 \alpha(\sigma(\xi_t), \sigma(\xi_0)) \|\langle \xi_t, B \rangle\|_{L^\infty(\mathbb{P})} \|\langle \xi_0, A \rangle\|_{L^\infty(\mathbb{P})} \\
&\leq \sum_{t=1}^{\infty} 16 c^2 \alpha(t - \eta) = 16 c^2 M,
\end{aligned}$$

where we use Ibragimov's covariance inequality for strongly mixing and bounded random variables (Ibragimov, 1962, Lemma 1.2) in the third step (note that $\langle \xi_t, B \rangle$ and $\langle \xi_0, A \rangle$ are centered real-valued random variables which are \mathbb{P} -a.e. bounded by $2c$ because of (4.3)). By symmetry, we obtain the same bound for $\|\sum_{t=1}^{\infty} \mathbb{E}[\xi_0 \otimes \xi_t]\|$ and we end up with the total norm bound

$$(A.3) \quad \|T\| \leq 4c^2 + 32c^2M,$$

which proves the claim in combination with (A.2). \blacksquare

Proof of Theorem 6.1. The key idea for this proof is to make use of the fact that the product RKHS $S_2(\mathcal{H}) \simeq \mathcal{H} \otimes \mathcal{H}$ is isometrically isomorphic to a Gaussian RKHS. This allows to interpret Γ as a (centered) convolution operator in order to apply classical results from the theory of integral equations.

Let \mathcal{G} denote the RKHS induced by the Gaussian kernel $\ell: E^2 \times E^2 \rightarrow \mathbb{R}$,

$$\ell(z, z') = \exp\left(-\frac{\|z - z'\|_{\mathbb{R}^{2d}}^2}{2\sigma^2}\right),$$

where $\|\cdot\|_{\mathbb{R}^{2d}}$ is the Euclidean norm on E^2 . Let $\psi: E^2 \rightarrow \mathcal{G}$ be the feature map corresponding to \mathcal{G} . Then the pointwise defined map

$$\begin{aligned}
\nu: \mathcal{H} \otimes \mathcal{H} &\rightarrow \mathcal{G} \\
\varphi(x) \otimes \varphi(y) &\mapsto \psi((x, y))
\end{aligned}$$

is an isometry, which can be seen by expressing the respective inner products in terms of the corresponding kernels and using the fact that $k(x, x')k(y, y') = \ell((x, y), (x', y'))$. Extending ν to linear combinations gives a bijective isometry from the dense subset $\text{span}\{\varphi(x) \otimes \varphi(x') \mid x, x' \in E\}$ of $\mathcal{H} \otimes \mathcal{H}$ to the dense subset $\text{span}\{\psi((x, x')) \mid (x, x') \in E^2\}$ of \mathcal{G} . Finally, extending ν continuously to the respective completions yields an isometric isomorphism from $\mathcal{H} \otimes \mathcal{H}$ to \mathcal{G} .

We now decompose $\Gamma = \Gamma_1 - \Gamma_2$, where $\Gamma_1 := \mathbb{E}[(\varphi(X_\eta) \otimes \varphi(X_0)) \otimes (\varphi(X_\eta) \otimes \varphi(X_0))]$ and $\Gamma_2 := C(\eta) \otimes C(\eta)$. Since Γ_2 is a rank-one operator, Γ has the same asymptotic eigenvalue behavior as Γ_1 (Gohberg and Krein, 1969, Corollary 2.1). It is therefore sufficient to only consider the eigenvalue decay of Γ_1 . The isomorphism ν

constructed above allows to interpret Γ_1 as an integral operator with respect to the Gaussian kernel ℓ , which makes the application of classical results from the theory of integral equations possible. For every operator $A \in \mathbb{S}_2(\mathcal{H}) \simeq \mathcal{H} \otimes \mathcal{H}$ and all $x, x' \in E$, we write $A(x, x') = \langle A, \varphi(x) \otimes \varphi(x') \rangle_{\mathcal{H} \otimes \mathcal{H}}$ where we identify A with its representation in $\mathcal{H} \otimes \mathcal{H}$ via its singular decomposition. We get the representation

$$\begin{aligned} (\Gamma_1 A)(y, y') &= \langle \Gamma_1 A, \varphi(y) \otimes \varphi(y') \rangle_{\mathcal{H} \otimes \mathcal{H}} \\ &= \int \langle \varphi(X_\eta) \otimes \varphi(X_0), \varphi(y) \otimes \varphi(y') \rangle_{\mathcal{H} \otimes \mathcal{H}} A(X_\eta, X_0) \, d\mathbb{P} \\ &= \int k(X_\eta, y) k(X_0, y') A(X_\eta, X_0) \, d\mathbb{P} \\ &= \int \ell((X_\eta, X_0), (y, y')) A(X_\eta, X_0) \, d\mathbb{P} \\ &= \int_E \ell(z, z') A(z) \, d\mathcal{L}(X_\eta, X_0)(z) \end{aligned}$$

for all $y, y' \in E$, where $z := (x, x')$ and $z' := (y, y')$. We can therefore consider the eigenvalue problem

$$(A.4) \quad (\Gamma_1 A)(z') = \int_E \ell(z, z') A(z) \, d\mathcal{L}(X_\eta, X_0)(z) = \lambda A(z'),$$

where A is interpreted as a real-valued function on E^2 . The solution of integral equations of the form (A.4) for $A \in L^2(E^2, \mathcal{F}_E^{\otimes 2}, \mathcal{L}(X_\eta, X_0); \mathbb{R})$ is well examined. Let $(\lambda_j)_{j>0}$ denote the eigenvalues of Γ_1 . When E is a compact domain, the eigenvalues have a super exponential decay of the form $O(\exp(-cj \log j))$ for some constant $c > 0$. When no assumptions about the domain E are made, exponential decay of the Lebesgue density of $\mathcal{L}(X_\eta, X_0)$ on E^2 leads to an exponential eigenvalue decay in terms of $O(\exp(-cj))$, which is a special case of results by [Widom \(1963\)](#) (see for example [Bach and Jordan, 2002](#), Appendix C.2 for the specific cases considered in this context). Without any additional assumptions about the domain or the underlying distribution, a nearly exponential decay of eigenvalues of the form $O(\exp(-cj^{1/2d}))$ is always guaranteed ([Belkin, 2018](#), Theorem 5).

Note that when we interpret (A.4) as an operator on product RKHS functions in $\mathcal{H} \otimes \mathcal{H}$ instead of $L^2(E^2, \mathcal{F}_E^{\otimes 2}, \mathcal{L}(X_\eta, X_0); \mathbb{R})$, the resulting operator Γ_1 has the same eigenvalues as its L^2 -analogue ([Rosasco et al., 2010](#), Proposition 8), which proves all assertions of the theorem. \blacksquare

Proof of Theorem 8.2. Note that since $\sup_{x \in E} k(x, x) = c < \infty$, we have the \mathbb{P} -a.e. bounds $\|\mu_z\|_{\mathcal{H}} \leq c^{1/2}$ as well as $\|C(\eta)\| \leq c$ for all $\eta \in \mathbb{N}$. Additionally, the regularized inverse can be bounded as $\|(C(0) + \gamma I_{\mathcal{H}})^{-1}\| \leq \frac{1}{\gamma}$, which is easy to see from the corresponding spectral decomposition. These bounds hold analogously for the empirical versions of all above objects.³ All following bounds below will be understood in the \mathbb{P} -a.e. sense for the remainder of this proof.

We now successively insert appropriate zero-sum terms into the total error and apply the triangle inequality multiple times to obtain the worst-case estimation

³For $\hat{\mu}_z$, estimators of the form $\hat{\mu}_z := \sum_i \beta_i \varphi(x_i)$ with coefficients $\sum_i |\beta_i| = 1$ naturally satisfy the bound.

error. We have the overall decomposition

$$(A.5) \quad \left\| U_n^{(\gamma)} \widehat{\mu}_z - U \mu_z \right\|_{\mathcal{H}} \leq \underbrace{\left\| U_n^{(\gamma)} \widehat{\mu}_z - U_n^{(\gamma)} \mu_z \right\|_{\mathcal{H}}}_{(I)} + \underbrace{\left\| U_n^{(\gamma)} \mu_z - U \mu_z \right\|_{\mathcal{H}}}_{(II)}.$$

For these two error components, we get the individual bounds

$$(I) \leq \|C_n(\eta)\| \left\| (C(0) + \gamma I_{\mathcal{H}})^{-1} (\widehat{\mu}_z - \mu_z) \right\|_{\mathcal{H}} \leq \frac{c}{\gamma} \|\widehat{\mu}_z - \mu_z\|_{\mathcal{H}}$$

as well as

$$(II) \leq \underbrace{\left\| C_n(\eta)(C_n(0) + \gamma I_{\mathcal{H}})^{-1} \mu_z - C_n(\eta)(C(0) + \gamma I_{\mathcal{H}})^{-1} \mu_z \right\|_{\mathcal{H}}}_{(*)} \\ + \underbrace{\left\| C_n(\eta)(C(0) + \gamma I_{\mathcal{H}})^{-1} \mu_z - C(\eta)C(0)^\dagger \mu_z \right\|_{\mathcal{H}}}_{(**)}.$$

For $(*)$, we give a bound by

$$(*) \leq \|C_n(\eta)\| \left\| (C_n(0) + \gamma I_{\mathcal{H}})^{-1} - (C(0) + \gamma I_{\mathcal{H}})^{-1} \right\| \|\mu_z\|_{\mathcal{H}} \\ \leq \frac{c^{3/2}}{\gamma^2} \|C_n(0) - C(0)\|,$$

where we use the identity $A^{-1} - B^{-1} = A^{-1}(B - A)B^{-1}$ for invertible operators A and B . To obtain a bound for $(**)$, we again insert a zero-sum:

$$(**) \leq \left\| C_n(\eta)(C(0) + \gamma I_{\mathcal{H}})^{-1} \mu_z - C(\eta)(C(0) + \gamma I_{\mathcal{H}})^{-1} \mu_z \right\|_{\mathcal{H}} \\ + \left\| C(\eta)(C(0) + \gamma I_{\mathcal{H}})^{-1} \mu_z - C(\eta)C(0)^\dagger \mu_z \right\|_{\mathcal{H}} \\ \leq \|C_n(\eta) - C(\eta)\| \left\| (C(0) + \gamma I_{\mathcal{H}})^{-1} \right\| \|\mu_z\|_{\mathcal{H}} \\ + \|C(\eta)\| \left\| (C(0) + \gamma I_{\mathcal{H}})^{-1} \mu_z - C(0)^\dagger \mu_z \right\|_{\mathcal{H}} \\ \leq \frac{c^{1/2}}{\gamma} \|C_n(\eta) - C(\eta)\| + c \left\| (C(0) + \gamma I_{\mathcal{H}})^{-1} \mu_z - C(0)^\dagger \mu_z \right\|_{\mathcal{H}}.$$

The sum of the bounds (I) , $(*)$, and $(**)$ yields the total bound as given in (8.8) after rearranging. \blacksquare

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