Learning linear operators: Infinite-dimensional regression as a well-behaved non-compact inverse problem

Mattes Mollenhauer\textsuperscript{1}  
Nicole Mücke\textsuperscript{2}  
T. J. Sullivan\textsuperscript{3}

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Abstract. We consider the problem of learning a linear operator $\theta$ between two Hilbert spaces from empirical observations, which we interpret as least squares regression in infinite dimensions. We show that this goal can be reformulated as an inverse problem for $\theta$ with the feature that its forward operator is generally non-compact (even if $\theta$ is assumed to be compact or of $p$-Schatten class). However, we prove that, in terms of spectral properties and regularisation theory, this inverse problem is equivalent to the known compact inverse problem associated with scalar response regression.

Our framework allows for the elegant derivation of dimension-free rates for generic learning algorithms under Hölder-type source conditions. The proofs rely on the combination of techniques from kernel regression with recent results on concentration of measure for sub-exponential Hilbertian random variables. The obtained rates hold for a variety of practically-relevant scenarios in functional regression as well as nonlinear regression with operator-valued kernels and match those of classical kernel regression with scalar response.

Keywords. statistical learning • inverse problems • spectral regularisation • concentration of measure • functional data analysis • kernel regression • conditional mean embedding

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1. Introduction

Let $X$ and $Y$ be Bochner square-integrable random variables taking values in separable Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$ respectively. We aim to solve the following regression problem:

$$\text{minimise } \mathbb{E}[\|Y - \theta X\|_2^2] \equiv \|Y - \theta X\|_{L^2(P,\mathcal{Y})}^2 \text{ with respect to } \theta \in L(X, \mathcal{Y}), \quad \text{(RP)}$$

where $L(X, \mathcal{Y})$ denotes the Banach space of bounded linear operators from $\mathcal{X}$ into $\mathcal{Y}$. If at least one of $\mathcal{X}$ and $\mathcal{Y}$ has infinite dimension, then so too does the search space $L(X, \mathcal{Y})$, and so (RP) is an infinite-dimensional regression problem. We are particularly motivated by the case of infinite-dimensional $\mathcal{Y}$, exemplified by relevant applications in functional linear regression with functional response (Ramsay and Silverman, 2005), non-parametric regression with vector-valued...
kernels (Caponnetto and De Vito, 2007; Li et al., 2024; Meunier et al., 2024), the conditional mean embedding (Park and Muandet, 2020; Li et al., 2022) and inference for Hilbertian time series (Bosq, 2000). We will discuss each of these applications in the context of our results in more detail in Section 5. We assume that the joint distribution \( \mathcal{L}(X,Y) \) of \( X \) and \( Y \) is not known explicitly and \((RP)\) must be solved approximately based on sample pairs drawn from \( \mathcal{L}(X,Y) \). We approach this problem by proposing an inverse problem framework which generalises finite-dimensional ridge regression, principal component regression and various other techniques including iterative learning algorithms (e.g. gradient descent methods).

In contrast to finite-dimensional linear regression, the infinite-dimensional analogue does not necessarily admit a minimiser. Under the assumption of a \textit{linear model}, i.e. the existence of a bounded linear operator \( \theta^\ast : X \to Y \) such that

\[
Y = \theta^\ast X + \varepsilon
\]

with an exogeneous \( Y \)-valued noise variable \( \varepsilon \) satisfying \( \mathbb{E}[\varepsilon|X] = 0 \) — which may be interpreted as the \textit{well-specified case} in the context of statistical learning theory — it is known that the regression problem \((RP)\) can be solved via the \textit{operator factorisation problem}

\[
C_{YX} = \theta C_{XX}, \quad \theta \in L(X,Y),
\]

\text{(OFP)}

where \( C_{YX} \in L(X,Y) \) and \( C_{XX} \in L(X,X) \) are the \textit{covariance operators} (Baker, 1973) associated with \( X \) and \( Y \), which is again related to an well-known set of range inclusion and operator majorisation conditions due to Douglas (1966) and the Moore–Penrose pseudoinverse (Engl et al., 1996). The representation of linear conditional expectations in terms of pseudoinverses of covariance operators has also been investigated recently by Klebanov et al. (2021).

The above operator factorisation problem \text{(OFP)} can be reformulated in terms of a (potentially ill-posed) \textit{linear inverse problem}

\[
A_{C_{XX}}[\theta] = C_{YX}, \quad \theta \in L(X,Y)
\]

\text{(IP)}

based on the (generally non-compact) \textit{forward operator} \( A_{C_{XX}} : L(X,Y) \to L(X,Y) \) given by

\[
A_{C_{XX}}[\theta] := \theta C_{XX}.
\]

We call the operator \( A_{C_{XX}} \) the \textit{precomposition operator} associated with \( C_{XX} \).

We show that, even in the \textit{misspecified case} (i.e. without the assumption of a linear model), the solution to the inverse problem \text{(IP)} still characterises the minimiser of the linear regression problem \((RP)\). We argue that, due to this fact, our viewpoint is the natural generalisation of finite-dimensional least squares regression. We will revisit this perspective later on and compare \text{(IP)} to the well-known inverse problem associated with scalar-valued response regression.

**Main results.** Motivated by the ultimate need for a regularised empirical solution to the inverse problem, we give a characterisation of the spectrum of the precomposition operator. In particular it turns out that, \textit{although} \( A_{C_{XX}} \) \textit{is generally non-compact, the spectra of} \( A_{C_{XX}} \) \textit{and} \( C_{XX} \) \textit{coincide} (Theorem 3.18). As \( C_{XX} \) is self-adjoint and compact, we show that the non-compact inverse problem \text{(IP)} can be regularised as if it were a compact inverse problem. Thus, one key message of this article is that, from a regularisation standpoint, when the random variable \( X \) is assumed to be infinite-dimensional,

\[
\text{predicting an infinite-dimensional random variable} \ Y \ \text{is “just as hard” as predicting a finite-dimensional random variable} \ Y \ \text{based on information provided by} \ X.
\]
We show that convergence proof techniques for functional regression and kernel regression with finite-dimensional $Y$ can be used — with surprisingly minor adaptations — for infinite-dimensional $Y$. As these techniques and the empirical theory of covariance operators have seen rapid development over recent years, this opens up a powerful arsenal of tools for the infinite-dimensional learning problem. We underline this point by proving basic rates for generic learning algorithms (i.e. regularisation strategies) by modifying approaches from the kernel community. The rates obtained match known rates for kernel regression under comparable assumptions.

**Scope of this paper.** This paper has two main goals.

(a) The primary focus of this paper is to investigate the *population formulation* of linear regression for Hilbert-valued random variables. Although this concept has gained interest in terms of *learning linear operators* in machine learning and functional data analysis, the mathematical background in the general context of inverse problems is novel.

(b) We also contribute to the population formulation by providing the functional-analytic framework for our secondary goal, namely the *statistical analysis of regularised empirical solutions*. We tackle this problem by modifying proof techniques developed by the statistical learning community for kernel-based regression in combination with concentration bounds for sub-exponential Hilbertian random variables. However, we do not yet provide an entirely exhaustive statistical analysis; instead we aim to lay the groundwork for a unified empirical theory, with further results such as *fast rates* and *optimal rates* under additional regularity assumptions deferred to future work.

**Remark 1.1 (Precomposition and operator factorisation).** Problem (OPP) is a special case of a general operator factorisation problem: given spaces $X$ and $Y$ and operators $B \in L(X,Y)$ and $C \in L(X,X)$, find an operator $\theta \in L(X,Y)$ such that $B = \theta C$. This problem can be approached as an inverse problem à la (IP), i.e. $A_C[\theta] = B$, and it would certainly be interesting to explore the power and limitations of this approach. However, it suffices for our present purposes to consider only instances of $B = \theta C$ arising from problem (RP), which offers several simplifications: the operators $B = C_{YX}$ and $C = C_{XX}$ are of trace class, $C_{XX}$ is self-adjoint and positive, and $C_{YX}$ is “almost” dominated by $C_{XX}$ in the sense that, for some operator $R$ of at most unit norm, $C_{YX} = C_{YY}^{1/2} R C_{XX}^{1/2}$ (Baker, 1973, Theorem 1).

**Remark 1.2 (Spectral theory of precomposition operators).** Although we investigate the spectrum of the precomposition operator in order to understand the regularisation of (IP), our spectral-theoretic results apply to general precomposition operators which are not necessarily related to covariance operators. As composition operators can be understood as *tensor products of linear operators* acting on tensor products of Hilbert spaces (Aubin, 2000, Section 12.4), these results may be relevant in other disciplines involving a similar functional-analytic background.

**Remark 1.3 (Related work).** The theory of learning linear operators on infinite-dimensional spaces has gained significant attention over the last years. However, in contrast to our present work, the current literature seems to almost exclusively consider problem settings and assumptions which are rather specific. Notable examples include the approximation of $L^p$-space operators based on reproducing kernels (e.g. Mollenhauer and Koltai, 2020, Li et al., 2022, Kostic et al., 2022, Jin et al., 2023) and functional regression with functional response (e.g. Crambes and Mas, 2013, Hörmann and Kidziński, 2015, Benatia et al., 2017, Imaizumi and Kato, 2018). As we discuss later, estimators for these settings can be viewed as special cases of our framework in some instances. We also point out the more recent work by de Hoop et al. (2023), who investigate a Bayesian estimator in a Hilbertian linear model when the eigenfunctions of the ground truth operator are known a priori, allowing for a detailed statistical investigation.
2. Notation and setup of the problem

Random variables of interest. Let $X$ and $Y$ be random variables defined on a common probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and taking values in separable real Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$ respectively. We require that $X$ and $Y$ each have finite second moment, i.e. that $X$ and $Y$ lie in the Bochner spaces $L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathcal{X})$ and $L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathcal{Y})$ respectively. To save space, we usually shorten $L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathcal{X})$ to $L^2(\mathbb{P}; \mathcal{X})$ or even to $L^2(\mathbb{P})$ when $\mathcal{X} = \mathbb{R}$. See e.g. Diestel and Uhl (1977, Section II.2) for a comprehensive treatment of the Bochner integral. We write $\mathcal{L}(\mathcal{X})$ for the distribution or law of $X$ on the measurable space $(\mathcal{X}, \mathcal{B}_\mathcal{X})$ (i.e. the pushforward measure of $\mathbb{P}$ under $X$), where $\mathcal{B}_\mathcal{X}$ denotes the Borel $\sigma$-algebra of $\mathcal{X}$. We write $\mathcal{F}_X$ for the $\sigma$-algebra generated by $X$, i.e. the coarsest one on $\Omega$ with respect to which $X$ is a measurable function from $(\Omega, \mathcal{F})$ into $(\mathcal{X}, \mathcal{B}_\mathcal{X})$.

Spaces of operators. We write $L(\mathcal{X}, \mathcal{Y})$ for the Banach space of bounded linear operators from $\mathcal{X}$ to $\mathcal{Y}$ and write either $\|A\|_{L(\mathcal{X}, \mathcal{Y})}$ or $\|A\|_{\mathcal{X} \to \mathcal{Y}}$ for the operator norm of a linear operator $A : \mathcal{X} \to \mathcal{Y}$. The Banach space of compact linear operators from $\mathcal{X}$ to $\mathcal{Y}$, also equipped with the operator norm, will be denoted $S_\infty(\mathcal{X}, \mathcal{Y})$. For $1 \leq p < \infty$, $S_p(\mathcal{X}, \mathcal{Y}) \subseteq S_\infty(\mathcal{X}, \mathcal{Y})$ denotes the Banach space of $p$-Schatten class operators from $\mathcal{X}$ to $\mathcal{Y}$, i.e. those whose singular value sequence is $p^{th}$-power summable, with the norm being the $\ell^p$ norm of the singular value sequence. For $p = 1$ we obtain the trace class operators; for $p = 2$ we obtain the Hilbert–Schmidt operators. We have $S_p(\mathcal{X}, \mathcal{Y}) \subseteq S_q(\mathcal{X}, \mathcal{Y})$ for $p \leq q$. The class $S_2(\mathcal{X}, \mathcal{Y})$ is a Hilbert space with respect to the inner product

$$\langle A, B \rangle_{S_2(\mathcal{X}, \mathcal{Y})} := \text{tr}(A^* B). \quad (2.1)$$

Naturally, we shorten $L(\mathcal{X}, \mathcal{Y})$ to $L(\mathcal{X})$, $S_p(\mathcal{X}, \mathcal{Y})$ to $S_p(\mathcal{X})$, etc.

Hilbert tensor products. For $y \in \mathcal{Y}$ and $x \in \mathcal{X}$, $y \otimes x \in L(\mathcal{X}, \mathcal{Y})$ is the rank-one operator

$$\mathcal{X} \ni v \mapsto (y \otimes x)(v) := \langle x, v \rangle_{\mathcal{X}} y \in \mathcal{Y}. \quad (2.2)$$

The Hilbert tensor product $\mathcal{Y} \otimes \mathcal{X}$ is defined to be the completion of the linear span of all such rank-one operators with respect to the inner product $\langle y \otimes x, y' \otimes x' \rangle_{\mathcal{Y} \otimes \mathcal{X}} := \langle y, y' \rangle_{\mathcal{Y}} \langle x, x' \rangle_{\mathcal{X}}$. We will freely use the isometric isomorphisms $S_2(\mathcal{X}, \mathcal{Y}) \cong \mathcal{Y} \otimes \mathcal{X}$ and $L^2(\mathbb{P}; \mathcal{X}) \cong L^2(\mathbb{P}; \mathbb{R}) \otimes \mathcal{X}$ (Aubin, 2000, Chapter 12). Note that

$$\|y \otimes x\|_{S_p(\mathcal{X}, \mathcal{Y})} = \|x\|_{\mathcal{X}} \|y\|_{\mathcal{Y}} \quad \text{for any } x \in \mathcal{X}, \ y \in \mathcal{Y}, \ \text{and } 1 \leq p \leq \infty. \quad (2.3)$$
Covariance operators. The (uncentred) covariance operators (Baker, 1973) of $Y$ with $X$, and of $X$ with itself, are given by

$$C_{YX} := \text{Cov}[Y, X] := E[Y \otimes X] \in S_1(\mathcal{X}, \mathcal{Y})$$
$$C_{XX} := \text{Cov}[X, X] := E[X \otimes X] \in S_1(\mathcal{X}).$$

(2.4)

(2.5)

Note that $C_{YX} = C_{XY}$, and so $C_{XX}$ is self-adjoint. The covariance operators are the unique operators satisfying

$$E[(y, Y)_Y(x, X)_X] = \langle y, C_{YX}x \rangle_\mathcal{Y} \quad \text{for all } x \in \mathcal{X}, y \in \mathcal{Y}.$$ 

Moreover, for all $X_1, X_2 \in L^2(\mathbb{P}; \mathcal{X})$,

$$(X_1, X_2)_{L^2(\mathbb{P}; \mathcal{X})} = \text{tr}(\text{Cov}[X_1, X_2]).$$

For any $\theta \in L(\mathcal{X}, \mathcal{Y})$, $\text{Cov}[Y, \theta X] = \text{Cov}[Y, X]\theta^*$ (Klebanov et al., 2021, Lemma A.6), which also implies that $\text{Cov}[^*\theta Y, X] = \theta \text{Cov}[Y, X]$. It can additionally be shown that $\mathbb{P}[X \in \text{ran}(C_{XX})] = 1$ (Hsing and Eubank, 2015, Theorem 7.2.5), and hence that $\mathbb{P}[X \in \ker(C_{XX}) \setminus \{0\}] = 0$.

Pseudoinverses. Given $A \in L(\mathcal{X}, \mathcal{Y})$, its Moore–Penrose pseudoinverse $A^\dagger : \text{dom}(A^\dagger) \to \mathcal{X}$ is the unique extension of the bijective operator

$$(A|_{\ker(A)}^{-1})^{-1} : \text{ran}(A) \to \ker(A)^{\perp}$$

to a linear operator $A^\dagger$ defined on $\text{dom}(A^\dagger) := \text{ran}(A) \oplus \ker(A)^{\perp} \subseteq \mathcal{Y}$ subject to the criterion that $\ker(A^\dagger) = \text{ran}(A)^{\perp}$. In general, $\text{dom}(A^\dagger)$ is a dense but proper subspace of $\mathcal{Y}$ and $A^\dagger$ is an unbounded operator; global definition and boundedness of $A^\dagger$ occur precisely when $\text{ran}(A)$ is closed in $\mathcal{Y}$. For $y \in \text{dom}(A^\dagger)$,

$$A^\dagger y = \arg \min \{ \|x\|_\mathcal{X} \mid x \text{ minimises } \|Ax - y\|_\mathcal{Y} \}.$$ 

In particular, for $y \in \text{ran} A$, $A^\dagger y$ is the minimum-norm solution of $Ax = y$. See e.g. Engl et al. (1996, Section 2.1) for a comprehensive treatment of the Moore–Penrose pseudoinverse.

3. Inverse problem: Identifying the optimal regressor

The purpose of this section is to characterise the solution of the infinite-dimensional regression problem (RP) in terms of an inverse problem involving the precomposition operator.

3.1. Precomposition operator

Here we define the precomposition operator $A_C$ induced by $C \in L(\mathcal{X})$ and establish its key properties. At this stage $C$ is not required to be the (self-adjoint, positive semi-definite, trace-class) covariance operator $C_{XX}$, although that is the main use case that we have in mind.

Definition 3.1 (Precomposition). Given $C \in L(\mathcal{X})$, the associated precomposition operator $A_C : L(\mathcal{X}, \mathcal{Y}) \to L(\mathcal{X}, \mathcal{Y})$ is defined by

$$A_C[\theta] := \theta C.$$ 

Lemma 3.2 (Basic properties of the precomposition operator). Let $C \in L(\mathcal{X})$ and $1 \leq p \leq \infty$. Then $A_C : L(\mathcal{X}, \mathcal{Y}) \to L(\mathcal{X}, \mathcal{Y})$ admits the following properties:
(a) \(A_C\) is bounded with \(\|A_C\|_{L(L(X,Y))} = \|C\|_{L(X)}\);
(b) \(A_{B+C} = cA_B + A_C\) for all \(c \in \mathbb{R}\) and \(B \in L(X)\);
(c) \(A_C\) is injective if and only if \(C^*\) is injective;
(d) if \(C \in S_p(X)\), then \(\text{ran}(A_C) \subseteq S_p(X,Y)\); and
(e) the subspaces \(S_p(X,Y) \subseteq L(X,Y)\) are invariant under the action of \(A_C\), i.e.
\[\text{ran}(A_C) \subseteq S_p(X,Y).\]

**Remark 3.3 (Precomposition on \(p\)-Schatten classes).** The invariance of the \(p\)-Schatten classes (Lemma 3.2(e)) allows the precomposition operator \(A_C\) to be considered as an operator on \(S_p(X,Y)\) instead — with its domain and range equipped with the corresponding \(p\)-Schatten norm. We indicate to which norm we refer by adding corresponding subscripts to the operator
\[\|A_C[\theta]\|_{S_p(X,Y)} \leq \|C\|_{L(X)} \|\theta\|_{S_p(X,Y)}.
\]
for all \(\theta \in S_p(X,Y)\) and \(1 \leq p \leq \infty\), and the proof strategy is the same as for Lemma 3.2(a).

**Proof of Lemma 3.2.** (a) The upper bound
\[\|A_C\|_{L(L(X,Y))} \leq \|C\|_{L(X)}\]
follows from submultiplicativity of the operator norm. To see that equality holds, let \(y \in Y\) have unit norm. Then
\[
\sup_{x \in X, \|x\|_X = 1} \|A_C[y \otimes x]\|_{L(X,Y)} = \sup_{x \in X, \|x\|_X = 1} \|(y \otimes x)C\|_{L(X,Y)} = \sup_{x \in X, \|x\|_X = 1} \|y \otimes (C^*x)\|_{L(X,Y)} = \|C^*\|_{L(X)} \quad \text{(by (2.3) with } p = \infty)\]
\[
= \|C\|_{L(X)}.
\]

(b) Let \(\theta \in L(X,Y)\) and \(x \in X\) be arbitrary. Then
\[A_{cB+C}[\theta](x) := \theta((cB+C)(x)) = \theta(cBx + Cx) = c(\theta B)x + (\theta C)x = cA_B[\theta](x) + A_C[\theta](x),\]
i.e. \(A_{cB+C}[\theta] = cA_B[\theta] + A_C[\theta]\), i.e. \(A_{cB+C} = cA_B + A_C\), as claimed.

(c) Suppose that \(C^*\) is injective. We see that \(A_C[\theta] = \theta C = 0\) is equivalent to the fact that we have \(\text{ran}(C) \subseteq \ker(\theta)\). As \(\ker(\theta)\) is closed, this implies \(\overline{\text{ran}(C)} \subseteq \ker(\theta)\). Using that \(\overline{\text{ran}(C)} = \ker(C^*\perp) = X\) by assumption, we see that \(\theta = 0\), i.e. \(A_C\) is injective.

Conversely, suppose that \(A_C\) is injective. Then, for every \(\theta \neq 0\), \(A_C[\theta] = \theta C \neq 0\). By letting \(\theta\) vary over all rank-one operators from \(X\) to \(Y\), we see that \(\text{ran}(C)\) is dense in \(X\), which is equivalent to \(\overline{\text{ran}(C)} = \ker(C^*\perp) = X\) and finally \(\ker(C^*) = \{0\}\).

(d) Suppose that \(C \in S_p(X)\) and \(\theta \in L(X,Y)\). Then \(A_C[\theta] := C\theta \in S_p(X,Y)\) by the well-known fact that the Schatten classes are operator ideals.

(e) The proof of this claim is similar to that of (d).

**Remark 3.4 (Precomposition as operator tensor product).** When the precomposition operator \(A_C\) acts on \(S_2(X,Y)\), it can be shown that it is isomorphically equivalent to the operator tensor product \(C \otimes \text{Id}_Y\) on the tensor product space \(X \otimes Y \cong S_2(X,Y)\). Some of the above properties of \(A_C\) are proven in a more convenient way when using this representation.
3.2. Regression solution and inverse problem

The solution of the regression problem can be described by an inverse problem with the forward operator \( A_{XX} \). Note that, unless we restrict the true solution to be an element of \( S_2(\mathcal{X}, \mathcal{Y}) \), this is an inverse problem with a forward operator acting on the Banach space \( L(\mathcal{X}, \mathcal{Y}) \).

**Proposition 3.5** (Inverse problem). There exists an operator \( \theta_\ast \in L(\mathcal{X}, \mathcal{Y}) \) solving the regression problem (RP) if and only if
\[
C_{YY} \in \text{ran}(A_{XX}^\perp).
\]
(3.1)

The set of solutions of (RP) is exactly given by the solutions of the inverse problem (IP).

**Proof.** Given some \( \theta \in L(\mathcal{X}, \mathcal{Y}) \), we expand the objective functional of (RP) as
\[
E[\|Y - \theta X\|_Y^2] = \|Y\|_{L^2(\mathcal{X}, \mathcal{Y})}^2 - 2\langle Y, \theta X \rangle_{L^2(\mathcal{X}, \mathcal{Y})} + \|\theta X\|_{L^2(\mathcal{X}, \mathcal{Y})}^2.
\]
The first term does not depend on \( \theta \). It therefore suffices to minimise the last two terms, which can be reformulated as
\[
-2\langle Y, \theta X \rangle_{L^2(\mathcal{X}, \mathcal{Y})} + \|\theta X\|_{L^2(\mathcal{X}, \mathcal{Y})}^2 = -2\text{tr}(\text{Cov}[Y, \theta X]) + \text{tr}(\text{Cov}[\theta X, \theta X])
\]
\[
= -2\text{tr}(C_{YY} \theta^*) + \text{tr}(\theta C_{XX} \theta^*)
\]
\[
= \text{tr}(-2C_{YY} \delta^* + \theta C_{XX} \delta^* + \delta^* C_{XX} \theta).
\]
The minimum of \( F(\theta) \) is attained at \( \theta_\ast \) satisfying \( \frac{d}{d\theta} F(\theta_\ast) = 0 \in L(L(\mathcal{X}, \mathcal{Y}), \mathbb{R}) = L(\mathcal{X}, \mathcal{Y})' \). Computing the derivative of \( F \) at a point \( \theta_\ast \in L(\mathcal{X}, \mathcal{Y}) \) in a direction \( \delta \in L(\mathcal{X}, \mathcal{Y}) \) yields
\[
\frac{d}{d\theta} F(\theta)[\delta] = \text{tr}(\theta C_{YY} \delta^* + 2\theta C_{XX} \delta^* + \delta^* C_{XX} \theta).
\]
Since the trace is linear and invariant under forming the adjoint, the above term simplifies to
\[
\frac{d}{d\theta} F(\theta)[\delta] = \text{tr}(\theta C_{YY} \delta^* + 2\theta C_{XX} \delta^*)
\]
\[
= \text{tr}(\theta C_{YY} \delta^* + 2A_{XX} [\theta] \delta^*),
\]
which vanishes at some \( \theta_\ast \in L(\mathcal{X}, \mathcal{Y}) \) in all directions \( \delta \in L(\mathcal{X}, \mathcal{Y}) \) if and only if \( C_{YY} = A_{XX} [\theta_\ast] \), as claimed.

**Corollary 3.6** (Set of solutions). Assume that the regression problem (RP) admits a minimiser \( \theta_\ast \in L(\mathcal{X}, \mathcal{Y}) \). Then the set of operators in \( L(\mathcal{X}, \mathcal{Y}) \) solving (RP) is exactly given by
\[
\theta_\ast + \ker(A_{XX}) = \theta_\ast + \{ \theta \in L(\mathcal{X}, \mathcal{Y}) \mid \ker(\theta)^\perp \subseteq \ker(C_{XX}) \}.
\]

**Proof.** The fact that \( \theta_\ast + \ker(A_{XX}) \) is the set of solutions of (RP) is the immediate consequence of Proposition 3.5. Furthermore, it is clear that \( \ker(A_{XX}) \) consists precisely of the operators \( \theta \in L(\mathcal{X}, \mathcal{Y}) \) which satisfy \( \theta C_{XX} = 0 \), which are exactly those operators that satisfy the condition \( \ker(\theta)^\perp \subseteq \text{ran}(C_{XX})^\perp = \ker(C_{XX}) \).

Intuitively, Corollary 3.6 describes the fact that an optimal regressor \( \theta_\ast \in L(\mathcal{X}, \mathcal{Y}) \) may be arbitrarily modified in basis directions of the space \( \mathcal{X} \) which do not lie in the support of \( L'(\mathcal{X}) \), while still leading to a minimiser of (RP). As a consequence, the minimiser \( \theta_\ast \) is unique whenever the distribution of \( X \) has support on all basis directions of \( \mathcal{X} \).
Definition 3.7 (Non-degenerate distribution). We call the distribution $\mathcal{L}(X)$ of $X$ on $(\mathcal{X}, \mathcal{B}_X)$ non-degenerate if $C_{XX}$ is injective. Note that this is equivalent to the condition $E[(x, X)^2] \neq 0$ for all $x \in \mathcal{X} \setminus \{0\}$.

Corollary 3.8 (Unique solution). Assume that a minimiser $\theta_* \in L(\mathcal{X}, \mathcal{Y})$ of the regression problem (RP) exists. Then $\theta_*$ is unique if and only if the distribution $\mathcal{L}(X)$ is non-degenerate.

Proof. This follows directly from Lemma 3.2(c).

Corollaries 3.6 and 3.8 assume the existence of a minimiser $\theta_*$ for (RP), and so we now turn our attention to necessary and sufficient conditions for this hypothesis to hold.

3.3. Existence of the minimiser $\theta_* \in L(\mathcal{X}, \mathcal{Y})$

In contrast to finite-dimensional regression problems, the existence of the regression solution $\theta_* \in L(\mathcal{X}, \mathcal{Y})$ is not clear, and so this issue deserves special attention in the Hilbertian case.

We now give alternative characterisations of the necessary and sufficient conditions for this hypothesis to hold.

Remark 3.9 (Range of $A_{CXX}$ is dense). Let us briefly consider the operator $A_{CXX}$ acting on the Hilbert space $S_2(\mathcal{X}, \mathcal{Y})$ as described in Remark 3.3. We assume that $C_{XX}$ is injective. Using the fact that $A_{CXX}$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_{S_2(\mathcal{X}, \mathcal{Y})}$ (proved in Theorem 3.18(b)) together with the equivalence $C_{XX}$ injective $\iff$ $A_{CXX}$ injective from Lemma 3.2(c), we see that

$$\text{ran}(A_{CXX})^\perp \|_{S_2(\mathcal{X}, \mathcal{Y})} = \text{ker}(A_{CXX})^\perp = S_2(\mathcal{X}, \mathcal{Y}),$$

i.e. $\text{ran}(A_{CXX})$ is dense in $S_2(\mathcal{X}, \mathcal{Y})$ with respect to the Hilbert–Schmidt norm. It follows that $\text{ran}(A_{CXX})$ is dense in $S_2(\mathcal{X}, \mathcal{Y})$ with respect to the operator norm.

Before investigating the condition for the existence of $\theta_*$ given in (3.1) in more detail, we justify our approach with a classical example: If the true relationship between $Y$ and $X$ is linear, then our theory naturally gives the “correct” solution to the regression problem.

Example 3.10 (Linear model). Assume that the relation between $Y$ and $X$ is given in terms of the linear model

$$Y = \theta_* X + \varepsilon \quad \text{(LM)}$$

for some $\theta_* \in L(\mathcal{X}, \mathcal{Y})$ and $\varepsilon \in L^2(\mathcal{P}; \mathcal{Y})$ such that the exogeneity condition $E[\varepsilon \mid X] = 0$ holds. In this case, $C_{YX} \in \text{ran}(A_{CXX})$, since (LM) yields

$$Y \otimes X = \theta_* X \otimes X + \varepsilon \otimes X \implies C_{YX} = \theta_* C_{XX} + C_{\varepsilon X}.$$

Since $C_{\varepsilon X} = E[\varepsilon \otimes X] = E[E[\varepsilon \mid X] \otimes X] = 0$, this implies $C_{YX} = A_{CXX}(\theta_*)$. This confirms Proposition 3.5 in the setting that the linear regression problem is well-specified in the context of statistical learning theory. Note that the linear model above is equivalent to assuming the validity of the linear conditional expectation (Klebanov et al., 2021) representation

$$E[Y \mid X] = \theta_* X \quad \text{P-a.s.} \quad \text{(LCE)}$$
This equivalence is easy to see, since (LM) and the exogeneity condition together yield (LCE). For the converse implication, we consider the orthogonal projection operator \( \Pi: L^2(\mathbb{P}; \mathcal{Y}) \rightarrow L^2(\mathbb{P}; \mathcal{Y}) \) onto the closed subspace \( L^2(\mathbb{R}, F^X, \mathbb{P}; \mathcal{Y}) \subseteq L^2(\mathbb{P}; \mathcal{Y}) \) of \( F^X \)-measurable functions and \( \Pi^\perp := \text{Id}_{L^2(\mathbb{P}; \mathcal{Y})} - \Pi \). Using this notation, the characterisation of the conditional expectation as an \( L^2 \)-projection yields that \( \Pi \mathcal{Y} = \mathcal{E}[\mathcal{Y}|X] \). Performing the orthogonal decomposition \( \mathcal{Y} = \Pi \mathcal{Y} + \Pi^\perp \mathcal{Y} \) and defining \( \varepsilon := \Pi^\perp \mathcal{Y} \) yield (LM). Note that \( \varepsilon \) satisfies the exogeneity assumption, since \( \mathcal{E}[\varepsilon|X] = \Pi \varepsilon = \Pi (\Pi^\perp \mathcal{Y}) = 0 \).

Moreover, the existence of \( \theta_* \) can be characterised alternatively in terms of a well-known range inclusion and majorisation condition due to Douglas (1966). Note that (3.1) can equivalently be expressed as
\[
C_{\mathcal{Y}X} = \theta_* C_{XX}, \quad \theta_* \in L(\mathcal{X}, \mathcal{Y}),
\] (3.2)
which can be interpreted a factorisation of \( C_{\mathcal{Y}X} \) into a known operator \( C_{XX} \) and some bounded operator \( \theta_* \). This fact links (RP) directly to Douglas’ work. We list important equivalent conditions for the existence of this factorisation here for completeness and give a closed-form solution of the regression problem.

**Proposition 3.11** (Existence of \( \theta_* \in L(\mathcal{X}, \mathcal{Y}) \) and closed form). The following conditions are equivalent to the existence of an operator \( \theta_* \in L(\mathcal{X}, \mathcal{Y}) \) which solves (RP):

(a) We have \( C_{\mathcal{Y}X} = A_{C_{XX}} [\theta_*] = \theta_* C_{XX} \) for some \( \theta_* \in L(\mathcal{X}, \mathcal{Y}) \).

(b) We have \( \text{ran}(C_{XY}) \subseteq \text{ran}(C_{XX}) \).

(c) The operator \( \beta C_{\mathcal{Y}X}^2 - C_{XY} C_{\mathcal{Y}X} \) is positive for some \( \beta \in \mathbb{R} \).

(d) The operator \( C_{XX}^\dagger C_{XY} : \mathcal{Y} \rightarrow \mathcal{X} \) is well-defined and bounded.

(e) For all \( y \in \mathcal{Y} \),
\[
\sup_{x \in \mathcal{X}} \frac{|\mathcal{E}[\langle x, X \rangle, \langle y, Y \rangle]|}{\|C_{XX} x\|_{\mathcal{X}}} < \infty.
\] (3.3)

If the above conditions are satisfied, then \( \theta_* := (C_{XX}^\dagger C_{XY})^* \) is a closed-form solution of (RP). Moreover, \( \theta_* = (C_{XX}^\dagger C_{XY})^* \) is the unique solution of (RP) satisfying
\[
\ker(\theta_*)^\perp \subseteq \ker(C_{XX})^\perp \quad \text{or equivalently} \quad \theta_*|_{\ker(C_{XX})} = 0
\] (3.4)
and its operator norm is given by
\[
\|\theta_*\|_{\mathcal{X} \rightarrow \mathcal{Y}} = \sup_{x \in \mathcal{X}} \frac{\|C_{YX} x\|_{\mathcal{Y}}}{\|C_{XX} x\|_{\mathcal{X}}},
\] (3.5)

**Proof.** The equivalence of (a)–(c) is due to Douglas (1966, Theorem 1), and the equivalence of (d) follows from Klebanov et al. (2021, Theorem A.1). The proof of the equivalence of (e) relies on a lesser known equivalent characterisation of Douglas’ range inclusion theorem due to Shmul’yan (1967, Lemma 1), which asserts that \( x_0 \in \mathcal{X} \) belongs to \( \text{ran}(C_{XX}) \) if and only if
\[
\sup_{x \in \mathcal{X}} \frac{|\langle x, x_0 \rangle_{\mathcal{X}}|}{\|C_{XX} x\|_{\mathcal{X}}} < \infty;
\]
see also Fillmore and Williams (1971, Corollary 2). Therefore, \( \text{ran}(C_{XY}) \subseteq \text{ran}(C_{XX}) \) if and only if the condition
\[
\sup_{x \in \mathcal{X}} \frac{|\langle x, C_{XX} y \rangle_{\mathcal{X}}|}{\|C_{XX} x\|_{\mathcal{X}}} < \infty,
\]
\footnote{See e.g. Kallenberg (2021, Chapter 8) for the real-valued conditional expectation. The vector-valued case follows analogously in the context of the Bochner-\( L^2 \) space.}
is satisfied for all \( y \in \mathcal{Y} \), proving the claim. The given uniqueness criteria in (3.4), various additional properties of the unique solution \( \theta = (C_{XX}^t C_{XY})^* \) as well as the role of the pseudoinverse are well known in the context of operator factorisation (Arias et al., 2008; Fillmore and Williams, 1971; Shmulyan, 1967). In order to obtain the norm of \( \theta_* \) given in (3.5), we apply Shmulyan (1967, Lemma 2c) to the adjoint of \( \theta_* \).

**Remark 3.12 (Existence of \( \theta_* \in L(\mathcal{X}, \mathcal{Y}) \)).** A few remarks about Proposition 3.11 are in order.

(a) We emphasise that, in general, \((C_{XX}^t C_{XX})^* \neq C_{XY} C_{XX}^t \). In particular, note that \( C_{XX}^t \) as well as \( C_{XX}^t C_{XX}^* \) are not globally defined whenever \( \mathcal{X} \) is infinite-dimensional. Indeed, as discussed in the proof above, \((C_{XX}^t C_{XX})^* \) is globally defined and bounded if and only if the equivalent conditions given in Proposition 3.11 hold. The closed-form characterisation of the regression solution as \( \theta_* = (C_{XX}^t C_{XY})^* \) can be understood as the mathematically informal representation

\[
\theta_* = A_{C_{XX}} [C_{YX}]
\]

in the context of our framework. Note that \( A_{C_{XX}} \) is not rigorously defined as an operator acting on \( L(\mathcal{X}, \mathcal{Y}) \). However, we argue that our approach is the natural way to discuss the solution of this problem, as the precomposition operator will later allow us to consider the direct regularisation of \( C_{XX} \) in the composition \( \theta_* = (C_{XX}^t C_{XY})^* \) in a convenient way.

(b) The characterisation of all solutions of (RP) given in Corollary 3.6 together with (3.4) shows that \( \theta_* = (C_{XX}^t C_{XY})^* \) is the unique solution with the largest nullspace. All other solutions of (RP) perform operations on \( \ker(C_{XX}) \) which are irrelevant for the regression.

(c) As also noted by Klebanov et al. (2021), it is easy to see that the equivalent conditions given in Proposition 3.11 are always satisfied whenever \( \mathcal{X} \) is finite-dimensional, as in this case \( C_{XX}^t \) is always bounded.

### 3.4. Constraining the problem: Hilbert–Schmidt regression

Instead of (RP), in which \( \theta \) is required merely to be a bounded operator, we may consider the constrained *Hilbert–Schmidt regression problem*

\[
\min_{\theta \in S_2(\mathcal{X}, \mathcal{Y})} \mathbb{E}[\|Y - \theta X\|_2^2]. \tag{HSRP}
\]

with the solution space \( S_2(\mathcal{X}, \mathcal{Y}) \). It is straightforward to see that the results from Section 3.2 remain valid for this constrained problem when \( A_{C_{XX}} : L(\mathcal{X}, \mathcal{Y}) \to L(\mathcal{X}, \mathcal{Y}) \) is replaced with the modified precomposition operator \( A_{C_{XX}} : S_2(\mathcal{X}, \mathcal{Y}) \to S_2(\mathcal{X}, \mathcal{Y}) \). Instead of (IP), we now consider the modified inverse problem

\[
A_{C_{XX}} [\theta] = C_{YX}, \quad \theta \in S_2(\mathcal{X}, \mathcal{Y}). \tag{HSIP}
\]

We emphasise that the “HS” in (HSIP) refers only to the fact that the search space consists of Hilbert–Schmidt operators \( \theta \); as we shall see, the forward operator \( A_{C_{XX}} \) is generally not even compact, let alone Hilbert–Schmidt. The restriction allows us to apply concepts from the rich theory of inverse problems in Hilbert spaces (Engl et al., 1996), which significantly simplifies the regularisation and empirical solution of the regression problem. The restriction to the solution space \( S_2(\mathcal{X}, \mathcal{Y}) \) in (HSIP) is quite standard in a multitude of practical applications of infinite-dimensional regression (see Section 5).

**Remark 3.13 (Existence of \( \theta_* \in S_2(\mathcal{X}, \mathcal{Y}) \)).** The existence of an operator \( \theta_* \in S_2(\mathcal{X}, \mathcal{Y}) \) which solves (HSRP) is clearly equivalent to \( C_{YX} \in \text{ran}(A_{C_{XX}}) \) with \( A_{C_{XX}} : S_2(\mathcal{X}, \mathcal{Y}) \to S_2(\mathcal{X}, \mathcal{Y}) \).
We now express solutions of \((\text{HSRP})\) in terms of the pseudoinverse operator

\[
A_{\text{XX}}^\dagger : S_2(\mathcal{X}, \mathcal{Y}) \supseteq \text{dom}(A_{\text{XX}}^\dagger) \to S_2(\mathcal{X}, \mathcal{Y}),
\]

where \(\text{dom}(A_{\text{XX}}^\dagger) = \text{ran}(A_{\text{XX}}) \oplus \text{ran}(A_{\text{XX}})^\perp\). The next result shows that, whenever a solution of \((\text{HSRP})\) exists, the known closed-form solution \(\theta_* = (C_{\text{XX}}^\dagger C_{\text{XY}})^*\) is not only bounded but even Hilbert–Schmidt, and it is recovered in a natural way when the inverse problem in \(S_2(\mathcal{X}, \mathcal{Y})\) is solved via the pseudoinverse operator.

**Proposition 3.14 (Pseudoinverse solution).** Assume there exists a solution of \((\text{HSRP})\), i.e. assume that \(C_{\text{XY}} \in \text{ran}(A_{\text{XX}})\) with \(A_{\text{XX}} : S_2(\mathcal{X}, \mathcal{Y}) \to S_2(\mathcal{X}, \mathcal{Y})\). Then

\[
\theta_* := (C_{\text{XX}}^\dagger C_{\text{XY}})^* = A_{\text{XX}}^\dagger [C_{\text{XY}}].
\]

In particular, \(\theta_*\) defined in this way is the unique solution of \((\text{HSRP})\) of minimal norm in \(S_2(\mathcal{X}, \mathcal{Y})\).

**Proof.** Assume \(C_{\text{XY}} \in \text{ran}(A_{\text{XX}})\) with \(A_{\text{XX}} : S_2(\mathcal{X}, \mathcal{Y}) \to S_2(\mathcal{X}, \mathcal{Y})\). By the construction of the pseudoinverse, this implies that the operator factorisation \(C_{\text{XY}} = (A_{\text{XX}}^\dagger C_{\text{XX}}) C_{\text{XX}}\) holds and hence \(A_{\text{XX}}^\dagger [C_{\text{XY}}] \in S_2(\mathcal{X}, \mathcal{Y})\) clearly solves the Hilbert–Schmidt regression problem \((\text{HSRP})\) (and therefore also the bounded regression problem \((\text{RP})\)) due to Proposition 3.5. Furthermore, according to Proposition 3.11, the operator \(\theta := (C_{\text{XX}}^\dagger C_{\text{XY}})^*\) is bounded and solves the bounded regression problem \((\text{RP})\). Due to the characterisation of the set of bounded solutions in Corollary 3.6, both solutions \(\theta_*\) and \(A_{\text{XX}}^\dagger [C_{\text{XY}}]\) can only differ on \(\ker(C_{\text{XX}})\). To prove their equivalence, it is thus sufficient to show that they coincide on \(\ker(C_{\text{XX}})\). By construction of the pseudoinverse, we have \(A_{\text{XX}}^\dagger [C_{\text{XY}}]|_{\ker(C_{\text{XX}})} = 0\), since it is the minimal \(S_2(\mathcal{X}, \mathcal{Y})\)-norm solution of the operator factorisation \(C_{\text{XY}} = \theta C_{\text{XX}}\) for \(\theta \in L(\mathcal{X}, \mathcal{Y})\). Furthermore,

\[
\ker(\theta_*) = \text{ran}(\theta_*)^\perp = \text{ran}(C_{\text{XX}}^\dagger C_{\text{XY}})^\perp \supseteq \text{ran}(C_{\text{XX}}^\dagger)^\perp = \ker(C_{\text{XX}}),
\]

where the last equality follows again from the definition of the pseudoinverse. Since this implies \(\theta_*|_{\ker(C_{\text{XX}})} = 0\), the claim is proven.

We now give an equivalent characterisation of the requirement that \(\theta_* = (C_{\text{XX}}^\dagger C_{\text{XY}})^* \in S_2(\mathcal{X}, \mathcal{Y})\) in terms of a moment condition which can be interpreted as the Hilbert–Schmidt analogue of the condition given in Proposition 3.11(e).

**Proposition 3.15 (Existence of \(\theta_* \in S_2(\mathcal{X}, \mathcal{Y})\)).** The operator \(\theta_* = (C_{\text{XX}}^\dagger C_{\text{XY}})^*\) satisfies

\[
\|\theta_*\|_{S_2(\mathcal{X}, \mathcal{Y})}^2 = \sum_{i \in I} \sup_{x \in \mathcal{X}} \frac{\|E(\langle x, X \rangle_X \langle e_i, Y \rangle_Y)\|^2}{\|C_{XX} x\|_{\mathcal{X}}^2} = \|C_{XX} x\|_{\mathcal{X}}^2 - \|C_{XX} x\|_{\mathcal{X}}^2,
\]

where \(\{e_i\}_{i \in I}\) is a complete orthonormal system in \(\mathcal{Y}\) (i.e. \(\langle e_i, e_j \rangle_\mathcal{Y} = 1\) if \(i = j\) and \(\overline{\text{span}}\{e_i\}_{i \in I} = \mathcal{Y}\)). In particular, the expression (3.6) is independent of the choice of complete orthonormal system and the solution \(\theta_*\) of \((\text{HSRP})\) exists if and only if (3.6) is finite.

**Proof.** Clearly, a necessary condition for \(\theta_* = (C_{\text{XX}}^\dagger C_{\text{XY}})^*\) to be Hilbert–Schmidt is that \(\theta_*\) is bounded. According to Proposition 3.11, \(\theta_*\) therefore satisfies \(\ker(\theta_*)^\perp \subseteq \text{ran}(C_{\text{XX}})\) which is exactly the required condition for Shmulylan (1967, Lemma 2b) to hold. This yields

\[
\|\theta_* y\|_{\mathcal{X}} = \sup_{x \in \mathcal{X}} \frac{\langle C_{\text{XY}} y, x \rangle_{\mathcal{X}}}{\|C_{XX} x\|_{\mathcal{X}}} = \sup_{x \in \mathcal{X}} \frac{\|E(\langle x, X \rangle_X \langle y, Y \rangle_\mathcal{Y})\|}{\|C_{XX} x\|_{\mathcal{X}}}
\]
for all \( y \in \mathcal{Y} \). Hence, by definition of the Hilbert–Schmidt norm,
\[
\| \theta_* \|^2_{S_2(\mathcal{X}, \mathcal{Y})} = \| \theta_* \|^2_{S_2(\mathcal{Y}, \mathcal{X})} = \sum_{i \in I} \| \theta_* e_i \|^2_{\mathcal{X}} = \sum_{i \in I} \| E[\langle x, X \rangle, X] e_i, Y \|^2_{\mathcal{Y}} \frac{\| C_{XX} x \|^2_{\mathcal{X}}}{\| C_{XX} x \|^2_{\mathcal{Y}}}
\]
and clearly this expression is independent of the choice of complete orthonormal system. 

If (HSRP) has a solution, then we can characterise the set of all solutions of (HSRP):

**Remark 3.16** (Set of Hilbert–Schmidt solutions). Whenever \( \theta_* = (C_{XX}^\dagger C_{XY})^* \in S_2(\mathcal{X}, \mathcal{Y}) \), the set of all solutions of (HSRP) is given by
\[
\theta_* + \ker(A_{CXX}) = \theta_* + \{ \theta \in S_2(\mathcal{X}, \mathcal{Y}) | \ker(\theta) \perp \ker(C_{XX}) \}
\]
with \( A_{CXX} : S_2(\mathcal{X}, \mathcal{Y}) \to S_2(\mathcal{X}, \mathcal{Y}) \), which is a standard characterisation in the theory of inverse problems (see Engl et al., 1996, Theorem 2.5).

We emphasise that in general, analogously to the discussion in Remark 3.12, we have \( A_{CXX}^\dagger \neq A_{CXX}^{-1} \), as the latter does clearly not map to the space \( S_2(\mathcal{X}, \mathcal{Y}) \) whenever \( C_{XX}^\dagger \) is unbounded.

**Remark 3.17** (Inverse problem). As is standard in linear inverse problems theory, one may distinguish three regimes for the problem \( C_{XX} = A_{CXX} \theta \) with \( \theta \in S_2(\mathcal{X}, \mathcal{Y}) \):
(a) \( C_{XX} \in \text{ran}(A_{CXX}) \), in which case \( \theta_* \) does exist, as previously discussed;
(b) \( C_{XX} \notin \text{ran}(A_{CXX}) \), which case \( C_{XX} \) can be arbitrarily well approximated by a sequence of \( C_{XX}^k \in \text{ran}(A_{CXX}) \), leading to approximate regression solutions \( \theta^k = A_{CXX}^\dagger C_{XX}^k \) which fail to converge in \( \mathcal{X} \) as \( k \to \infty \) due to the unboundedness of the pseudoinverse operator \( A_{CXX}^\dagger \);
(c) \( C_{XX} \notin \text{ran}(A_{CXX}) \), which is ruled out as soon as \( C_{XX} \) is injective (cf. Lemma 3.2(c) and Remark 3.9).

### 3.5. Spectral properties of \( A_C \)

The characterisation of the minimiser \( \theta_* \) in terms of an inverse problem motivates us to investigate the spectral properties of the operator \( A_C \) before we address the regularisation and corresponding empirical solutions.

Recall the following definitions of the point, continuous, and residual spectrum of a linear operator \( T \in L(\mathcal{X}) \):
\[
\sigma_p(T) = \{ \lambda \in \mathbb{C} | T - \lambda \text{Id}_{\mathcal{X}} \text{ is not injective} \},
\sigma_c(T) = \{ \lambda \in \mathbb{C} | T - \lambda \text{Id}_{\mathcal{X}} \text{ is injective, not surjective, and } \text{ran}(T - \lambda \text{Id}_{\mathcal{X}}) = \mathcal{X} \},
\sigma_r(T) = \{ \lambda \in \mathbb{C} | T - \lambda \text{Id}_{\mathcal{X}} \text{ is injective, not surjective, and } \text{ran}(T - \lambda \text{Id}_{\mathcal{X}}) \neq \mathcal{X} \}.
\]

For \( \lambda \in \mathbb{C} \), we write
\[
eig_\lambda(T) \coloneqq \ker(T - \lambda \text{Id}_{\mathcal{X}}) = \{ v \in \mathcal{X} | Tv = \lambda v \},
\]
which is a non-trivial subspace of \( \mathcal{X} \) if and only if \( \lambda \in \sigma_p(T) \).

**Theorem 3.18** (Spectral properties of the precomposition operator). Let \( C \in L(\mathcal{X}) \) and consider the operator \( A_C : L(\mathcal{X}, \mathcal{Y}) \to L(\mathcal{X}, \mathcal{Y}) \).
Moreover, the operator $A$: $\mathcal{S}_2(\mathcal{X}, \mathcal{Y}) \rightarrow \mathcal{S}_2(\mathcal{X}, \mathcal{Y})$ admits the following properties:

(b) The adjoint of $A$ with respect to $\langle \cdot, \cdot \rangle_{\mathcal{S}_2(\mathcal{X}, \mathcal{Y})}$ is given by $A^* = A_{\mathcal{C}^*}$. In particular, if $C$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_\mathcal{X}$, then $A_C$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_{\mathcal{S}_2(\mathcal{X}, \mathcal{Y})}$.

(c) The spectra of $A_C$ and $C^*$ coincide, i.e.

\[
\sigma_p(A_C) = \sigma_p(C^*), \quad \text{(already covered in (a))}
\]
\[
\sigma_c(A_C) = \sigma_c(C^*),
\]
\[
\sigma_r(A_C) = \sigma_r(C^*).
\]

(d) Let $C$ be compact and self-adjoint with spectral decomposition

\[
C = \sum_{\lambda \in \sigma_p(C)} \lambda P_{\text{eig}_\lambda(C)},
\]

where $P_{\text{eig}_\lambda(C)}: \mathcal{X} \rightarrow \mathcal{X}$ denotes the orthogonal projection operator onto $\text{eig}_\lambda(C)$ and the above series expression converges in operator norm. Then $A_C$ has the spectral decomposition given by

\[
A_C = \sum_{\lambda \in \sigma_p(C)} \lambda P_{\mathcal{Y} \otimes \text{eig}_\lambda(C)},
\]

where $P_{\mathcal{Y} \otimes \text{eig}_\lambda(C)}: \mathcal{S}_2(\mathcal{X}, \mathcal{Y}) \rightarrow \mathcal{S}_2(\mathcal{X}, \mathcal{Y})$ denotes the orthogonal projection operator onto $\mathcal{Y} \otimes \text{eig}_\lambda(C)$ and the above series converges in operator norm.

(e) Let $C$ be compact and self-adjoint. $A_C$ is compact if and only if $\mathcal{Y}$ is finite-dimensional.

**Proof.**

(a) We first characterise the nullspace $\ker(A_C)$. Let $\theta \in L(\mathcal{X}, \mathcal{Y})$. Then

\[
0 = A_C[\theta] = \theta C \iff \text{ran}(C) \subseteq \ker(\theta)
\]
\[
\iff \overline{\text{ran}(C)} \subseteq \ker(\theta) \quad \text{(since $\ker(\theta)$ is closed)}
\]
\[
\iff \ker(C^*)^\perp \subseteq \ker(\theta),
\]

which is again equivalent to the condition that $\theta P_{\ker(C^*)} = 0$, where $P_{\ker(C^*)} \in L(\mathcal{X})$ is the orthogonal projection operator onto $\ker(C^*)$ and $P_{\ker(C^*)} := \text{Id}_\mathcal{X} - P_{\ker(C^*)}$ its complement. In total, for every $C \in L(\mathcal{X})$, the nullspace $\ker(A_C)$ consists exactly of the operators $\theta \in L(\mathcal{X}, \mathcal{Y})$ which satisfy

\[
\theta = \theta P_{\ker(C^*)}.
\]

Let now $\lambda \in \mathbb{C}$. Since we can easily verify $A_C - \lambda \text{Id}_{L(\mathcal{X}, \mathcal{Y})} = A_{C - \lambda \text{Id}_{\mathcal{X}}}$, we can apply the above reasoning and obtain

\[
eig_\lambda(A_C) = \ker(A_C - \lambda \text{Id}_{L(\mathcal{X}, \mathcal{Y})}) = \ker(A_{C - \lambda \text{Id}_{\mathcal{X}}}) = \{ \theta \in L(\mathcal{X}, \mathcal{Y}) \mid \theta = \theta P_{\ker(C^* - \lambda \text{Id}_{\mathcal{X}})} \}
\]
\[
= \{ \theta \in L(\mathcal{X}, \mathcal{Y}) \mid \theta = \theta P_{\text{eig}_\lambda(C^*)} \}.
\]

It is straightforward to verify that this set is exactly given by tensors in $\mathcal{Y} \otimes \text{eig}_\lambda(C^*)$, proving the claim.
(b) Let \( \theta_1, \theta_2 \in S_2(\mathcal{X}, \mathcal{Y}) \) and let \( C \in L(\mathcal{X}) \). Then
\[
(A_C[\theta_1], \theta_2)_{S_2(\mathcal{X}, \mathcal{Y})} = \text{tr}((\theta_1 C)^* \theta_2) = \text{tr}(C^* \theta_1^* \theta_2) = \text{tr}(\theta_1^* A_C^* \theta_2) = (\theta_1, A_C^* \theta_2)_{S_2(\mathcal{X}, \mathcal{Y})}.
\]
(c) Let \( \lambda \in \mathbb{C} \). We have already covered the equality of the point spectra of \( A_C \) and \( C^* \) in (a). We now address the continuous and the residual spectrum. First, we note that \( C^* - \lambda \text{Id}_\mathcal{X} \) is injective if and only if \( A_C - \lambda \text{Id}_{\mathcal{X}} = A_C - \text{Id}_{S_2(\mathcal{X}, \mathcal{Y})} \) is injective by Lemma 3.2(c). Furthermore,
\[
\text{ran}(C^* - \lambda \text{Id}_\mathcal{X}) = \ker(C - \lambda \text{Id}_\mathcal{X})^\perp \quad \text{and} \quad \text{ran}(A_C - \lambda \text{Id}_{S_2(\mathcal{X}, \mathcal{Y})}) = \ker(A_C^* - \lambda \text{Id}_\mathcal{X})^\perp = \ker((A_C - \lambda \text{Id}_\mathcal{X})^*)^\perp,
\]
where we use part (b) of this theorem and \( A_C - \lambda \text{Id}_{S_2(\mathcal{X}, \mathcal{Y})} = A_C - \lambda \text{Id}_\mathcal{X} \) in the second line. We have \( \ker(C - \lambda \text{Id}_\mathcal{X}) = \{0\} \iff \ker(A_C^* - \lambda \text{Id}_\mathcal{X}) = \{0\} \) by Lemma 3.2(c). This implies that
\[
\text{ran}(C^* - \lambda \text{Id}_\mathcal{X}) = \mathcal{X} \iff \text{ran}(A_C - \lambda \text{Id}_{S_2(\mathcal{X}, \mathcal{Y})}) = S_2(\mathcal{X}, \mathcal{Y}).
\]

Therefore, as claimed, \( \lambda \in \sigma_c(C^*) \iff \lambda \in \sigma_c(A_C) \) and \( \lambda \in \sigma_p(C^*) \iff \lambda \in \sigma_p(A_C) \).

(d) Applying (a) to the spectral decomposition of \( C \) immediately proves the claim.

(e) By the spectral theorem for self-adjoint operators, \( A_C \) is compact if and only if each of its eigenspaces is finite-dimensional and its spectral decomposition series converges in operator norm. Combined with the fact that \( \text{eig}_\lambda(A_C) = \mathcal{Y} \otimes \text{eig}_\lambda(C) \) is finite-dimensional if and only if \( \mathcal{Y} \) is finite-dimensional, this proves the claim.

An important consequence of the above discussion is that, once \( C \) is self-adjoint and compact, the self-adjoint but generally non-compact \( A_C \) can be conveniently manipulated (and, in particular, regularised) using the functional calculus (Reed and Simon, 1980, Chapter VII).

**Corollary 3.19 (Compatibility with the functional calculus).** Let \( C \in L(\mathcal{X}) \) be compact and self-adjoint with the spectral decomposition \( C = \sum_{\lambda \in \sigma_p(C)} \lambda P_{\text{eig}_\lambda(C)} \). If \( g: \mathbb{R} \rightarrow \mathbb{R} \) is extended to act on self-adjoint Hilbert space operators with a discrete spectrum in terms of their spectral decompositions via
\[
g(C) := \sum_{\lambda \in \sigma_p(C)} g(\lambda) P_{\text{eig}_\lambda(C)},
\]
then \( A_C \) as an operator on \( S_2(\mathcal{X}, \mathcal{Y}) \) satisfies
\[
A_{g(C)} = g(A_C),
\]
with each series converging in operator norm if and only if the other does.

**Proof.** By Theorem 3.18, \( A_C: S_2(\mathcal{X}, \mathcal{Y}) \rightarrow S_2(\mathcal{X}, \mathcal{Y}) \) has the spectral decomposition
\[
A_C = \sum_{\lambda \in \sigma_p(C)} \lambda P_{\mathcal{Y} \otimes \text{eig}_\lambda(C)}.
\]
Thus,
\[
g(A_C) = \sum_{\lambda \in \sigma_p(C)} g(\lambda) P_{\mathcal{Y} \otimes \text{eig}_\lambda(C)} = A_{g(C)},
\]
which proves the claim.\[\]
4. Regularisation of Hilbert–Schmidt regression

Having discussed the general spectral theory of the precomposition operator \( A_C \) for some bounded operator \( C \in L(\mathcal{X}) \), we now return to our setting of Hilbert–Schmidt regression and the Hilbert space inverse problem (HSIP). It is noteworthy that the theory of regularisation in Banach spaces is technically more involved than the concepts we discuss here (e.g. Schuster et al., 2012). In our investigation, we mainly rely on Theorem 3.18 and Corollary 3.19, as they are sufficient for a basic understanding of the regularisation of our inverse problem (HSIP) in \( S_2(\mathcal{X}, \mathcal{Y}) \).

According to Proposition 3.14, we may consider the solution \( \theta_* = A_{C_{XX}}^\dagger [C_{YY}] \) whenever we assume that a solution of (HSRP) exists. Theorem 3.18(e) shows that the inverse problem is non-compact whenever \( \mathcal{Y} \) is infinite-dimensional. However, as the covariance operator \( C_{XX} \) is always Hilbert–Schmidt and self-adjoint, the operator \( A_{C_{XX}} \) is self-adjoint on \( S_2(\mathcal{X}, \mathcal{Y}) \) and Theorem 3.18(d) yields the spectral representation

\[
A_{C_{XX}} = \sum_{\lambda \in \sigma_p(C_{XX})} \lambda P_{YY|\sigma_{\lambda}(C_{XX})}.
\]

We now recall the concept of regularisation strategies for inverse problems in Hilbert spaces.

**Definition 4.1.** We call a family of functions \( g_{\alpha} : [0, \infty) \rightarrow \mathbb{R} \), indexed by a regularisation parameter \( \alpha > 0 \), a spectral regularisation strategy (Engl et al., 1996, Section 4) if it satisfies the following properties for all choices of \( \alpha \):

(R1) \( \sup_{\lambda \in [0,\infty)} |\lambda g_{\alpha}(\lambda)| \leq D \) for some constant \( D \),

(R2) \( \sup_{\lambda \in [0,\infty)} |1 - \lambda g_{\alpha}(\lambda)| \leq \gamma_0 \) for some constant \( \gamma_0 \), and

(R3) \( \sup_{\lambda \in [0,\infty)} |g_{\alpha}(\lambda)| \leq B \alpha^{-1} \), for some constant \( B \).

It will be convenient later to have the shorthand notation

\[
r_{\alpha}(\lambda) := 1 - \lambda g_{\alpha}(\lambda)
\]

for the residual associated to the regularisation scheme \( g_{\alpha} \), and both \( g_{\alpha} \) and \( r_{\alpha} \) will be applied to compact self-adjoint operators using the continuous functional calculus. Additionally, we define the qualification of \( g_{\alpha} \) as the maximal \( q \) such that

\[
\sup_{\lambda \in [0,\infty)} \lambda^q |r_{\alpha}(\lambda)| \equiv \sup_{\lambda \in [0,\infty)} \lambda^q |1 - \lambda g_{\alpha}(\lambda)| \leq \gamma_q \alpha^q
\]

for some constant \( \gamma_q \) which does not depend on \( \alpha \). If (4.2) holds for every positive number \( q \), then we say the regularisation strategy has arbitrary qualification. The above requirements for regularisation strategies are also commonly found in the context of learning theory (see e.g. Bauer et al., 2007; Gerfo et al., 2008; Dicker et al., 2017; Blanchard and Mücke, 2018).

We call \( g_{\alpha}(A_{C_{XX}}) \) the regularised inverse of \( A_{C_{XX}} \). According to Corollary 3.19,

\[
g_{\alpha}(A_{C_{XX}}) = A_{g_{\alpha}(C_{XX})} = \sum_{\lambda \in \sigma_p(C_{XX})} g_{\alpha}(\lambda) P_{YY|\sigma_{\lambda}(C_{XX})},
\]

i.e. the regularisation of \( A_{C_{XX}} \) is exactly given by the precomposition operation associated with the correspondingly regularised covariance operator. We may think of the regularised inverse \( g_{\alpha}(A_{C_{XX}}) \) as approximating the pseudoinverse \( A_{C_{XX}}^\dagger \) pointwise on its domain as \( \alpha \rightarrow 0 \).
**Regularised population solution.** The regularised inverse \( g_\alpha(A_{\mathcal{C}XX}) \) is bounded for every \( \alpha \) and hence we may define the regularised population solution to (HSIP) as

\[
\theta_\alpha := g_\alpha(A_{\mathcal{C}XX})(C_{\mathcal{Y}X}) = C_{\mathcal{Y}X}g_\alpha(C_{\mathcal{XX}}).
\]

(REG)

Note that as \( C_{\mathcal{Y}X} \) is always trace class, so is \( \theta_\alpha \).

**Remark 4.2 (Regularisation strategies).** The solution arising from standard regularisation strategies leads to well-known statistical methodologies. Two classical examples are ridge regression, which is obtained from the Tikhonov–Phillips regularisation \( g_\alpha(\lambda) := (\alpha + \lambda)^{-1} \), and principal component regression, which is obtained from the spectral truncation \( g_\alpha(\lambda) := \lambda^{-1}\mathbb{1}[\lambda > \alpha] \).

Tikhonov–Phillips regularisation satisfies our definition of a spectral regularisation strategy with \( D = \gamma_0 = B = 1 \) and has qualification \( q = 1 \) with \( \gamma_q = 1 \). Principal component regression satisfies \( D = \gamma_0 = B = 1 \) as well but has arbitrary qualification with \( \gamma_q = 1 \).

Both of these approaches are classically used in finite-dimensional regression as well as kernel regression (Dicker et al., 2017; Blanchard and Mücke, 2018). We show in Section 5.3 that kernel regression can be formulated in terms of our infinite-dimensional linear regression problem. Moreover, we emphasise that this perspective yields a formalism for gradient descent learning, as it is well-known that various iterative regularisation strategies lead to specific implementations of gradient descent (see e.g. Yao et al., 2007 for the context of Landweber iteration).

**Empirical solution.** The random variables \( X \) and \( Y \) are in practice only accessible through sample pairs \((X_i, Y_i) \in \mathcal{X} \times \mathcal{Y} \) for \( i = 1, \ldots, n \). For simplicity, we assume that these sample pairs are obtained i.i.d. from the joint law \( \mathcal{L}(X, Y) \). However, ergodic sampling schemes for time series applications or Markov chain Monte Carlo methods or even deterministic approaches in the context of quasi-Monte Carlo methods would be interesting to explore here.

Given the sample pairs above, we define the *empirical covariance operators* by

\[
\hat{C}_{XX} := \frac{1}{n}\sum_{i=1}^{n} X_i \otimes X_i \quad \text{and} \quad \hat{C}_{YX} := \frac{1}{n}\sum_{i=1}^{n} Y_i \otimes X_i.
\]

Note that \( \hat{C}_{XX} \) and \( \hat{C}_{YX} \) are \( \mathbb{P} \)-a.s. of rank at most \( n \). We obtain the *regularised empirical solution* straightforwardly as the empirical analogue of the regularised population solution (REG) for some regularisation parameter \( \alpha \), i.e.

\[
\hat{\theta}_\alpha := g_\alpha(A_{\hat{C}_{XX}})(\hat{C}_{YX}) = \hat{C}_{YX}g_\alpha(\hat{C}_{XX}).
\]

(EMP)

**4.1. Risk and excess risk**

We introduce the shorthand notation \( R(\theta) := \mathbb{E}[\|Y - \theta X\|_2^2] \) for the risk associated with some \( \theta \in S_2(\mathcal{X}, \mathcal{Y}) \). The Pythagorean theorem in \( L^2(\mathbb{P}; \mathcal{Y}) \) implies that the risk decomposes as

\[
R(\theta) = \|\Pi(Y - \theta X)\|_{L^2(\mathbb{P}; \mathcal{Y})}^2 + \|\Pi^\perp(Y - \theta X)\|_{L^2(\mathbb{P}; \mathcal{Y})}^2
= \|\mathbb{E}[Y|X] - \theta X\|_{L^2(\mathbb{P}; \mathcal{Y})}^2 + \|Y - \mathbb{E}[Y|X]\|_{L^2(\mathbb{P}; \mathcal{Y})}^2.
\]

(4.3)

Here, just as in Example 3.10, \( \Pi: L^2(\mathbb{P}; \mathcal{Y}) \to L^2(\mathbb{P}; \mathcal{Y}) \), denotes the orthogonal projection operator onto \( L^2(\Omega, \mathcal{F}^X, \mathbb{P}; \mathcal{Y}) \) such that \( \Pi Y := E[Y|X] \), and \( \Pi^\perp := \text{Id}_{L^2(\mathbb{P}; \mathcal{Y})} - \Pi \). The second summand in the risk decomposition (4.3) is an irreducible noise term associated with the learning problem itself and is independent of the choice of \( \theta \).

We introduce the *excess risk* of the estimator \( \hat{\theta}_\alpha \) as

\[
\mathcal{E}(\hat{\theta}_\alpha) := R(\hat{\theta}_\alpha) - \inf_{\theta \in S_2(\mathcal{X}, \mathcal{Y})} R(\theta) \geq 0.
\]
Remark 4.3 (Excess risk and notation). Note that as we interpret the estimator \( \hat{\theta}_\alpha \) as a random variable depending on the sample pairs \((X_i, Y_i)\). Consequently, \( R(\hat{\theta}_\alpha) \) and \( E(\hat{\theta}_\alpha) \) are also interpreted as random variables depending on \((X_i, Y_i)\). However, note that the risk and the excess risk contain the expectation operator \( E \) with respect to \( X \) and \( Y \). To prevent ambiguity and confusion, we introduce the convention that we write expectations and probabilities with respect to \( (X_i, Y_i) \) distributed according to the product law \( \mathcal{L}(X, Y)^{\otimes n} \) on the measurable product space \( (\mathcal{X} \times \mathcal{Y})^n, \mathcal{B}^{\otimes n}_{\mathcal{X} \otimes \mathcal{Y}} \) as \( \mathbb{E}^{\otimes n} \) and \( \mathbb{P}^{\otimes n} \), while \( \mathbb{E} \) and \( \mathbb{P} \) will always be interpreted with respect to \( (X, Y) \).

Lemma 4.4 (Excess risk). Assume that the minimiser \( \theta_* = A^I_{\mathcal{L}X} [G_{\mathcal{L}X}] \in S_2(\mathcal{X}, \mathcal{Y}) \) exists. Then

\[
E(\hat{\theta}_\alpha) \leq \| \theta_* X - \hat{\theta}_\alpha X \|^2_{L^2(\mathbb{P};Y)} + 2M_* \| \theta_* X - \hat{\theta}_\alpha X \|^2_{L^2(\mathbb{P};Y)} \quad \mathbb{P}^{\otimes n}\text{-a.s.,}
\]

where \( M_* := \| \mathbb{E}[Y|X] - \theta_* X \|^2_{L^2(\mathbb{P};Y)} \) is the misspecification error of the linear regression problem.

Remark 4.5 (Well-specified case). Note that \( M_* = 0 \) if and only if the problem is well specified, i.e. the LCE representation \( \mathbb{E}[Y|X] = \theta_* X \) holds \( \mathbb{P}\text{-a.s.} \) with \( \theta_* \in S_2(\mathcal{X}, \mathcal{Y}) \) — or, equivalently, if the linear model (LM) holds with \( \theta_* \in S_2(\mathcal{X}, \mathcal{Y}) \).

Proof of Lemma 4.4. All inequalities in this proof are to be understood in the \( \mathbb{P}^{\otimes n}\text{-a.s.} \) sense. Assuming that the minimiser \( \theta_* = A^I_{\mathcal{L}X} [G_{\mathcal{L}X}] \in S_2(\mathcal{X}, \mathcal{Y}) \) exists, we can insert the risk decomposition (4.3) into the definition of the excess risk \( E(\hat{\theta}_\alpha) \) and obtain

\[
E(\hat{\theta}_\alpha) = R(\hat{\theta}_\alpha) - R(\theta_*) \leq \| \mathbb{E}[Y|X] - \hat{\theta}_\alpha X \|^2_{L^2(\mathbb{P};Y)} - \| \mathbb{E}[Y|X] - \theta_* X \|^2_{L^2(\mathbb{P};Y)} \leq \left( \| \mathbb{E}[Y|X] - \theta_* X \|^2_{L^2(\mathbb{P};Y)} + \| \theta_* X - \hat{\theta}_\alpha X \|^2_{L^2(\mathbb{P};Y)} \right) - \| \mathbb{E}[Y|X] - \theta_* X \|^2_{L^2(\mathbb{P};Y)} \leq \| \theta_* X - \hat{\theta}_\alpha X \|^2_{L^2(\mathbb{P};Y)} + 2 \| \mathbb{E}[Y|X] - \theta_* X \|^2_{L^2(\mathbb{P};Y)} \| \theta_* X - \hat{\theta}_\alpha X \|^2_{L^2(\mathbb{P};Y)} \leq \leq M_* \text{ as claimed.}
\]

Combining the bound in Lemma 4.4 with the fact that

\[
\| \theta_* X - \hat{\theta}_\alpha X \|^2_{L^2(\mathbb{P};Y)} = \mathbb{E}[\| (\theta_* - \hat{\theta}_\alpha) X \|^2_{Y}]
\]

\[
= \text{tr} \left( (\theta_* - \hat{\theta}_\alpha) C_{XX} (\theta_* - \hat{\theta}_\alpha)^* \right) = \| (\theta_* - \hat{\theta}_\alpha) C_{XX}^{1/2} \|^2_{S_2(\mathcal{X}, \mathcal{Y})} \quad \mathbb{P}^{\otimes n}\text{-a.s.,}
\]

we see that the performance of \( \hat{\theta}_\alpha \) may be assessed by bounding the quantity

\[
\| (\theta_* - \hat{\theta}_\alpha) C_{XX}^s \|^2_{S_2(\mathcal{X}, \mathcal{Y})} = \| A^s_{\mathcal{L}X} [\theta_* - \hat{\theta}_\alpha] \|^2_{S_2(\mathcal{X}, \mathcal{Y})} \quad \text{for } 0 \leq s \leq 1/2
\]
either with high \( \mathbb{P}^{\otimes n}\)-probability or in terms of moment bounds with respect to \( \mathbb{E}^{\otimes n} \). The case \( s = 0 \) corresponds to the classical reconstruction error \( \| \theta_* - \hat{\theta}_\alpha \|^2_{S_2(\mathcal{X}, \mathcal{Y})} \). A similar approach can be found in the literature on kernel regression with scalar response, see e.g. Blanchard and Mücke (2018).

Alternatively, it is also possible to investigate the performance of the estimator in terms of the weaker operator norm \( \| \theta_* - \hat{\theta}_\alpha \|_{\mathcal{L}_X \to \mathcal{Y}}, \) since

\[
\| (\theta_* - \hat{\theta}_\alpha) C_{XX}^{1/2} \|^2_{S_2(\mathcal{X}, \mathcal{Y})} \leq \text{tr}(C_{XX}) \| (\theta_* - \hat{\theta}_\alpha) \|^2_{\mathcal{L}_X \to \mathcal{Y}} \quad \mathbb{P}^{\otimes n}\text{-a.s.}
\]
4.2. Source conditions

We assume that \( \theta_* := A^{1}_{C_{XX}}[C_{XY}] \) exists, i.e., by Proposition 3.14, \( \theta_* \) is the unique operator of minimal norm in \( S_2(\mathcal{X}, \mathcal{Y}) \) solving (HSRP). In general, the convergence of \( \| (\theta_* - \theta_0) C_{XX} \|_{S_2(\mathcal{X}, \mathcal{Y})} \) and \( \| \theta_* - \theta_0 \|_{\mathcal{X} \rightarrow \mathcal{Y}} \) as \( \alpha \rightarrow 0 \) can be arbitrarily slow. In order to alleviate this problem, one usually imposes source conditions (e.g., Engl et al., 1996, Section 3.2) for the inverse problem (HSIP), which we are able to express in terms of the functional calculus derived in Corollary 3.19. Equivalent conditions are commonly imposed in order to derive convergence rates in functional response regression (Benatia et al., 2017; Kutta et al., 2022) and kernel regression with vector-valued response variables (Li et al., 2022, 2024; Meunier et al., 2024).

Assumption 4.6 (Hölder source condition). For \( 0 < \nu < \infty \) and \( 0 < R < \infty \), we define the source set

\[
\Omega(\nu, R) := \{ A^\nu_{C_{XX}}[\theta] \mid \theta \in S_2(\mathcal{X}, \mathcal{Y}), \| \theta \|_{S_2(\mathcal{X}, \mathcal{Y})} \leq R \} \subseteq S_2(\mathcal{X}, \mathcal{Y}).
\] (4.4)

We assume that the solution satisfies the source condition \( \theta_* \in \Omega(\nu, R) \).

Remark 4.7 (Source condition on \( C_{XY} \)). Using Corollary 3.19, we may rewrite the above source condition as the constrained operator factorisation problem

\[
\theta_* = \hat{\theta} C_{XX}^\nu \text{ for some } \hat{\theta} \in S_2(\mathcal{X}, \mathcal{Y}) \text{ with } \| \hat{\theta} \|_{S_2(\mathcal{X}, \mathcal{Y})} \leq R.
\]

By assumption, as \( C_{XY} = \theta_* C_{XX} \), this factorisation is clearly equivalent to

\[
C_{XY} = \hat{\theta} C_{XX}^\nu \text{ with } \| \hat{\theta} \|_{S_2(\mathcal{X}, \mathcal{Y})} \leq R.
\] (4.5)

This shows that the source condition \( \theta_* \in \Omega(\nu, R) \) is equivalent to \( C_{XY} \in \Omega(\nu + 1, R) \). In the classical context of inverse problems and kernel regression, source conditions are usually interpreted as smoothness assumptions about the underlying problem. In our setting, the interpretation is not immediately clear. However, we can straightforwardly apply the approach in Proposition 3.15 to this factorisation problem (4.5) by replacing \( A_{C_{XX}} \) with \( A_{C_{XX}^{\nu+1}} \) and express its solubility in terms of an equivalent moment condition.

Corollary 4.8 (Source condition). The source condition \( \theta_* \in \Omega(\nu, R) \) is satisfied if and only if

\[
\sum_{i \in I} \sup_{x \in \mathcal{X}} \frac{\| \mathbb{E}[\langle x, \mathcal{X} \rangle \langle e_i, Y \rangle_{\mathcal{Y}} \] \|^2}{\| C_{XX}^{\nu+1} x \|^2_{\mathcal{X}}} \leq R^2
\] (4.6)

for some (indeed, any) complete orthonormal system \( \{ e_i \}_{i \in I} \) in \( \mathcal{Y} \).

Proof. Proceeding analogously to the proof of Proposition 3.15, we see that the factorisation (4.5) admits a solution if and only if \( \hat{\theta} := (C_{XX}^{\nu+1})^*[C_{XY}]^* \) satisfies the condition \( \| \hat{\theta} \|_{S_2(\mathcal{X}, \mathcal{Y})} \leq R \), which is clearly equivalent to (4.6). Note that the left-hand side of (4.6) is equivalent to \( \| \hat{\theta} \|^2_{S_2(\mathcal{X}, \mathcal{Y})} \) and hence independent of the choice of complete orthonormal system. \( \blacksquare \)

We note that Corollary 4.8 can be interpreted as a special case of the so-called Picard criterion for Hölder source conditions (Engl et al., 1996, Proposition 3.13). Under the assumption of suitable source conditions, convergence rates depending on \( \alpha \rightarrow 0 \) can be derived. The details of this theory under more general assumptions are not in the scope of this work, as there is a plethora of results concerning general source conditions in the literature on inverse problems. However, our results serve as a starting point for the investigation of source conditions in the context of infinite-dimensional regression.
4.3. Convergence analysis

We demonstrate how our framework allows derivation of rates for Hilbert–Schmidt regression based on Hölder source conditions. We begin by decomposing the error \( \theta_\ast - \hat{\theta}_\alpha \) associated with the regularised empirical solution \( \hat{\theta}_\alpha \). In particular, we are interested both in the Hilbert–Schmidt norm of this error and in the mean-square prediction error\(^2\)

\[
\mathbb{E}[\| \theta_\ast - \hat{\theta}_\alpha \|^2_X] \equiv \| \theta_\ast - \hat{\theta}_\alpha \|_{S_2(X,\mathcal{Y})}^{1/2}
\]

and in order to treat these in a unified way we will examine

\[
\| \theta_\ast - \hat{\theta}_\alpha \|_{S_2(X,\mathcal{Y})}^s \text{ for } 0 \leq s \leq \frac{1}{2}.
\]

Error decomposition. Na"ively, one would decompose this error norm using the triangle inequality as follows: \( \mathbb{P}^\otimes n\)-a.s. with respect to the samples \((X_i, Y_i)_{i=1}^n\),

\[
\| \theta_\ast - \hat{\theta}_\alpha \|_{S_2(X,\mathcal{Y})} \leq \underbrace{\| \theta_\ast - \theta_\alpha \|_{S_2(X,\mathcal{Y})}}_{=\text{approximation error}} + \underbrace{\| \theta_\alpha - \hat{\theta}_\alpha \|_{S_2(X,\mathcal{Y})}}_{=\text{variance}}.
\] (4.7)

However, this decomposition turns out to be less than ideal and we shall consider the following alternative \( \mathbb{P}^\otimes n\)-a.s. decomposition:

\[
\theta_\ast - \hat{\theta}_\alpha = \theta_\ast - \theta_\ast \hat{C}_{XX} g_\alpha(\hat{C}_{XX}) + \theta_\ast \hat{C}_{XX} g_\alpha(\hat{C}_{XX}) - \hat{\theta}_\alpha
\]

\[
= \theta_\ast r_\alpha(\hat{C}_{XX}) + \theta_\ast \hat{C}_{XX} g_\alpha(\hat{C}_{XX}) - \hat{\theta}_\alpha
\]

\[
= \theta_\ast r_\alpha(\hat{C}_{XX}) + (\theta_\ast \hat{C}_{XX} - \hat{C}_{XX}) g_\alpha(\hat{C}_{XX}),
\]

where \( r_\alpha \) is as in (4.1), and so

\[
\| \theta_\ast - \hat{\theta}_\alpha \|_{S_2(X,\mathcal{Y})} \leq \| \theta_\ast r_\alpha(\hat{C}_{XX}) \|_{S_2(X,\mathcal{Y})} + \| (\theta_\ast \hat{C}_{XX} - \hat{C}_{XX}) g_\alpha(\hat{C}_{XX}) \|_{S_2(X,\mathcal{Y})} \text{ \( \mathbb{P}^\otimes n\)-a.s.}
\] (4.8)

Again, we think of the two terms on the right-hand side of (4.8) as an approximation error and a variance term. Crucially, though, the approximation error in the decomposition (4.8) is random — as opposed to the deterministic approximation term in (4.7) — and both terms in (4.8) will be amenable to analysis using concentration-of-measure techniques. Our approach combines error decomposition techniques from kernel-based learning theory by Blanchard and Mücke (2018) with concentration results for sub-exponential random operators which derive based on recent results by Maurer and Pontil (2021). Before bounding both these error terms, we introduce sub-Gaussian and sub-exponential norms for Hilbertian random variables.

Concentration bound for empirical covariance operators. We begin by defining notions of sub-exponentiality and sub-Gaussianity of real-valued random variables (e.g. Buldygin and Kozachenko, 2000), which we generalise to vector-valued random variables. For a real-valued random variable \( \xi \) defined on \((\Omega, \mathcal{F}, \mathbb{P})\), we introduce the Banach spaces \( L_{\psi_1}(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}) = L_{\psi_1}(\mathbb{P}) \) and \( L_{\psi_2}(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}) = L_{\psi_2}(\mathbb{P}) \) via the norms

\[
\| \xi \|_{L_{\psi_1}(\mathbb{P})} := \sup_{1 \leq p < \infty} \frac{\| \xi \|_{L^p(\mathbb{P})}}{p} \quad \text{and} \quad \| \xi \|_{L_{\psi_2}(\mathbb{P})} := \sup_{1 \leq p < \infty} \frac{\| \xi \|_{L^p(\mathbb{P})}}{p^{1/2}};
\]

\(^2\)Note well that the expectation here is with respect to \( X \) and that both sides are random quantities, being functions of the sample data \((X_i, Y_i)_{i=1}^n\); cf. Remark 4.3.
see Maurer and Pontil (2021). We extend this definition to the case that $\xi$ takes values in a separable Hilbert space $\mathcal{H}$ by defining

$$
\|\xi\|_{L_{psi}(\mathcal{P};\mathcal{H})} := \|\|\xi\|_{\mathcal{H}}\|_{L_{psi}(\mathcal{P})} = \sup_{1 \leq p < \infty} \frac{\|\xi\|_{L^p(\mathcal{P};\mathcal{H})}}{p}
$$

and analogously for $\|\xi\|_{L_{psi_2}(\mathcal{P};\mathcal{H})} := \|\|\xi\|_{\mathcal{H}}\|_{L_{psi_2}(\mathcal{P})}$. For the real-valued case, these norms are equivalent to the usual sub-exponential and sub-Gaussian norms (see e.g. Vershynin, Propositions 2.5.2 and 2.7.1). In the vector-valued case, the sub-Gaussian and sub-exponential norms of $\xi$ are sometimes defined as the supremum of the real sub-exponential and sub-Gaussian norms over all one-dimensional projections $\langle x, \xi \rangle_{\mathcal{H}}$ for $x \in \mathcal{H}$ — the norms of $L_{\psi_1}(\mathcal{P};\mathcal{H})$ and $L_{\psi_2}(\mathcal{P};\mathcal{H})$ discussed here are stronger. Note that $L_{\psi_2}(\mathcal{P};\mathcal{H}) \subseteq L_{\psi_1}(\mathcal{P};\mathcal{H})$.

**Remark 4.9** (Bernstein condition). Let $\xi$ take values in the separable Hilbert space $\mathcal{H}$. In statistical learning theory, the vector-valued Bernstein condition (Pinelis and Sakhanenko, 1986) given by

$$
\mathbb{E}\left[\|\xi - \mathbb{E}[\xi]\|^p_{\mathcal{H}}\right] \leq \frac{1}{2^p p!} \sigma^2 L^{p-2} \text{ for all } p \geq 2
$$

with parameters $\sigma < \infty$ and $L < \infty$ is a standard assumption in order to derive tail bounds for Hilbertian random variables. Condition (4.9) can be interpreted as the classical real-valued Bernstein condition applied to the random variable $\|\xi - \mathbb{E}[\xi]\|_{\mathcal{H}}$ (see e.g. Buldygin and Kozachenko, 2000, Section 1.4). However, it is possible to prove that the real-valued Bernstein condition is equivalent to sub-exponentiality (see Appendix A.2). Hence, the vector-valued Bernstein condition (4.9) is equivalent to $\|\xi\|_{L_{psi}(\mathcal{P};\mathcal{H})} < \infty$.

Analogously to the fact that products of real-valued sub-Gaussians are sub-exponential, we show that such a property holds for tensor products of sub-Gaussians in the vector-valued case.

**Lemma 4.10** (Tensor products of sub-Gaussians are sub-exponential). We have

$$
\|Y \otimes X\|_{L_{psi}(\mathcal{P};S_2(\mathcal{X},\mathcal{Y}))} \leq 2\|X\|_{L_{psi}(\mathcal{P};\mathcal{X})}\|Y\|_{L_{psi}(\mathcal{P};\mathcal{Y})}.
$$

**Proof.** We have

$$
\|Y \otimes X\|_{L_{psi}(\mathcal{P};S_2(\mathcal{X},\mathcal{Y}))}^2 = \sup_{1 \leq p < \infty} \frac{\mathbb{E}\left[\|X\|_{\mathcal{X}}^p\|Y\|_{\mathcal{Y}}^p\right]^{2/p}}{p^2} \leq 4 \sup_{1 \leq p < \infty} \frac{\mathbb{E}\left[\|X\|_{L^2(\mathcal{P};\mathcal{X})}^{2p}\right]^{1/p} \mathbb{E}\left[\|Y\|_{L^2(\mathcal{P};\mathcal{Y})}^{2p}\right]^{1/p}}{p^2} \leq 4\|X\|_{L_{psi}(\mathcal{P};\mathcal{X})}^2\|Y\|_{L_{psi}(\mathcal{P};\mathcal{Y})}^2.
$$

Taking square roots completes the proof.

We now summarise the concentration-of-measure results that will be used to control both the approximation error and the variance. We call particular attention to the fact that, although these are stated as five inequalities, some are deterministic consequences of others (e.g. (4.11) follows from (4.10) pointwise for all events in a subset of the underlying sample space), and this allows us to minimise the number of overall appeals to concentration of measure and the union bound.
Theorem 4.11 (Simultaneous concentration bounds). Suppose that \( X \in L_{\psi^2}(P;\mathcal{X}), Y \in L_{\psi^2}(P;\mathcal{Y}), \) and that \((X_1, Y_1), \ldots, (X_n, Y_n)\) are sampled i.i.d. from \( P(X, Y) \), i.e. with joint distribution \( \mathbb{P}^\otimes n \). Let \( \alpha \in (0, 1), \delta \in (0, \frac{1}{2}], n \geq \log(1/\delta), \) and \( r \in [0, 1]. \) Also let \( T \in L(\mathcal{X}, \mathcal{Y}) \). Then, with \( \mathbb{P}^\otimes n \)-probability at least \( 1 - 2\delta \), all the following bounds hold simultaneously (i.e. for the same subset of the underlying sample space):

\[
\| \hat{\theta} - C_{X,Y} \|_{S_2(\mathcal{X}, \mathcal{Y})} \leq 24\sqrt{2}e\|X\|_{L_{\psi^2}(P;\mathcal{X})}^2 \sqrt{\frac{\log(1/\delta)}{n}}, \tag{4.10}
\]

\[
\| \hat{\theta} - C_{X,Y} \|_{S_2(\mathcal{X}, \mathcal{Y})} \leq 24\sqrt{2}e\|X\|_{L_{\psi^2}(P;\mathcal{X})}^2 \sqrt{\frac{\log(1/\delta)}{n}}, \tag{4.11}
\]

\[
2 \geq \| (\hat{\theta} - C_{X,Y})^{-1} (C_{X,Y} + \alpha \text{Id}_{\mathcal{Y}})^{-1} (C_{X,Y} + \alpha \text{Id}_{\mathcal{Y}}) \|_{L(\mathcal{X}, \mathcal{Y})}, \tag{4.12}
\]

\[
\| T\hat{\theta} \|_{L(\mathcal{X}, \mathcal{Y})} \leq 2^r \cdot \| T(\hat{\theta} - C_{X,Y}) \|_{L(\mathcal{X}, \mathcal{Y})}, \tag{4.13}
\]

and,

\[
\| (\hat{\theta} - C_{X,Y}) (C_{X,Y} + \alpha \text{Id}_{\mathcal{Y}})^{-1/2} \|_{S_2(\mathcal{X}, \mathcal{Y})} \leq 16\sqrt{2}eB_{\psi^2} \cdot \frac{\log(1/\delta)}{\alpha}, \tag{4.14}
\]

where

\[
B_{\psi^2} := \| \theta_r \|_{L(\mathcal{X}, \mathcal{Y})} \| X \|_{L_{\psi^2}(P;\mathcal{X})} + \| X \|_{L_{\psi^2}(P;\mathcal{X})} \| Y \|_{L_{\psi^2}(P;\mathcal{Y})}. \tag{4.15}
\]

and inequalities (4.12) and (4.13) require the additional assumption that

\[
n \geq \max \left\{ 1, \frac{1152 \cdot e^2 \|X\|_{L_{\psi^2}(P;\mathcal{X})}^4}{\alpha^2} \right\} \cdot \log(1/\delta). \tag{4.16}
\]

Proof. Inequalities (4.10) to (4.14) are proven separately in the appendix as Lemmas A.7 to A.11 respectively. Bearing in mind the dependency structure of these results, as illustrated in Figure 4.1, we see that there are only two statements that each hold with probability at least \( 1 - \delta \), namely (4.10) and (4.14), and the remainder are pointwise corollaries of those two. Thus, by the union bound, the complete set of inequalities holds simultaneously on a set of \( \mathbb{P}^\otimes n \)-probability at least \( 1 - 2\delta \).

We remark that the condition (4.16) is deliberately chosen such that it implies the bound

\[
24\sqrt{2}e\|X\|_{L_{\psi^2}(P;\mathcal{X})}^2 \sqrt{\frac{\log(1/\delta)}{n}} \leq \alpha. \tag{4.17}
\]

We make use of this implication multiple times.

Bounding the approximation error. We now bound the approximation error \( \theta_r a (\hat{\theta}) \) in the \( C_{X,Y}^\alpha \)-weighted Hilbert–Schmidt norm using the properties of \( a \) defined in Definition 4.1 and the qualification introduced in (4.2); we introduce the shorthand \( \bar{\alpha} := \max \{\alpha_0, \gamma_q\}. \) In what follows, \( \kappa_{a,b,c} \) denotes a positive, finite constant depending on some generic quantities \( a, b, c. \)

Proposition 4.12 (High-probability bound on approximation error in (4.8)). In addition to the assumptions of Theorem 4.11, suppose the regularisation strategy \( a \) has qualification \( q \geq \nu + s. \) Suppose that \( \theta_r \in \Omega(\nu, R) \) and \( s \in [0, \frac{1}{2}] \) and assume that \( n \) satisfies (4.16). There exists a constant \( \kappa_{a,b,c} < \infty, \) exclusively depending on \( \nu \) and \( \| C_{X,Y} \|_{L(\mathcal{X}, \mathcal{Y})}, \) such that with \( \mathbb{P}^\otimes n \)-probability at least \( 1 - \delta, \)

\[
\| \theta_r a (\hat{\theta}) \|_{S_2(\mathcal{X}, \mathcal{Y})} \leq \kappa_{a,b,c} \bar{\alpha}^R \left( \alpha^{\nu} + \| X \|_{L_{\psi^2}(P;\mathcal{X})}^2 \right) \sqrt{\frac{\log(1/\delta)}{n}}. \tag{4.18}
\]
Figure 4.1: The dependency structure of the concentration results used in this paper. The implications following on from Lemma A.7 hold pointwise in the sample space, and so two appeals to Proposition A.6, each valid with \(\mathbb{P}^\otimes n\)-probability at least \(1 - \delta\), for \(n \geq \log(1/\delta)\), suffice to establish all the necessary bounds simultaneously with \(\mathbb{P}^\otimes n\)-probability at least \(1 - 2\delta\) (by the union bound). The two shaded bounds require an additional lower bound on \(n\), given in (4.16).

**Proof.** In view of Theorem 4.11, we may restrict attention to an event of \(\mathbb{P}^\otimes n\)-probability at least \(1 - \delta\) on which (4.10) and its pointwise consequences (4.11) and (4.13) all hold. In what follows, all statements are to be understood pointwise for outcomes in this event.

Applying the assumption \(\theta_* \in \Omega(\nu, R)\) and (4.13), we have
\[
\|\theta_\star r_\alpha (\hat{C}_{XX})C_{XX} \|_{s_2(\mathcal{X}, \mathcal{Y})} \leq 2^\star R \cdot \|C_{XX}^\nu r_\alpha (\hat{C}_{XX}) (\hat{C}_{XX} + \alpha \text{Id}_\mathcal{X})^s \|_{L(\mathcal{X})} \tag{4.18}
\]
We now bound the right-hand side of (4.18) by treating the two cases \(\nu \in (0, 1)\) and \(\nu \geq 1\) separately.

**Case I:** \(\nu \in (0, 1)\). In this case we apply (4.13) and Lemma A.3 and obtain
\[
\|C_{XX}^\nu r_\alpha (\hat{C}_{XX}) (\hat{C}_{XX} + \alpha \text{Id}_\mathcal{X})^s \|_{L(\mathcal{X})} \leq 2^\nu \|r_\alpha (\hat{C}_{XX}) (\hat{C}_{XX} + \alpha \text{Id}_\mathcal{X})^{\nu + s} \|_{L(\mathcal{X})} \leq 4\gamma \alpha^{\nu + s},
\]

**Case II:** \(\nu \geq 1\). In this case we follow Blanchard and M"ucke (2018, Eq. (5.10)):
\[
\|C_{XX}^\nu r_\alpha (\hat{C}_{XX}) (\hat{C}_{XX} + \alpha \text{Id}_\mathcal{X})^s \|_{L(\mathcal{X})} \leq \|\hat{C}_{XX}^\nu r_\alpha (\hat{C}_{XX}) (\hat{C}_{XX} + \alpha \text{Id}_\mathcal{X})^s \|_{L(\mathcal{X})} + \| (\hat{C}_{XX}^\nu - \hat{C}_{XX}^\nu) r_\alpha (\hat{C}_{XX}) (\hat{C}_{XX} + \alpha \text{Id}_\mathcal{X})^s \|_{L(\mathcal{X})}
\]
and the terms on the right-hand side can be bounded individually. For the first term we use the qualification of \(g_\alpha\) and apply Lemma A.3:
\[
\|\hat{C}_{XX}^\nu r_\alpha (\hat{C}_{XX}) (\hat{C}_{XX} + \alpha \text{Id}_\mathcal{X})^s \|_{L(\mathcal{X})} \leq 2\gamma \alpha^{\nu + s}.
\]
For the second term we obtain
\[
\| (C_{XX} - \hat{C}_{XX}) r_\alpha ((\hat{C}_{XX} + \alpha \text{Id}_X)^s) \|_{L(X)} \leq 2\gamma \alpha^s \| C_{XX}^\nu - \hat{C}_{XX}^\nu \|_{L(X)} \tag{4.19}
\]
again by the qualification of \( g_\alpha \) and Lemma A.3. We now address bounding \( \| C_{XX}^\nu - \hat{C}_{XX} \|_{L(X)} \).

The combination of (4.11) and (4.17) implies
\[
\| \hat{C}_{XX} \|_{L(X)} \leq \| C_{XX} \|_{S_2(X)} + \alpha.
\]

Together with the assumption \( \alpha \leq 1 \), we see that \( \| \hat{C}_{XX} \|_{L(X)} \) is bounded by an absolute constant depending on \( \| C_{XX} \|_{L(X)} \), allowing us to apply Proposition A.1, yielding the existence of a constant \( \kappa'_\nu C_{XX} \) such that \( \| C_{XX}^\nu - \hat{C}_{XX}^\nu \|_{L(X)} \leq \kappa'_\nu C_{XX} \| C_{XX} - \hat{C}_{XX} \|_{L(X)} \). We may finally proceed bounding (4.19) as
\[
2\gamma \alpha^s \| C_{XX}^\nu - \hat{C}_{XX}^\nu \|_{L(X)} \leq 2\gamma \alpha^s \| C_{XX} - \hat{C}_{XX} \|_{L(X)}
\]
\[
\leq 48\sqrt{2} e \kappa'_\nu C_{XX} \gamma \alpha^s \| X \|_{\psi_2(P,X)}^2 \sqrt{\log(1/\delta)} \sqrt{n},
\]
where the last step follows from (4.10). The final assertion follows from collecting all estimates.

**Bounding the variance term.** We now bound the variance term \((\theta, \hat{C}_{XX} - \hat{C}_{YX}) g_\alpha(\hat{C}_{XX}) \) in the \( C_{XX}^\nu \)-weighted Hilbert–Schmidt norm, again using properties of the regularisation scheme and concentration of measure.

**Proposition 4.13 (High-probability bound on variance term in (4.8)).** Under the assumptions of Theorem 4.11, let \( \kappa_{D,B} := (D + 1)B \geq 0 \) with \( D \) and \( B \) as in Definition 4.1, and let \( B_{\psi_2} \) be as in (4.15). Then, with \( \mathbb{P}^n \)-probability at least \( 1 - 2\delta \) and for \( n \) satisfying (4.16) as well as \( s \in [0,1/2] \),
\[
\| (\theta, \hat{C}_{XX} - \hat{C}_{YX}) g_\alpha(\hat{C}_{XX}) C_{XX}^\nu \|_{S_2(X,Y)} \leq 64\kappa_{D,B} e B_{\psi_2} \alpha^{s-1} \sqrt{\log(1/\delta)} / n.
\]

**Proof.** Define (random) linear operators \( T_1 : X \to Y \) and \( T_2, T_3 : X \to X \) by
\[
T_1 := (\theta, \hat{C}_{XX} - \hat{C}_{YX})(C_{XX} + \alpha \text{Id}_X)^{-1/2},
T_2 := (C_{XX} + \alpha \text{Id}_X)^{1/2}(\hat{C}_{XX} + \alpha \text{Id}_X)^{-1/2},
T_3 := (\hat{C}_{XX} + \alpha \text{Id}_X)^{1/2} g_\alpha(C_{XX})(\hat{C}_{XX} + \alpha \text{Id}_X)^s = g_\alpha(\hat{C}_{XX})(\hat{C}_{XX} + \alpha \text{Id}_X)^{s+1/2}.
\]

In view of Theorem 4.11, we may restrict attention to an event of \( \mathbb{P}^n \)-probability at least \( 1 - 2\delta \) on which both (4.10) (and hence both (4.12) and (4.13)) and (4.14) hold. Then, pointwise for outcomes in this event,
\[
\| (\theta, \hat{C}_{XX} - \hat{C}_{YX}) g_\alpha(\hat{C}_{XX}) C_{XX}^\nu \|_{S_2(X,Y)} \leq 2^s \| (\theta, \hat{C}_{XX} - \hat{C}_{YX}) g_\alpha(\hat{C}_{XX}) (\hat{C}_{XX} + \alpha \text{Id}_X)^s \|_{S_2(X,Y)} \quad \text{(by (4.13))}
\]
\[
= 2^s \| T_1 T_2 T_3 \|_{S_2(X,Y)} \quad \text{(by (4.12) and Lemma A.4)}
\]
\[
\leq 2 \cdot 2^s \kappa_{D,B} \alpha^{s-1/2} \sqrt{\log(1/\delta)} / \sqrt{n} \quad \text{(by (4.14))}
\]
\[
\leq 64\kappa_{D,B} e B_{\psi_2} \alpha^{s-1} \sqrt{\log(1/\delta)} / n.
\]
This completes the proof.

**Overall error bounds and rates.** Combining the estimates for the approximation and variance in (4.8) yields the following:

**Corollary 4.14 (Convergence rates in probability).** Suppose the regularisation strategy \( g_\alpha \) has qualification \( q \geq \nu + s \). Suppose that \( Y \in L_{\psi_2}(\mathbb{P}; Y) \), \( X \in L_{\psi_2}(\mathbb{P}; X) \), \( \theta_\star \in \Omega(\nu, R) \), and \( 0 < \alpha < 1 \). Let \( \delta \in (0, \frac{1}{e}) \) and \( s \in [0, \frac{1}{2}] \). If the regularisation parameter \( \alpha = \alpha_n \) is chosen to depend on the number \( n \) of data points via

\[
\alpha_n := \left( \frac{1}{\sqrt{n}} \right)^{\frac{1}{1+\nu}},
\]

then, for

\[
n \geq n_0 := \max \left\{ \| X \|_{L_{\psi_2}(\mathbb{P}; X)}^4, \left( 1152e^2 \| X \|_{L_{\psi_2}(\mathbb{P}; X)}^4 \log(1/\delta) \right)^{\frac{1}{2}} \right\}^{1+\nu},
\]

with \( \mathbb{P}^n \)-probability at least \( 1 - 2\delta \),

\[
\| (\theta_\star - \hat{\theta}_n) C_{XX}^s \|_{S_2(X, Y)} \leq \bar{\kappa} \sqrt{\log(1/\delta)} \left( \frac{1}{\sqrt{n}} \right)^{\frac{s+\nu}{\nu+1}},
\]

where \( \bar{\kappa} := \max \{ \kappa_{\nu,C_{XX}} \gamma R, 64\kappa_{D,B} e B_{\psi_2} \} < \infty \) is obtained from the constants appearing in Propositions 4.12 and 4.13.

**Proof.** For the chosen regularisation parameter schedule \( \alpha_n = n^{-1/(2+2\nu)} \), condition (4.16) reduces to

\[
n \geq 1152e^2 \| X \|_{L_{\psi_2}(\mathbb{P}; X)}^4 \log(1/\delta)n^{\frac{1}{1+\nu}},
\]

which is satisfied by those \( n \) exceeding the stated value of \( n_0 \). Thus, we may appeal to Propositions 4.12 and 4.13.

Since both these results are derived from Theorem 4.11, their assertions hold simultaneously (i.e. for the same subset of the sample space) with \( \mathbb{P}^n \)-probability at least \( 1 - 2\delta \). Applying Propositions 4.12 and 4.13 to the error decomposition (4.8) yields

\[
\| (\theta_\star - \hat{\theta}_n) C_{XX}^s \|_{S_2(X, Y)} \leq \bar{\kappa} \alpha_n^s + \| X \|_{L_{\psi_2}(\mathbb{P}; X)}^2 \sqrt{\frac{\log(1/\delta)}{n}} + \sqrt{\frac{\log(1/\delta)}{\alpha_n^2 n}}
\]

(4.20)

for all \( n \geq n_0 \) with \( \bar{\kappa} = \max \{ \kappa_{\nu,C_{XX}} \gamma R, 64\kappa_{D,B} e B_{\psi_2} \} \). A short calculation shows that

\[
\alpha_n^{s+\nu} = \frac{\alpha_n^s}{\sqrt{\alpha_n^2 n}} = \left( \frac{1}{\sqrt{n}} \right)^{\frac{s+\nu}{\nu+1}}.
\]

As for the middle term on the right-hand side of (4.20),

\[
\frac{\alpha_n^s}{\sqrt{n}} = \left( \frac{1}{\sqrt{n}} \right)^{\frac{s+\nu}{\nu+1} + 1}.
\]

Thus,

\[
\| (\theta_\star - \hat{\theta}_n) C_{XX}^s \|_{S_2(X, Y)} \leq \bar{\kappa} \left( \frac{1}{\sqrt{n}} \right)^{\frac{s+\nu}{\nu+1}} \left( 1 + \| X \|_{L_{\psi_2}(\mathbb{P}; X)}^2 \sqrt{\frac{\log(1/\delta)}{n}} + \sqrt{\log(1/\delta)} \right),
\]

and the claim now follows from the hypotheses that \( \delta < \frac{1}{e} \) and \( n \geq n_0 \).
Two remarks concerning the above rates are in order.

**Remark 4.15 (Fast rates).** Merely imposing source conditions is insufficient to characterise regression problems allowing for rates faster than $1/\sqrt{n}$ with high probability. We conjecture that, analogously to results in kernel regression, the use of a Bernstein-type inequality (e.g. Maurer and Pontil, 2021, Proposition 7(iii)) combined with a sufficiently fast decay of eigenvalues of $C_{XX}$ will lead to the desired results. However, this requires linking the eigenvalue decay — in terms of some notion of an effective dimension (e.g. Caponnetto and De Vito, 2007; Blanchard and Mücke, 2018) — to the variance proxy in the Bernstein bound in order to find the optimal schedule for the regularisation parameter. For kernel problems, this is commonly done based on the classical Bernstein bound by Pinelis and Sakhanenko (1986) under assumption of the vector-valued Bernstein condition (4.9). However, we deliberately choose to work with sub-Gaussian and sub-exponential norms instead, as these concepts allow a convenient analysis of unbounded random variables and their tensor products. This is a major difference compared to kernel regression, where the kernel and therefore the embedded random variables in the reproducing kernel Hilbert space are assumed to be bounded.

**Remark 4.16 (Optimal rates and comparison to kernel setting).** The rates in Corollary 4.14 match those of kernel regression with scalar and finite-dimensional response variables under a Hölder source condition and with no additional assumptions on the eigenvalue decay of $C_{XX}$; see e.g. Caponnetto and De Vito (2007), Blanchard and Mücke (2018), and Lin et al. (2020). Minimax optimality of these rates is only derived by Caponnetto and De Vito (2007) and Blanchard and Mücke (2018) under the additional assumption that the eigenvalues of $C_{XX}$ decay rapidly enough, which is an implicit assumption on the marginal distribution of $X$. To establish minimax optimality in our setting, we would have to repeat the standard arguments, e.g. apply a general reduction scheme in conjunction with Fano’s method (Tsybakov, 2009). However, we show in Section 5.3 that the Hilbert–Schmidt regression problem (HSRP) contains scalar response kernel regression as well as some settings of kernel regression with vector-valued response as special cases.

5. Related work, applications and examples

In this section, we discuss some specific applications of the infinite-dimensional regression setting. We compare our approach to existing results in the literature and comment on the insights obtained from our general framework as well as potential directions for future research.

5.1. Functional data analysis

When the Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$ are chosen to be the space of square integrable functions over some interval with respect to the Lebesgue measure $L^2([a, b])$, the infinite-dimensional linear regression problem (RP) becomes functional linear regression with functional response, which is ubiquitous in functional data analysis. However, it is important to note that virtually all results for this problem derived in context of functional data analysis assume the well-specified case (LM), i.e. $Y = \theta_\star X + \varepsilon$, which is usually called the functional linear model. We refer the reader to the monographs by Ramsay and Silverman (2005) and Horváth and Kokoszka (2012) for comprehensive introductions to the functional linear model. We emphasise that the operator $\theta_\star$ is often assumed to be Hilbert–Schmidt whenever it is expressed in terms of a convolution with respect to some suitable integral kernel. The functional linear model with functional response is particularly important for for autoregressive models and the theory of linear processes in
functional time series (Mas and Pumo, 2010, Horváth and Kokoszka, 2012). We will address these topics separately in a more general setting of Hilbertian time series in the next section.

In the existing literature on functional linear regression, estimators are derived by assuming the well-specified case based on the equation $C_{YX} = \theta \star C_{XX}$ (this is easily obtained from the functional linear model as shown in Example 3.10). However, instead of solving this identity for $\theta \star$ in terms of a more general inversion of a precomposition operation (or equivalently by solving an operator factorisation), estimators of $\theta$ are obtained by heuristically applying some specific regularisation strategy to $C_{XX}$ directly and performing an operator composition. This approach has led to various estimators based on the functional linear model with functional response (we refer the reader to Crambes and Mas (2013), Hörmann and Kidziński (2015), Benatia et al. (2017), Imaizumi and Kato (2018) and the references therein). While most of these estimators do allow for a statistical analysis, they bypass the application of standard consistency arguments for classical inverse problems almost entirely (see e.g. Engl et al., 1996). This renders the analysis of the regularised estimators fairly complicated, as the underlying spectral theory requires a manual investigation of the composition of $C_{YX}$ and the regularised version of $C_{XX}$. In fact, known approaches from inverse problem theory are essentially implicitly reconstructed in these proofs in the much more challenging context of operator composition. The severity of this problem arising from the singularity of $C_{XX}$ and the involved composition is sometimes even mentioned explicitly by the aforementioned authors; see also Mas and Pumo (2010, Section 3.2) and Bosq (2000, Section 8.2).

Although our results in Section 3 (and in particular Corollary 3.19) show that this approach is mathematically equivalent to the inverse problem framework we propose here, we argue below that our perspective has several advantages:

(a) It combines the existing estimators for functional linear regression into a unified framework which allows for a comparison and simplified investigation in the language of inverse problems. We emphasise that for kernel-based regression, an analogous approach has lead to a vast variety of important results and has now become a standard setup for the investigation of supervised learning (Caponnetto and De Vito, 2007; we refer the reader to Blanchard and Mücke, 2018 and the references therein for a more recent analysis based on this framework and an overview of existing results).

(b) It generalises the functional linear regression problem to a least-squares setting in which is not necessarily required to assume the functional linear model (i.e. the well-specified case) in order to construct estimators.

(c) It reduces the construction and the investigation of new solution algorithms for functional linear regression to the choice of new regularisation strategies in our framework.

5.2. Linear autoregression of Hilbertian time series

We consider a time series $(Y_t)_{t \in \mathbb{N}}$ taking values in the Hilbert space $\mathcal{Y}$. For the sake of clarity in our presentation, we will assume that $(Y_t)_{t \in \mathbb{N}}$ is strictly stationary and centered. Our framework can be generalised to the non-stationary case straightforwardly. For some fixed time horizon $r \in \mathbb{N}$, we may seek to solve the linear autoregression problem

$$\min_{\theta_1, \ldots, \theta_r \in L(\mathcal{Y})} \mathbb{E} \left\| Y_t - \sum_{i=1}^{r} \theta_i Y_{t-i} \right\|_{\mathcal{Y}}^2.$$

(5.1)

In the well-specified case, there exist operators $\theta_{s_1}, \ldots, \theta_{s_r} \in L(\mathcal{Y})$ such that

$$Y_t = \sum_{i=1}^{r} \theta_{s_i} Y_{t-i} + \varepsilon_t \text{ for all } t \in \mathbb{N} \quad \text{(ARH-} r \text{)}$$
with a family of pairwise independent \(Y\)-valued noise variables \((\varepsilon_t)_{t \in \mathbb{N}}\) satisfying \(\mathbb{E}[\varepsilon_t | Y_{t-1}] = 0\) for all \(1 \leq i \leq r\), i.e. the process \((Y_t)_{t \in \mathbb{N}}\) satisfies the linear Hilbertian autoregressive model of order \(r\) (ARH-\(r\), see Bosq, 2000). In practice, depending on the scenario of application (e.g. in the context of functional time series), it may be reasonable to directly restrict the linear autoregression problem (5.1) to a minimisation over \(p\)-Schatten class operators instead of bounded operators.

We can directly reformulate the linear autoregression problem (5.1) as a special case of the general linear regression problem (RP). We define the Hilbert space \(X := \mathcal{Y}^r = \bigoplus_{i=1}^r Y\) via the external direct sum of normed spaces. We note that every operator \(\theta \in L(X, \mathcal{Y})\) corresponds to a unique sequence of operators \(\theta_1, \ldots, \theta_r \in L(\mathcal{Y})\) such that

\[
\theta x = \sum_{i=1}^r \theta_i y_i \text{ for every } x = (y_1, \ldots, y_r) \in X
\]

and vice versa. Moreover, the same statement holds when the classes of bounded operators are replaced with \(p\)-Schatten operators. In fact, is is straightforward to check that the above correspondence (5.2) defines the isomorphisms

\[
L(X, \mathcal{Y}) \cong \bigoplus_{i=1}^r L(\mathcal{Y}) \text{ and } S_p(X, \mathcal{Y}) \cong \bigoplus_{i=1}^r S_p(\mathcal{Y}) \text{ for all } p \geq 1.
\]

As a consequence of (5.2) and (5.3), the linear autoregression problem (5.1) is equivalent to the linear regression problem (RP) given by

\[
\min_{\theta \in L(X, \mathcal{Y})} \mathbb{E}[|y_t - \theta x_t|^2] \text{ with } X_t := (Y_{t-1}, \ldots, Y_{t-r}) \in X \text{ and } \theta X_t := \sum_{i=1}^r \theta_i Y_{t-i}.
\]

for the family of operators \(\theta_1, \ldots, \theta_r \in L(\mathcal{Y})\). This equivalence still holds if the classes of bounded operators are replaced with \(p\)-Schatten operators in both descriptions of the problem. The latter problem can be solved in terms of the inverse problem approach proposed in the preceding sections. In particular, we seek to solve the inverse problem

\[
A_{C_{X_t, X_t}}[\theta] = C_{X_{t+1}, X_t},
\]

where we may express the covariance operators in block format on \(X = \mathcal{Y}^r\) as

\[
C_{X_t, X_t} = \begin{bmatrix}
C_{Y_{t-1}Y_{t-1}} & \cdots & C_{Y_{t-1}Y_{t-r}} \\
\vdots & \ddots & \vdots \\
C_{Y_{t-r+1}Y_{t-1}} & \cdots & C_{Y_{t-r+1}Y_{t-r}}
\end{bmatrix}
\]

and

\[
C_{X_{t+1}, X_t} = \begin{bmatrix}
C_{Y_{t+1}Y_{t-1}} & \cdots & C_{Y_{t+1}Y_{t-r}} \\
\vdots & \ddots & \vdots \\
C_{Y_{t+r+1}Y_{t-1}} & \cdots & C_{Y_{t+r+1}Y_{t-r}}
\end{bmatrix}.
\]

A detailed discussion of the potential regularisation schemes arising are out the scope of this paper, as are the approaches for proving consistency under the assumption of ergodicity and relevant concepts for measuring probabilistic temporal dependence.

Applying our inverse problem framework to the reformulated autoregression problem (5.4) has some advantages for the theory of linear prediction for Hilbertian time series. The inverse problem perspective may lead to directions of research with the potential of extending the available literature (Bosq, 2000; Mas and Pumo, 2010):

(a) It allows us to express solutions of the forecasting problem in terms of the generic spectral regularisation approach, giving a theoretical foundation for heuristically designed estimators relying on the (approximate) inversion of \(C_{X_t, X_t}\).
b) It allows us to consider the more general least squares forecasting problem instead of assuming the well-specified ARH-1 model as commonly done in the literature.

c) It allows the direct regularisation of the $r$th-order forecasting problem, potentially leading to a broad class of solutions schemes designed for the inverse problem involving the block operators $C_{X_t}X_t$ and $C_{X_{t+1}}X_t$.

5.3. Vector-valued kernel regression

We now show that our linear regression setting includes a case of nonlinear regression with vector-valued reproducing kernels (Carmeli et al., 2006, 2010) for infinite-dimensional response variables. In fact, it is known that standard proof techniques for obtaining convergence rates for this problem (e.g. Caponnetto and De Vito, 2007) may fail for a commonly used type of kernel in the infinite-dimensional case, as the compactness of the involved inverse problem is explicitly assumed. This has been remarked independently by several authors over the last years (e.g. Grünewälder et al., 2012; Kadri et al., 2016; Park and Muandet, 2020; Mollenhauer, 2022).

An important special case of the setting described here is the conditional mean embedding, for which optimal rates (matching those of the scalar response kernel regression) have recently been derived for the special case of Tikhonov–Phillips regularisation; we refer the reader to Klebanov et al. (2020), Park and Muandet (2020) and Li et al. (2022) and the references therein. For the general infinite-dimensional response kernel regression, our approach shows that the resulting non-compact inverse problem behaves as in the real-valued learning case from a spectral regularisation perspective.

We elaborate on this statement in what follows. We introduce the concept of a vector-valued reproducing kernel Hilbert space (vv-RKHS) in terms of an operator-based description as formulated by Mollenhauer (2022). See Carmeli et al. (2006) and Carmeli et al. (2010) for a comprehensive and more general construction of vv-RKHSSs from corresponding operator-valued reproducing kernels, their topological properties and the theory of corresponding inclusion operators.

Let $E$ be a second-countable locally compact Hausdorff space equipped with its Borel $\sigma$-algebra $B_E$, and let $X$ be an RKHS consisting of $\mathbb{R}$-valued functions on $E$ with reproducing kernel $k: E^2 \to \mathbb{R}$ and canonical feature map $\varphi: E \to X$. Assume further that $(E, B_E)$ is equipped with a probability measure $\mu$, with a compact embedding operator $i: X \hookrightarrow L^2(\mu)$ (e.g. Christmann and Steinwart, 2008, Section 4.3).

Let $Y$ be another separable real Hilbert space. Consider $G := \{A\varphi(\cdot) \mid A \in S_2(X, Y)\}$; this is a vv-RKHS of $Y$-valued functions with operator-valued reproducing kernel

$$K: E^2 \to L(Y)$$

$$(x, x') \mapsto k(x, x') \text{Id}_Y$$

and we have a bounded linear embedding operator

$$I := i \otimes \text{Id}_Y: G \cong X \otimes Y \hookrightarrow L^2(\mu) \otimes Y \cong L^2(\mu; Y).$$

As the embedding $i: X \hookrightarrow L^2(\mu)$ is compact, the embedding $I := i \otimes \text{Id}_Y$ is compact precisely when $\dim Y < \infty$. The operator-valued kernel $K$ defined above plays a fundamental role for learning problems with infinite-dimensional response variables.

We now consider an $E$-valued random variable $\xi$ with law $\mathcal{L}(\xi) := \mu$ on $(E, B_E)$ and a $Y$-valued random variable $Y$, both defined on a common probability space. We can now immediately see that our nonlinear kernel regression problem

$$\min_{F \in G} \mathbb{E}[\|Y - F(\xi)\|_Y^2]$$

(5.5)
is equivalent to our linear regression problem \((RP)\) with \(X := \varphi(\xi)\), as we have
\[
\min_{\theta \in \mathbb{S}^2(X, Y)} \mathbb{E}[\|Y - \theta \varphi(\xi)\|^2],
\]
which we would then reformulate as the inverse problem \((IP)\) in terms of cross-covariance and covariance operators.

Remark 5.1 (Kernel trick). Replacing the nonlinear regression problem \((5.5)\) with the linearised problem \((5.6)\) can be interpreted as the well-known kernel trick for vector-valued regression.

The well-specified kernel regression scenario given by the assumption
\[
F_{\star}(\cdot) := \mathbb{E}[Y|\xi = \cdot] \in I(\mathcal{G}) \subseteq L^2(\mathcal{L}(\xi); \mathcal{Y})
\]
is equivalent to the linear model in the RKHS (or equivalently the linear conditional expectation property by Klebanov et al. 2021) where there exists \(\theta \in \mathbb{S}^2(\mathcal{X}, \mathcal{Y})\) such that
\[
F_{\star}(\cdot) = \theta \varphi(\cdot) \mathcal{L}(\xi)\text{-a.s.}
\]
In particular, this example motivates minimisation of the above objective function over the more restrictive space \(\mathbb{S}^2(\mathcal{X}, \mathcal{Y})\) instead of \(L(\mathcal{X}, \mathcal{Y})\) in a theoretical discussion of convergence based on our framework.

Remark 5.2 (Spectrum of non-compact inverse problem). In kernel learning theory (see e.g. Caponnetto and De Vito, 2007), the regression problem \((5.5)\) is solved via the fundamentally important normal equation
\[
TF = I^*F_{\star}, \quad F \in \mathcal{G}
\]
based on the (generalised) kernel covariance operator \(T := I^*I^*\mathcal{G} \rightarrow \mathcal{G}\), which is sometimes also called frame operator. Under the isomorphism \(\mathcal{G} \cong \mathcal{X} \otimes \mathcal{Y}\) we have
\[
T = I^*I^* = (i \otimes \text{Id}_Y)^*(i \otimes \text{Id}_Y) = i^*i \otimes \text{Id}_Y = C_{XX} \otimes \text{Id}_Y,
\]
where we apply Aubin (2000, Proposition 12.4.1) together with the well-known fact that \(C_{XX} = i^*i\) (Christmann and Steinwart, 2008, Theorem 4.26). Aubin (2000, Chapter 12.4) also shows that the tensor product operator \(C_{XX} \otimes \text{Id}_Y\): \(\mathcal{X} \otimes \mathcal{Y} \rightarrow \mathcal{X} \otimes \mathcal{Y}\) is again isomorphically equivalent to the precomposition \(A_{C_{XX}}: S_2(\mathcal{X}, \mathcal{Y}) \rightarrow S_2(\mathcal{X}, \mathcal{Y})\). Therefore, \(T \cong A_{C_{XX}}\) (where we abuse notation and write \(\cong\) for the isomorphism of operators arising from the isomorphisms of the domain and codomain spaces). Hence, Theorem 3.18(d) shows that
\[
T \cong \sum_{\lambda \in \sigma_p(C_{XX})} \lambda P_{\mathcal{Y} \otimes \text{eig}_{\lambda}(C_{XX})}.
\]
In particular, \(T\) has the same spectrum as \(C_{XX}\), which is the forward operator of the inverse problem associated with scalar response kernel regression. We revisit this fact in a more general setting in the next section.

Remark 5.3 (Convergence rates). The rates derived in Corollary 4.14 appear to be the first convergence results obtained for general regression with operator-valued kernels which do not require the assumption of compactness of the underlying inverse problem, hence allowing for infinite-dimensional response variables. For the special case of the conditional mean embedding, they appear to be the first rates covering generic regularisation strategies.
6. General interpretation and implications of our work

Let us briefly consider the well-known scalar response regression problem with $\mathcal{Y} = \mathbb{R}$. This setting allows the discussion of generic regularisation schemes for standard finite-dimensional linear least squares regression (for the case $\mathcal{X} = \mathbb{R}^d$) and various nonlinear kernel regression settings (in this case, $\mathcal{X}$ is a reproducing kernel Hilbert space, e.g. Bauer et al., 2007; Blanchard and Mücke, 2018), including kernel distribution regression (Szabó et al., 2016) and kernel regression over general Hilbert spaces (Lin et al., 2020). To emphasise that we are dealing with a scalar response learning problem, we will use the notation $y := Y$ for the real-valued response variable here.

We identify every operator $\theta \in L(\mathcal{X}, \mathbb{R})$ with some unique vector $\vartheta \in \mathcal{X}$ via Riesz representation theorem as $\theta x = \langle \vartheta, x \rangle_\mathcal{X}$ for all $x \in \mathcal{X}$ (i.e. we consider the canonical isomorphism $L(\mathcal{X}, \mathbb{R}) \cong \mathcal{X}$) and rewrite the regression problem (RP) in its dual formulation given by

$$\min_{\vartheta \in \mathcal{X}} \mathbb{E}\|y - \langle \vartheta, X \rangle \|^2.$$

It is straightforward to check that the covariance operator $C_{YX} = \mathbb{E}[y \otimes X] \in L(\mathcal{X}, \mathbb{R})$ satisfies $C_{YX}x = \langle \mathbb{E}[y | X], x \rangle_\mathcal{X}$ for all $x \in \mathcal{X}$, i.e. it is identified with the vector $\mathbb{E}[y | X] \in \mathcal{X}$ under the above isomorphism. Furthermore, the dual analogue of the inverse problem (IP) clearly becomes

$$C_{XX}\vartheta = \mathbb{E}[y | X], \quad \vartheta \in \mathcal{X},$$

which is well-known across all statistical disciplines in a variety of formulations.

This shows that in the scalar response setting, the forward operator $A_{C_{XX}}$ of the inverse problem (IP) is isomorphically equivalent to $C_{XX}$. This can also be seen directly by considering the spectral theorem from Theorem 3.18(d) together with the fact that the eigenspaces of $A_{C_{XX}}$ and $C_{XX}$ are isomorphic, i.e. $\mathbb{R} \otimes \text{eig}_\lambda(C_{XX}) \cong \text{eig}_\lambda(C_{XX})$ for all $\lambda \in \sigma(C_{XX})$, which follows from the definition of the Hilbert tensor product.

We gain several insights and potential directions of future research for the general infinite-dimensional learning setting from considering the scalar response regression problem. Most importantly, the discussion above shows that the formalism derived in this article can be interpreted as the natural generalisation of the inverse problem associated with scalar response least squares regression given by (6.1).

Regularising infinite-dimensional response regression. Theorem 3.18 and Corollary 3.19 show that the infinite-dimensional response regression problem (RP) with its inverse problem (IP) and the scalar response regression problem with its inverse problem (6.1) are equivalent in the sense that they share the same spectrum and essentially require “only” regularising the operator $C_{XX}$, even though the infinite dimensionality of $\mathcal{Y}$ introduces non-compactness of (IP) via infinite-dimensional eigenspaces of the forward operator $A_{C_{XX}}$. However, it is possible to measure the estimation error in operator norm, which is independent of the dimensionality of the corresponding eigenspaces. In particular, $\|A_{g_\alpha(C_{XX})}\|_{S_2(\mathcal{X}, \mathcal{Y}) \to S_2(\mathcal{X}, \mathcal{Y})} = \|g_\alpha(C_{XX})\|_{\mathcal{X} \to \mathcal{X}}$, which holds analogously for operator norm distances between regularised precomposition operators and the corresponding regularised covariance operators (Lemma 3.2 combined with Corollary 3.19). Consequently, the inverse problem (IP) and its convergence analysis can be conveniently reduced to the analysis of (6.1) to some extent. In general, even the interpretation of the source conditions is identical in both settings according to Corollary 4.8. However, an infinite-dimensional response of course requires square summability of the source condition across all dimensions, analogously to the existence criterion for Hilbert–Schmidt solutions in Proposition 3.15.
**Existence of a solution, model misspecification, and covariance bounds.** Although we are able to give basic existence criteria of minimisers of the infinite-dimensional regression problem in terms of alternative characterisations of range inclusions of bounded linear operators based on ideas by Douglas (1966), the results formulated in Proposition 3.11, Remark 3.12 and Proposition 3.15 seem a bit unspecific in our context of covariance operators (we also refer to the recent discussion by Klebanov et al., 2021). In fact, the importance of range inclusion properties is already mentioned by Baker (1973) in his seminal paper on covariance operators. However, to the best of our knowledge, no analysis of functional models for \(X\) and \(Y\) satisfying this property are available in the literature. Under the assumption that \(Y = f(X) + \varepsilon\) \(\mathbb{P}\)-a.s. for some nonlinear transformation \(f: \mathcal{X} \to \mathcal{Y}\) and noise variable \(\varepsilon\), does there exist some finite positive constant \(\beta_{X,Y,f,\varepsilon}\) such that

\[
C_{XY} C_{YX} \leq \beta_{X,Y,f,\varepsilon} C_{XX}^2,
\]

where \(\beta_{X,Y,f,\varepsilon}\) may depend on reasonable assumptions about smoothness and regularity properties of \(f\) and \(X\), \(Y\) and \(\varepsilon\) and their joint distributions? Such a bound implies the range inclusion property due to Proposition 3.11(c) and hence describes classes of nonlinear infinite-dimensional statistical models which could still be reasonably empirically approximated by performing linear regression in a misspecified setting. For finite-dimensional \(X\), this is always satisfied.

**Inverse problem and empirical theory for bounded operators.** We have derived our empirical framework in the context of an inverse problem in the Hilbert space \(S_2(\mathcal{X})\). This allowed us to straightforwardly derive the form of \(\hat{\theta}_\alpha\) and \(\hat{\theta}_\alpha\) in the context of the regularised precomposition operator and its empirical analogue. In our investigation, the precomposition operator serves mainly as a tool to establish a connection to the known theory of inverse problems and derive source conditions. However, note that the regularised population solution \(\theta_\alpha = C_{YX} g_\alpha(C_{XX})\) and its empirical analogue can still be defined when we merely expect the true solution \(\theta^\star = (C_{XX}^{-1} C_{XY})^+\) to be bounded, bypassing the need for the precomposition operator. In this case, the prediction error \(\|((\theta^\star - \hat{\theta}_\alpha) C_{XX}^{1/2}) \|_{S_2(\mathcal{X}, \mathcal{Y})}\) is of course still guaranteed to be finite, as \(C_{XX}\) is trace class and hence \(C_{XX}^{1/2}\) is Hilbert–Schmidt. It seems reasonable that under this choice of (semi)-norm, the bounded operator \(\theta^\star\) can still be approximated by the Hilbert–Schmidt (or even finite-rank) estimate \(\hat{\theta}_\alpha\). Under modified source conditions imposed on \(\theta^\star\) allowing for mere boundedness, we expect that rates for the bounded regression problem can be obtained. Interestingly, the Hölder-type source condition \(\theta^\star = \hat{\theta} C_{XX}^{\nu}\) for some bounded operator \(\hat{\theta}\) with \(\|\hat{\theta}\|_{L(\mathcal{X}, \mathcal{Y})} \leq R\) already implies that \(\theta^\star\) is Hilbert–Schmidt whenever \(\nu \geq 1/2\). This indicates that the investigation of more general source conditions is relevant for this problem. The theory of learning bounded operators in the context of our framework is a highly interesting field to explore in the future.

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A. Technical results

We collect here supporting material for the results in the main text. Appendix A.1 contains deterministic results on the perturbation and spectral regularisation of operators. Appendix A.2 sets out the relationship between sub-exponential Hilbertian random variables and the Bernstein condition. Appendix A.3 contains concentration-of-measure results for sub-exponential Hilbertian random variables, which were summarised in the main text as Theorem 4.11.

A.1. Operator perturbation and spectral regularisation

**Proposition A.1** (Cf. Blanchard and Mücke, 2018, Proposition 5.6). Let $\mathcal{H}$ be a Hilbert space, $T_1, T_2 \in L(\mathcal{H})$ positive semi-definite. Then, for all $0 < a < \infty$ and $1 \leq \nu < \infty$, there exists a constant $\kappa_{a,\nu} < \infty$ such that, whenever $\max\{\|T_1\|_{L(\mathcal{H})}, \|T_2\|_{L(\mathcal{H})}\} \leq a$,

$$\|T_1^\nu - T_2^\nu\|_{L(\mathcal{H})} \leq \kappa_{a,\nu}\|T_1 - T_2\|_{L(\mathcal{H})}.$$  

**Lemma A.2** (Cf. Blanchard and Mücke, 2018, Lemma 2.15). Let $g_\alpha$ be a spectral regularisation strategy (Definition 4.1) with qualification $q$. Then, for all $0 < \nu < q$ and $0 < \alpha < \infty$, we have

$$\sup_{0<\lambda<\infty} |r_\alpha(\lambda)\lambda^\nu| \leq \gamma_\nu \alpha^\nu,$$

with the constant $\gamma_\nu := \frac{1}{q} \frac{\nu}{\nu - q}$.  

**Proof.** The result presented in Lemma 2.15 by Blanchard and Mücke (2018) is given for regularisation strategies $g_\alpha$ formally defined on $[0,1]$ for every $\alpha > 0$. However, it is obtained as a special case from a more general result given by Mathé and Pereverzev (2003, Proposition 3), which also implies the assertion given here. □

**Lemma A.3** (Cf. Blanchard and Mücke, 2018, Eq. (5.11)). Let $\mathcal{H}$ be a Hilbert space, $T \in L(\mathcal{H})$ self-adjoint and positive semi-definite, and $g_\alpha$ a spectral regularisation strategy (Definition 4.1) with qualification $q \geq s + \nu$, where $s, \nu > 0$. Then, for $\bar{\gamma} := \max\{\gamma_0, \gamma_q\}$,

$$(T + \alpha \operatorname{Id}_\mathcal{H})^s r_\alpha(T) \|_{L(\mathcal{H})} \leq 2\bar{\gamma} \alpha^s$$

and

$$(T + \alpha \operatorname{Id}_\mathcal{H})^s r_\alpha(T)^\nu \|_{L(\mathcal{H})} \leq 2\bar{\gamma} \alpha^{s+\nu}.$$  

**Proof.** For the first bound, we have

$$\| (T + \alpha \operatorname{Id}_\mathcal{H})^s r_\alpha(T) \|_{L(\mathcal{H})} = \sup \{ |\mu| : \mu \in \sigma_p((T + \alpha \operatorname{Id}_\mathcal{H})^s r_\alpha(T)) \}$$

$$= \sup_{\lambda \in \sigma_p(T)} |(\lambda + \alpha)^s r_\alpha(\lambda)|$$

$$\leq \sup_{\lambda \in \sigma_p(T)} |r_\alpha(\lambda)|\lambda^s + \alpha^s \sup_{\lambda \in \sigma_p(T)} |r_\alpha(\lambda)|$$

$$\leq 2\bar{\gamma} \alpha^s$$

by the qualification of $g_\alpha$, where in the last step Lemma A.2 is applied to the first summand. We analogously obtain the second bound as

$$\| (T + \alpha \operatorname{Id}_\mathcal{H})^s r_\alpha(T)^\nu \|_{L(\mathcal{H})} = \sup \{ |\mu| : \mu \in \sigma_p((T + \alpha \operatorname{Id}_\mathcal{H})^s r_\alpha(T)^\nu) \}$$

$$= \sup_{\lambda \in \sigma_p(T)} |(\lambda + \alpha)^s r_\alpha(\lambda)^\nu|$$

$$\leq \sup_{\lambda \in \sigma_p(T)} |r_\alpha(\lambda)|\lambda^{s+\nu} + \alpha^s \sup_{\lambda \in \sigma_p(T)} |r_\alpha(\lambda)|\lambda^\nu$$

$$\leq 2\bar{\gamma} \alpha^{s+\nu},$$
where in the last step Lemma A.2 is applied to each summand.

\begin{align*}
\|g_\alpha(T)(T + \alpha \text{Id}_\mathcal{H})^{s+1/2}\|_{L(\mathcal{H})} &\leq \kappa_{D,B}\alpha^{s-1/2}. \\
\end{align*}

**Proof.** We calculate directly as follows:

\[
\begin{align*}
\|g_\alpha(T)(T + \alpha \text{Id}_\mathcal{H})^{s+1/2}\|_{L(\mathcal{H})} &= \sup_{\mu} \{ |\mu| : \mu \in \sigma_p(g_\alpha(T)(T + \alpha \text{Id}_\mathcal{H})^{s+1/2}) \} \\
&= \sup_{\lambda \in \sigma_p(T)} |g_\alpha(\lambda)(\lambda + \alpha)^{s+1/2}| \\
&\leq \sup_{\lambda \in \sigma_p(T)} |g_\alpha(\lambda)\lambda^{s+1/2}| + \sup_{\lambda \in \sigma_p(T)} |g_\alpha(\lambda)\alpha^{s+1/2}| \\
&\leq \sup_{\lambda \in \sigma_p(T)} |g_\alpha(\lambda)\lambda^{s+1/2}| \cdot \sup_{\lambda \in \sigma_p(T)} |g_\alpha(\lambda)|^{1/2-s} + B\alpha^{s-1/2} & \text{(by (R3))} \\
&\leq D^{s+1/2} \cdot B\alpha^{s-1/2} + B\alpha^{s-1/2} & \text{(by (R1) and (R3))}
\end{align*}
\]

which proves the claim with \( \kappa_{D,B} := (D + 1)B \).

**A.2. Sub-exponentiality**

An integrable real-valued random variable \( \xi \) is said to be sub-exponential (Buldygin and Kozachenko, 2000, Section 1.3), if it satisfies

\[ \mathbb{E}[e^{t(\xi - \mathbb{E}[\xi])}] \leq e^{at^2/2} \quad \text{for all } |t| \leq \tau \]

for some \( \tau > 0 \) and \( a > 0 \). It is said to satisfy the Bernstein condition (Buldygin and Kozachenko, 2000, Section 1.4) with parameters \( \sigma < \infty \) and \( L < \infty \) if

\[ |\mathbb{E}[(\xi - \mathbb{E}[\xi])^p]| \leq \frac{1}{2^p}p!\sigma^2L^{p-2} \quad \text{for all } p \geq 2. \quad (A.1) \]

Note that in its classical form, the real-valued Bernstein condition is stated with parameters \( \sigma \) and \( L \) such that it bounds the absolute value of the \( p \)-th centred moment, while the vector-valued analogue (4.9) usually bounds the expectation of the \( p \)-power of the (not necessarily centred) norm interpreted as a random variable. Hence, it may be important to keep track of the parameters when moving from a centered bound to an uncentered one. The fact that the real-valued Bernstein condition implies sub-exponentiality is well-known. We have not found a converse implication explicitly stated in the literature, and so for completeness we briefly deduce it from a known property of sub-exponentials.

**Lemma A.5** *(Bernstein condition and sub-exponentiality).* Let \( \xi \) be an integrable real-valued random variable. Then \( \xi \) satisfies the Bernstein condition with some parameters \( \sigma < \infty \) and \( L < \infty \) if and only if \( \xi \) is sub-exponential.

**Proof.** As previously mentioned, the fact that (A.1) implies sub-exponentiality of \( \xi \) can be found in the literature (e.g. Buldygin and Kozachenko, 2000, Theorem 4.2). We consider the converse implication. Under the assumption of sub-exponentiality, it is known that \( \xi \) satisfies

\[
\sup_{p \geq 1} \left( \frac{\mathbb{E}[(\xi - \mathbb{E}[\xi])^p]}{p!} \right)^{1/p} =: L < \infty
\]
see e.g. Buldygin and Kozachenko (2000, Theorem 3.2). From this, we directly obtain
\[ |E[(\xi - E[\xi])^p]| \leq E[|\xi - E[\xi]|^p] \leq p!L^p \quad \text{for all } p \geq 2 \]
which clearly implies (A.1) with \( \sigma^2 := 2L^2 \).

### A.3. Concentration bounds

A central ingredient for our analysis is the following Hoeffding-type bound for sub-exponential Hilbertian random variables.

**Proposition A.6** (Maurer and Pontil 2021, Proposition 7(ii)). Let \( \xi, \xi_1, \ldots, \xi_n \) be i.i.d. random variables with joint law \( \mathbb{P}^{\otimes n} \) taking values in a separable Hilbert space \( \mathcal{H} \) such that \( E[\xi] = 0 \) and \( \|\xi\|_{L^2(\mathbb{P}, \mathcal{H})} < \infty \). Then, for all \( \delta \in (0, \frac{1}{2}] \) and \( n \geq \log(1/\delta) \), with \( \mathbb{P}^{\otimes n} \)-probability at least \( 1 - \delta \),
\[
\left\| \frac{1}{n} \sum_{i=1}^{n} \xi_i \right\|_{\mathcal{H}} \leq 8\sqrt{2}e\|\xi\|_{L^2(\mathbb{P}, \mathcal{H})} \sqrt{\frac{\log(1/\delta)}{n}}.
\]

We now use Proposition A.6 to derive several supporting results for our covariance operators.

**Lemma A.7** (Sampling error of empirical covariance operators). Assume that \( X \in L^{p_2}(\mathbb{P}, \mathcal{X}) \), \( Y \in L^{p_2}(\mathbb{P}, \mathcal{Y}) \), and that the data pairs \((X_i, Y_i)_{i=1}^{n} \in \mathcal{X} \times \mathcal{Y} \) are sampled i.i.d. from the joint law \( \mathcal{L}(X, Y) \). Then, for all \( \delta \in (0, \frac{1}{2}] \) and \( n \geq \log(1/\delta) \), the bound
\[
\|\hat{C}_{XY} - C_{XY}\|_{S_2(\mathcal{X}, \mathcal{Y})} \leq 24\sqrt{2}e\|Y\|_{L^{p_2}(\mathbb{P}, \mathcal{Y})}\|X\|_{L^{p_2}(\mathbb{P}, \mathcal{X})} \sqrt{\frac{\log(1/\delta)}{n}}
\]
holds with \( \mathbb{P}^{\otimes n} \)-probability at least \( 1 - \delta \). An analogous bound holds for the sampling error of \( \hat{C}_{XX} \) when \( \|Y\|_{L^{p_2}(\mathbb{P}, \mathcal{Y})} \) is replaced with \( \|X\|_{L^{p_2}(\mathbb{P}, \mathcal{X})} \) in the right-hand side of the inequality.

**Proof.** First observe that
\[
\|Y \otimes X - E[Y \otimes X]\|_{L^{p_1}(\mathbb{P}, \mathcal{X} \otimes \mathcal{Y})} \leq \|Y \otimes X\|_{L^{p_1}(\mathbb{P}, \mathcal{X} \otimes \mathcal{Y})} + \|E[Y \otimes X]\|_{L^{p_1}(\mathbb{P}, \mathcal{X} \otimes \mathcal{Y})} \leq 2\|Y\|_{L^{p_2}(\mathbb{P}, \mathcal{Y})}\|X\|_{L^{p_2}(\mathbb{P}, \mathcal{X})} + \|E[Y \otimes X]\|_{\mathcal{Y} \otimes \mathcal{X}} \quad (\text{Lemma 4.10})
\]
and
\[
\|Y \otimes X\|_{L^{p_2}(\mathbb{P}, \mathcal{Y})}\|X\|_{L^{p_2}(\mathbb{P}, \mathcal{X})} \leq \frac{8\sqrt{2}e\|Y \otimes X - E[Y \otimes X]\|_{L^{p_1}(\mathbb{P}, \mathcal{Y} \otimes \mathcal{X})} \sqrt{\frac{\log(1/\delta)}{n}}}{\sqrt{\frac{\log(1/\delta)}{n}}},
\]
and this establishes the claim. \( \blacksquare \)
The bound below can be obtained straightforwardly by applying the reverse triangle inequality to the assertion of Lemma A.7.

**Lemma A.8 (High-probability boundedness of empirical covariance operator).** Assume that we have $X \in L_{\psi_2}(\mathcal{P}; \mathcal{X})$ and that $X_1, \ldots, X_n$ are sampled i.i.d. from $\mathcal{L}(X)$. Then, for all $\delta \in (0, \frac{1}{2}]$ and $n \geq \log(1/\delta)$,

$$
\|\hat{C}_{XX}\|_{S_2(\mathcal{X})} \leq \|C_{XX}\|_{S_2(\mathcal{X})} + 24\sqrt{2}e\|X\|_{L_{\psi_2}(\mathcal{P};\mathcal{X})}^2 \sqrt{\log(1/\delta)/n}
$$

with $\mathbb{P}^\otimes n$-probability at least $1 - \delta$. In particular, if $n$ satisfies (A.3) for some $\alpha > 0$, we obtain

$$
\|\hat{C}_{XX}\|_{S_2(\mathcal{X})} \leq \|C_{XX}\|_{S_2(\mathcal{X})} + \alpha
$$

with $\mathbb{P}^\otimes n$-probability at least $1 - \delta$ under the above assumptions.

**Proof.** The first bound follows directly from Lemma A.7, the second bound follows since the constraint (A.3) for $n$ was specifically chosen in the proof of Lemma A.9 such that it implies

$$
24\sqrt{2}e\|X\|_{L_{\psi_2}(\mathcal{P};\mathcal{X})}^2 \sqrt{\log(1/\delta)/n} \leq \alpha. \tag{A.2}
$$

**Lemma A.9 (High-probability boundedness of empirical identity operators).** Suppose that we have $X \in L_{\psi_2}(\mathcal{P}; \mathcal{X})$, $\alpha > 0$ and the $X_1, \ldots, X_n$ are sampled i.i.d. from $\mathcal{L}(X)$. Then

$$
\|((\hat{C}_{XX} + \alpha \text{Id}_X)^{-1}(C_{XX} + \alpha \text{Id}_X))\|_{L(\mathcal{X})} \leq 2
$$

with $\mathbb{P}^\otimes n$-probability at least $1 - \delta$, for all $n \in \mathbb{N}$ and $\delta \in (0, \frac{1}{2}]$ satisfying (4.16), i.e.

$$
n \geq \max\left\{1, \frac{1152e^2\|X\|_{L_{\psi_2}(\mathcal{P};\mathcal{X})}^2}{\alpha^2}\right\} \log(1/\delta). \tag{A.3}
$$

The same also holds for $\|((C_{XX} + \alpha \text{Id}_X)(\hat{C}_{XX} + \alpha \text{Id}_X)^{-1})\|_{L(\mathcal{X})}$. 

**Proof.** We use the decomposition $A^{-1}B = A^{-1}(B - A) + \text{Id}_\mathcal{X}$ with $A := \hat{C}_{XX} + \alpha \text{Id}_\mathcal{X}$ and $B := C_{XX} + \alpha \text{Id}_\mathcal{X}$. Since

$$
\|((\hat{C}_{XX} + \alpha \text{Id}_X)^{-1})\|_{L(\mathcal{X})} \leq \frac{1}{\alpha}
$$

and since the operator norm is dominated by the Hilbert–Schmidt norm, we may write, appealing to Lemma A.7 for the last inequality,

$$
\|((\hat{C}_{XX} + \alpha \text{Id}_X)^{-1}(C_{XX} + \alpha \text{Id}_X))\|_{L(\mathcal{X})} \leq \|((\hat{C}_{XX} + \alpha \text{Id}_X)^{-1}(C_{XX} - \hat{C}_{XX}))\|_{L(\mathcal{X})} + 1
\leq \frac{1}{\alpha}\|C_{XX} - \hat{C}_{XX}\|_{L(\mathcal{X})} + 1
\leq \frac{1}{\alpha}\|C_{XX} - \hat{C}_{XX}\|_{S_2(\mathcal{X})} + 1
\leq 24\sqrt{2}e\|X\|_{L_{\psi_2}(\mathcal{P};\mathcal{X})}^2 \sqrt{\log(1/\delta)/n} + 1,
$$

holding with $\mathbb{P}^\otimes n$-probability at least $1 - \delta$, provided that $n \geq \log(1/\delta)$. A short calculation shows that, if $n \in \mathbb{N}$ satisfies (A.3), then

$$
24\sqrt{2}e\|X\|_{L_{\psi_2}(\mathcal{P};\mathcal{X})}^2 \sqrt{\log(1/\delta)/n} \leq 1.
$$
The bound for \( \| (C_{XX} + \alpha \text{Id}_X)(\hat{C}_{XX} + \alpha \text{Id}_X)^{-1} \|_{L(X)} \) follows from the previous case by taking adjoints and using the fact that \(|T|_{L(X)} = |T^*|_{L(X)}\).

Lemma A.9 yields the following result.

**Lemma A.10 (Upper bounds for \( C_{XX}^\alpha \)-weighted norms).** Suppose that \( X_1, \ldots, X_n \) are sampled i.i.d. from \( \mathcal{L}(X) \). Let \( T \in L(X,\mathcal{Y}) \), \( X \in L_{\psi_2}(\mathbb{P};\mathcal{X}) \), and \( r \in [0,1] \). For all \( n \in \mathbb{N} \), \( \delta \in (0,1] \) and \( \alpha > 0 \) satisfying (A.3), with \( \mathbb{P}^\otimes n \)-probability at least \( 1 - \delta \),

\[
\|TC_{XX}^\alpha\|_{L(X,\mathcal{Y})} \leq 2^r \cdot \|T(\hat{C}_{XX} + \alpha \text{Id}_X)^r\|_{L(X,\mathcal{Y})},
\]

If \( T \in S_2(X,\mathcal{Y}) \), then, under the above conditions, with \( \mathbb{P}^\otimes n \)-probability at least \( 1 - \delta \),

\[
\|TC_{XX}^\alpha\|_{S_2(X,\mathcal{Y})} \leq 2^r \cdot \|T(\hat{C}_{XX} + \alpha \text{Id}_X)^r\|_{S_2(X,\mathcal{Y})}.
\]

**Proof.** Let \( T \in L(X) \). We write

\[
TC_{XX} = T(\hat{C}_{XX} + \alpha \text{Id}_X)^r(\hat{C}_{XX} + \alpha \text{Id}_X)^{-r}(C_{XX} + \alpha \text{Id}_X)^{-r}C_{XX}^\alpha.
\]

Using the Cordes inequality \( \|T_1 \cdot T_2\| \leq \|T_1\| \cdot \|T_2\| \), valid for self-adjoint, positive semi-definite operators \( T_1, T_2 \in L(X) \) and all \( r \in [0,1] \) (e.g. Furuta, 1989), we have

\[
\|(C_{XX} + \alpha)^{-r}C_{XX}^\alpha\|_{L(X)} \leq \|(C_{XX} + \alpha)^{-1}C_{XX}\|_{L(X)} \leq 1,
\]

Thus, we obtain from Lemma A.9 that, with \( \mathbb{P}^\otimes n \)-probability at least \( 1 - \delta \),

\[
\|TC_{XX}^\alpha\|_{L(X,\mathcal{Y})} \leq \|T(\hat{C}_{XX} + \alpha \text{Id}_X)^r\|_{L(X,\mathcal{Y})} \cdot \|(\hat{C}_{XX} + \alpha \text{Id}_X)^{-1}(C_{XX} + \alpha \text{Id}_X)\|_{L(X)} \leq 2^r \cdot \|T(\hat{C}_{XX} + \alpha \text{Id}_X)^r\|_{L(X,\mathcal{Y})},
\]

provided that (A.3) holds. This proves the first bound. The second bound for \( T \in S_2(X,\mathcal{Y}) \) follows analogously from considering that

\[
\|TC_{XX}^\alpha\|_{S_2(X,\mathcal{Y})} \leq \|T(\hat{C}_{XX} + \alpha \text{Id}_X)^r\|_{S_2(X,\mathcal{Y})} \cdot \|(\hat{C}_{XX} + \alpha \text{Id}_X)^{-1}(C_{XX} + \alpha \text{Id}_X)\|_{L(X)}
\]

holds \( \mathbb{P}^\otimes n \)-a.s. and applying Lemma A.9. Note in particular that the involved Hilbert–Schmidt norms are finite in this case, as \( T \in S_2(X,\mathcal{Y}) \) implies that \( TB \in S_2(X,\mathcal{Y}) \) for any \( B \in L(X) \).

An additional consequence of Proposition A.6 is the following result, which bounds the Tikhonov–Phillips-regularised precision norm of the residual operator that arises when the exact solution \( \theta_\star \) to (RP) is inserted into the unregularised empirical problem \( \hat{C}_{XX} = \theta \hat{C}_{XX} \).

**Lemma A.11 (Weighted residual operator).** Suppose that \( X \in L_{\psi_2}(\mathbb{P};\mathcal{X}) \) and \( Y \in L_{\psi_2}(\mathbb{P};\mathcal{Y}) \) and \((X_1,Y_1),\ldots,(X_n,Y_n)\) are sampled i.i.d. from \( \mathcal{L}(X,Y) \). Let \( \theta_\star \) be a solution of (RP) and set

\[
B_{\psi_2} := \|\theta_\star\|_{L(X,\mathcal{Y})}^2_{L_{\psi_2}(\mathbb{P};\mathcal{X})} + \|X\|_{L_{\psi_2}(\mathbb{P};\mathcal{X})} \|Y\|_{L_{\psi_2}(\mathbb{P};\mathcal{Y})}.
\]

Then, for any \( \alpha > 0 \), \( \delta \in (0,\frac{1}{2}] \), and \( n \geq \log(1/\delta) \), with \( \mathbb{P}^\otimes n \)-probability at least \( 1 - \delta \),

\[
\| (\theta_\star \hat{C}_{XX} - \hat{C}_{YY})(C_{XX} + \alpha \text{Id}_X)^{-1/2} \|_{S_2(X,\mathcal{Y})} \leq \frac{16\sqrt{e}B_{\psi_2}}{\sqrt{\alpha}} \cdot \sqrt{\frac{\log(1/\delta)}{n}}.
\]
Proof. For $j = 1, \ldots, n$ let

$$\xi_j := (\theta_*(X_j \otimes X_j) - Y_j \otimes X_j)(C_{XX} + \alpha \text{Id}_X)^{-1/2}.$$  

Then $E[\xi_j] = 0$, since $\theta_*$ as a solution of (RP) satisfies $C_{YX} = \theta_* C_{XX}$. Moreover,

$$\frac{1}{n} \sum_{j=1}^{n} \xi_j = (\theta_* \hat{C}_{XX} - \hat{C}_{YX})(C_{XX} + \alpha \text{Id}_X)^{-1/2}. $$

We now show that the $\xi_j$ are sub-Gaussian. Since $\|(C_{XX} + \alpha \text{Id}_X)^{-1/2}\|_{L(\mathcal{X})} \leq \alpha^{-1/2}$, we have

$$\|\xi_j\|_{S_2(\mathcal{X},\mathcal{Y})} \leq \frac{1}{\sqrt{\alpha}} \left( \|\theta_*\|_{L(\mathcal{X},\mathcal{Y})} \|X_j \otimes X_j\|_{S_2(\mathcal{X},\mathcal{Y})} + \|Y_j \otimes X_j\|_{S_2(\mathcal{X},\mathcal{Y})} \right).$$

Hence, applying Lemma 4.10 then gives

$$\|\xi_j\|_{L_{p_1}(\mathcal{P}; S_2(\mathcal{X},\mathcal{Y}))} \leq \frac{1}{\sqrt{\alpha}} \left( \|\theta_*\|_{L(\mathcal{X},\mathcal{Y})} \|X_j \otimes X_j\|_{L_{p_1}(\mathcal{P}; S_2(\mathcal{X},\mathcal{Y}))} + \|Y_j \otimes X_j\|_{L_{p_1}(\mathcal{P}; S_2(\mathcal{X},\mathcal{Y}))} \right) \leq \frac{2}{\sqrt{\alpha}} \left( \|\theta_*\|_{L(\mathcal{X},\mathcal{Y})} \|X_j\|_{L_{p_1}(\mathcal{P}; \mathcal{X})}^2 + \|X_j\|_{L_{p_1}(\mathcal{P}; \mathcal{X})} \|Y_j\|_{L_{p_1}(\mathcal{P}; \mathcal{Y})} \right).$$

Since the $\xi_j$ are i.i.d., the claim now follows from Proposition A.6.

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