Abstract

We study the interplay between surrogate methods for structured prediction and techniques from multitask learning designed to leverage relationships between surrogate outputs. We propose an efficient algorithm based on trace norm regularization which, differently from previous methods, does not require explicit knowledge of the coding/decoding functions of the surrogate framework. As a result, our algorithm can be applied to the broad class of problems in which the surrogate space is large or even infinite dimensional. We study excess risk bounds for trace norm regularized structured prediction, implying the consistency and learning rates for our estimator. We also identify relevant regimes in which our approach can enjoy better generalization performance than previous methods. Numerical experiments on ranking problems indicate that enforcing low-rank relations among surrogate outputs may indeed provide a significant advantage in practice.

1 Introduction

The problem of structured prediction is receiving increasing attention in machine learning, due to its wide practical importance [Bakir et al., 2007, Nowozin et al., 2011] and the theoretical challenges in designing principled learning procedures [Taskar et al., 2004, 2005, London et al., 2016, Cortes et al., 2016]. A key aspect of this problem is the non-vectorial nature of the output space, e.g. graphs, permutations, and manifolds. Consequently, traditional regression and classification algorithms are not well-suited to these settings and more sophisticated methods need to be developed.

Among the most well-established strategies for structured prediction are the so-called surrogate methods [Bartlett et al., 2006]. Within this framework, a coding function is designed to embed the structured output into a linear space, where the resulting problem is solved via standard supervised learning methods. Then, the solution of the surrogate problem is pulled back to the original output space by means of a decoding procedure, which allows one to recover the structured prediction estimator under suitable assumptions. In most cases, the
surrogate learning problem amounts to a vector-valued regression in a possibly infinite dimensional space. The prototypical choice for such surrogate estimator is given by regularized least squares in a reproducing kernel Hilbert space, as originally considered in [Weston et al., 2003, Cortes et al., 2005, Bartlett et al., 2006] and then explored in [Mroueh et al., 2012, Kadri et al., 2013, Brouard et al., 2016, Ciliberto et al., 2016, Osokin et al., 2017].

The principal goal of this paper is to extend the surrogate approaches to methods that encourage structure among the outputs. Indeed, a large body of work from traditional multi-task learning has shown that leveraging the relations among multiple outputs may often lead to better estimators [see e.g. Maurer, 2006, Caponnetto and De Vito, 2007, Micchelli et al., 2013, and references therein]. However, previous methods that propose to apply multitask strategies to surrogate frameworks [see e.g. Alvarez et al., 2012, Fergus et al., 2010] heavily rely on the explicit knowledge of the encoding function. As a consequence they are not applicable when the surrogate space is large or even infinite dimensional.

Contributions. We propose a new algorithm based on low-rank regularization for structured prediction that builds upon the surrogate framework in [Ciliberto et al., 2016, 2017]. Differently from previous methods, our algorithm does not require explicit knowledge of the encoding function. In particular, by leveraging approaches based on the variational formulation of trace norm regularization [Srebro et al., 2005], we are able to derive an efficient learning algorithm also in the case of infinite dimensional surrogate spaces.

We characterize the generalization properties of the proposed estimator by proving excess risk bounds for the corresponding least-squares surrogate estimator that extend previous results [Bach, 2008]. In particular, in line with previous work on the topic [Maurer and Pontil, 2013], we identify settings in which the trace norm regularizer can provide significant advantages over standard $\ell_2$ regularization. While similar findings have been obtained in the case of a Lipschitz loss, to our knowledge this is a novel result for least-squares regression with trace norm regularization. In this sense, the implications of our analysis extend beyond structured prediction and apply to settings such as collaborative filtering with side information [Abernethy et al., 2009]. We evaluate our approach on a number of learning-to-rank problems. In our experiments the proposed method significantly outperforms all competitors, suggesting that encouraging the surrogate outputs to span a low-rank space can be beneficial also in structured prediction settings.

Paper Organization. Sec. 2 reviews surrogate methods and the specific framework adopted in this work. Sec. 3 introduces the proposed approach to trace norm regularization and proves that it does not leverage explicit knowledge of coding and surrogate space. Sec. 4 describes the statistical analysis of the proposed estimator both in a vector-valued and multi-task learning setting. Sec. 5 reports on experiments and Sec. 6 discusses future research directions.

2 Background

Our proposed estimator belongs to the family of surrogate methods [Bartlett et al., 2006]. This section reviews the main ideas behind these approaches.
2.1 Surrogate Methods

Surrogate methods are general strategies to address supervised learning problems. Their goal is to learn a function \( f : \mathcal{X} \to \mathcal{Y} \) minimizing the expected risk of a distribution \( \rho \) on \( \mathcal{X} \times \mathcal{Y} \)

\[
\mathcal{E}(f) := \int_{\mathcal{X} \times \mathcal{Y}} \ell(f(x), y) \, d\rho(x, y),
\]

given only \( n \) observations \((x_i, y_i)_{i=1}^n\) independently drawn from \( \rho \), which is unknown in practice. Here \( \ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R} \) is a loss measuring prediction errors.

Surrogate methods have been conceived to deal with so-called structured prediction settings, namely supervised problems where \( \mathcal{Y} \) is not a vector space but rather a “structured” set (of e.g. strings, graphs, permutations, points on a manifold, etc.). Surrogate methods have been successfully applied to problems such as classification [Bartlett et al., 2006], multi-labeling [Gao and Zhou, 2013, Mroueh et al., 2012] or ranking [Duchi et al., 2010]. They follow an alternative route to standard empirical risk minimization (ERM), which instead consists in directly finding the model that best explains training data within a prescribed hypotheses space.

Surrogate methods are characterized by three phases:

1. **Coding.** Define an embedding \( c : \mathcal{Y} \to \mathcal{H} \), where \( \mathcal{H} \) is a Hilbert space. Map \((x_i, y_i)_{i=1}^n\) to a “surrogate” dataset \((x_i, c(y_i))_{i=1}^n\).

2. **Learning.** Define a surrogate loss \( L : \mathcal{H} \times \mathcal{H} \to \mathbb{R} \). Learn a surrogate estimator \( \hat{g} : \mathcal{X} \to \mathcal{H} \) via ERM on \((x_i, c(y_i))_{i=1}^n\).

3. **Decoding.** Define a decoding \( d : \mathcal{H} \to \mathcal{Y} \) and return the structured prediction estimator \( \hat{f} = d \circ \hat{g} : \mathcal{X} \to \mathcal{Y} \).

Below we give an well-known example of surrogate framework often used in multi-class classification settings.

**Example 1** (One Vs All). \( \mathcal{Y} = \{1, \ldots, T\} \) is a set of \( T \) classes and \( \ell \) is the 0-1 loss. Then:

1) The coding is \( c : \mathcal{Y} \to \mathcal{H} = \mathbb{R}^T \) with \( c(i) = e_i \), the vector of all 0s but 1 at the \( i \)-th entry. 2) \( \hat{g} : \mathcal{X} \to \mathbb{R}^T \) is learned by minimizing a surrogate loss \( L : \mathbb{R}^T \times \mathbb{R}^T \to \mathbb{R} \) (e.g. least-squares). 3) The classifier is \( \hat{f}(x) = d(\hat{g}(x)) \), with decoding \( d(v) = \text{argmax}_{i=1}^T \{v_i\} \) for any \( v \in \mathbb{R}^T \).

A key element of surrogate methods is the choice of the loss \( L \). Indeed, since \( \mathcal{H} \) is linear (e.g. \( \mathcal{H} = \mathbb{R}^T \) in Ex. 1), if \( L \) is convex it is possible to learn \( \hat{g} \) efficiently by means of standard ERM. However, this opens the question of characterizing how the surrogate risk

\[
\mathcal{R}(g) = \int L(g(x), c(y)) \, d\rho(x, y)
\]

is related to the original risk \( \mathcal{E}(f) \). In particular let \( f_* : \mathcal{X} \to \mathcal{Y} \) and \( g_* : \mathcal{X} \to \mathcal{H} \) denote the minimizers of respectively \( \mathcal{E}(f) \) and \( \mathcal{R}(g) \). We require the two following conditions:

- **Fisher Consistency.** \( \mathcal{E}(d \circ g_*) = \mathcal{E}(f_*) \).
Comparison Inequality. For any \( g : \mathcal{X} \to \mathcal{H} \), there exists a continuous nondecreasing function \( \sigma : \mathbb{R} \to \mathbb{R}_+ \), such that \( \sigma(0) = 0 \)

\[
\mathcal{E}(d \circ g) - \mathcal{E}(f_*) \leq \sigma(R(g) - R(g_*)).
\] (3)

Fisher consistency guarantees the coding/decoding framework to be coherent with the original problem. The comparison inequality suggests to focus the theoretical analysis on \( \hat{g} \), since learning rates for \( \hat{g} \) directly lead to learning rates for \( \hat{f} = d \circ \hat{g} \).

2.2 SELF Framework

A limiting aspect of surrogate methods is that they are often tailored around individual problems. An exception is the framework in [Ciliberto et al., 2016], which provides a general strategy to identify coding, decoding and surrogate space for a variety of learning problems. The key condition in this setting is for the loss \( \ell \) to be SELF:

**Definition 1 (SELF).** A function \( \ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R} \) is a Structure Encoding Loss Function (SELF) if there exist a separable Hilbert space \( \mathcal{H}_Y \), a continuous map \( \psi : \mathcal{Y} \to \mathcal{H}_Y \) and \( V : \mathcal{H}_Y \to \mathcal{H}_Y \) a bounded linear operator, such that for all \( y,y' \in \mathcal{Y} \)

\[
\ell(y,y') = \langle \psi(y), V\psi(y') \rangle_{\mathcal{H}_Y}.
\] (4)

The condition above is quite technical, but it turns out to be very general: it was shown in [Ciliberto et al., 2016, 2017] that most loss functions used in machine learning in settings such as regression, robust estimation, classification, ranking, etc., are SELF.

We can design surrogate frameworks “around” a SELF \( \ell \), by choosing (Coding) the map \( c = \psi : \mathcal{Y} \to \mathcal{H}_Y \), the least-squares (Surrogate loss) \( L(h,h') = \|h - h'\|_{\mathcal{H}_Y}^2 \) and (Decoding) \( d : \mathcal{H}_Y \to \mathcal{Y} \), defined for any \( h \in \mathcal{H}_Y \) as

\[
d(h) = \arg\min_{y \in \mathcal{Y}} \langle \psi(y), Vh \rangle_{\mathcal{H}_Y}.
\] (5)

The resulting is a sound surrogate framework as summarized by the theorem below.

**Theorem 1** (Thm. 2 in [Ciliberto et al., 2016]). Let \( \ell \) be SELF and \( \mathcal{Y} \) a compact set. Then, the SELF framework introduced above is Fisher consistent. Moreover, it satisfies the comparison inequality (3) with \( \sigma(\cdot) = q_\ell \sqrt{\cdot} \), where \( q_\ell = \|V\| \sup_{y \in \mathcal{Y}} \|\psi(y)\|_{\mathcal{H}_Y} \).

**Loss trick.** A key aspect of the SELF framework is that, in practice, the resulting algorithm does not require explicit knowledge of the coding/decoding and surrogate space (only needed for the theoretical analysis). To see this, let \( \mathcal{X} = \mathbb{R}^d \) and \( \mathcal{H}_Y = \mathbb{R}^T \) and consider the parametrization \( g(x) = Gx \) of functions \( g : \mathcal{X} \to \mathcal{H}_Y \), with \( G \in \mathbb{R}^{T \times d} \) a matrix. We can perform Tikhonov regularization to learn the matrix \( \hat{G} \) minimizing the (surrogate) empirical risk

\[
\min_{G \in \mathbb{R}^{d \times T}} \frac{1}{n} \sum_{i=1}^{n} \|Gx_i - \psi(y_i)\|_{\mathcal{H}_Y}^2 + \lambda\|G\|_{\mathcal{H}_S}^2.
\] (6)
where $||G||_{HS}$ is a Hilbert-Schmidt (HS) (or Frobenius) norm regularizer and $\lambda > 0$. A direct computation gives a closed form expression for $\hat{g} : \mathcal{X} \rightarrow \mathcal{H}_y$, namely
\begin{equation}
\hat{g}(x) = \hat{G}x = \sum_{i=1}^{n} \alpha_i(x)\psi(y_i), \quad \text{with} \quad \alpha(x) = (\alpha_1(x), \ldots, \alpha_n(x))^\top = (K_x + n\lambda I)^{-1}v_x,
\end{equation}
for every $x \in \mathcal{X}$ [see e.g. Alvarez et al., 2012]. Here $K_x \in \mathbb{R}^{n \times n}$ is the empirical kernel matrix of the linear kernel $k_x(x, x') = x^\top x'$ and $v_x \in \mathbb{R}^n$ is the vector with $i$-th entry $(v_x)_i = k_x(x, x_i)$.

Applying the SELF decoding in Eq. (5) to $\hat{g}$, we have for all $x \in \mathcal{X}$
\begin{equation}
\hat{f}(x) = d(\hat{g}(x)) = \arg\min_{y \in \mathcal{Y}} \sum_{i=1}^{n} \alpha_i(x)\ell(y, y_i).
\end{equation}
This follows by combining the SELF property $\ell(y, y_i) = \langle \psi(y), V \psi(y_i) \rangle_{\mathcal{H}_y}$ with $\hat{g}$ in Eq. (7) and the linearity of the inner product. Eq. (9) was originally dubbed “loss trick” since it avoids explicit knowledge of the coding $\psi$, similarly to the feature map for the kernel trick [Schölkopf et al., 2002].

The characterization of $\hat{f}$ in terms of an optimization problem over $\mathcal{Y}$ (like in Eq. (9)) is a common practice to most structured prediction algorithms. In the literature, such decoding process is referred to as the inference [Nowozin et al., 2011] or pre-image [Brouard et al., 2016, Cortes et al., 2005, Weston et al., 2003] problem. We refer to [Honeine and Richard, 2011, Bakir et al., 2007, Nowozin et al., 2011] for examples on how these problems are addressed in practice.

**General Setting.** The derivation above holds also when $\mathcal{H}_y$ is infinite dimensional and when using a positive definite kernel $k_x : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ on $\mathcal{X}$. Let $\mathcal{H}_x$ be the reproducing kernel Hilbert space (RKHS) induced by $k_x$ and $\phi : \mathcal{X} \rightarrow \mathcal{H}_x$ a corresponding feature map [Aronszajn, 1950]. We can parametrize $g : \mathcal{X} \rightarrow \mathcal{H}_y$ as $g(\cdot) = G\phi(\cdot)$, with $G \in \mathcal{H}_y \otimes \mathcal{H}_x$ the space of Hilbert-Schmidt operators from $\mathcal{H}_x$ to $\mathcal{H}_y$ (the natural generalization of $\mathbb{R}^{d \times T} = \mathbb{R}^d \otimes \mathbb{R}^T$ to the infinite setting). The problem in Eq. (6) can still be solved in closed form analogously to Eq. (7), with now $K_x$ the empirical kernel matrix of $k$ [Caponnetto and De Vito, 2007]. This leads to the decoding for $\hat{f}$ as in Eq. (9).

### 3 Low-Rank SELF Learning

Building upon the SELF framework, we discuss the use of multitask regularizers to exploit potential relations among the surrogate outputs. Our analysis is motivated by observing that Eq. (6) is equivalent to learning multiple (possibly infinitely many) scalar-valued functions
\begin{equation}
\min_{\{g_t\} \in \mathcal{H}_x} \frac{1}{n} \sum_{t \in \mathcal{T}} \sum_{i=1}^{n} (g_t(x_i) - \varphi_t(y_i))^2 + \lambda \|g_t\|^2_{\mathcal{H}_x},
\end{equation}
where, given a basis $\{e_t\}_{t \in \mathcal{T}}$ of $\mathcal{H}_y$, with $\mathcal{T} \subseteq \mathbb{N}$, we have denoted $\varphi_t(y) = \langle e_t, \psi(y) \rangle_{\mathcal{H}_y}$ for any $y \in \mathcal{Y}$ and $t \in \mathcal{T}$ (for instance, in the case of Eq. (6) we have $t \in \{1, \ldots, T\}$). Indeed, from
the literature on vector-valued learning in RKHS [see e.g. Micchelli and Pontil, 2005], we have that for \( g : \mathcal{X} \rightarrow \mathcal{H}_y \) parametrized by an operator \( G \in \mathcal{H}_y \otimes \mathcal{H}_x \), any \( g_t : \mathcal{X} \rightarrow \mathbb{R} \) defined by \( g_t(\cdot) = \langle e_t, g(\cdot) \rangle_{\mathcal{H}_y} \), is a function in the RKHS \( \mathcal{H}_x \) and, moreover, \( \|G\|_{\text{HS}}^2 = \sum_{t \in \mathcal{T}} \|g_t\|_{\mathcal{H}_x}^2 \).

The observation above implies that we are learning the surrogate “components” \( g_t \) as separate problems or tasks, an approach often referred to as “independent task learning” within the multitask learning (MTL) literature [see e.g. Micchelli and Pontil, 2005, Evgeniou et al., 2005, Argyriou et al., 2008]. In this respect, a more appropriate strategy would be to leverage potential relationships between such components during learning. In particular, we consider the problem

\[
\min_{G \in \mathcal{H}_y \otimes \mathcal{H}_x} \frac{1}{n} \sum_{i=1}^{n} \|G\phi(x_i) - \psi(y_i)\|_{\mathcal{H}_y}^2 + \lambda \|G\|_s,
\]

where \( \|G\|_s \) denotes the trace norm, namely the sum of the singular values of \( G \). Similarly to the \( \ell_1 \)-norm on vectors, the trace norm favours sparse (and thus low-rank) solutions. Intuitively, encouraging \( G \) to be low-rank reduces the degrees of freedom allowed to the individual tasks \( g_t \). This approach has been extensively investigated and successfully applied to several MTL settings, [see e.g. Argyriou et al., 2008, Bach, 2008, Abernethy et al., 2009, Maurer and Pontil, 2013].

In general, the idea of combining MTL methods with surrogate frameworks has already been studied in settings such as classification or multi-labeling [see e.g. Alvarez et al., 2012, Fergus et al., 2010]. However, these approaches require to explicitly use the coding/decoding and surrogate space within the learning algorithm. This is clearly unfeasible when \( \mathcal{H}_y \) is large or infinite dimensional.

**SELF and Trace Norm MTL.** In this work we leverage the SELF property outlined in Sec. 2 to derive an algorithm that overcomes the issues above and does not require explicit knowledge of the coding map \( \psi \). However, our approach still requires to access the matrix \( K_y \in \mathbb{R}^{n \times n} \) of inner products \( (K_y)_{ij} = \langle \psi(y_i), \psi(y_j) \rangle_{\mathcal{H}_y} \) between the training outputs. When the surrogate space \( \mathcal{H}_y \) is a RKHS, \( K_y \) corresponds to an empirical output kernel matrix, which can be efficiently computed. This motivates us to introduce the following assumption.

**Assumption 1 (SELF & RKHS).** The loss \( \ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R} \) is SELF with \( \mathcal{H}_y \) a RKHS on \( \mathcal{Y} \) with reproducing kernel \( k_y(y, y') = \langle \psi(y), \psi(y') \rangle_{\mathcal{H}_y} \) for any \( y, y' \in \mathcal{Y} \).

The assumption above imposes an additional constraint on \( \ell \) and thus on the applicability of Alg. 1. However, it was shown in [Ciliberto et al., 2016] that this requirement is always satisfied by any loss when \( \mathcal{Y} \) is a discrete set. In this case the output kernel is the 0-1 kernel, that is, \( k_y(y, y') = \delta_{y=y'} \). Moreover, it was recently shown that Asm. 1 holds for any smooth \( \ell \) on a compact set \( \mathcal{Y} \) by choosing \( k_y(y, y') = \exp(-\|y-y\|/\sigma) \), the Abel kernel with hyperparameter \( \sigma > 0 \) [Luise et al., 2018].

**Algorithm.** Standard methods to solve Eq. (11), such as forward-backward splitting, require to perform the singular value decomposition of the estimator at every iteration [Mazumder et al., 2016].
This is prohibitive for large scale applications and, to overcome these drawbacks, algorithms exploiting the variational form of the trace norm
\[
\|G\|_* = \frac{1}{2} \inf \left\{ \|A\|_{\text{HS}}^2 + \|B\|_{\text{HS}}^2 : G = AB^*, \ r \in \mathbb{N}, \ A \in \mathcal{H}_y \otimes \mathbb{R}^r, \ B \in \mathcal{H}_x \otimes \mathbb{R}^r \right\},
\]
have been considered [see e.g. Srebro et al., 2005] (here $B^*$ denotes the adjoint of $B$). Using this characterization, Eq. (11) is reformulated as the problem of minimizing
\[
\frac{1}{n} \sum_{i=1}^{n} \|AB^* \phi(x_i) - \psi(y_i)\|^2_{\mathcal{H}_y} + \lambda(\|A\|_{\text{HS}}^2 + \|B\|_{\text{HS}}^2),
\]
over the operators $A \in \mathcal{H}_y \otimes \mathbb{R}^r$ and $B \in \mathcal{H}_x \otimes \mathbb{R}^r$, where $r \in \mathbb{N}$ is now a further hyperparameter. The functional in Eq. (12) is smooth and methods such as gradient descent can be applied. Interestingly, despite the functional being non-convex, guarantees on the global convergence in these settings have been explored [Journé et al., 2010].

In the SELF setting, minimizing Eq. (12) has the additional advantage that it allows us to derive an analogous of the loss trick introduced in Eq. (9). In particular, the following result shows how each iterate of gradient descent can be efficiently “decoded” into a structured prediction estimator according to Alg. 1.

**Theorem 2** (Loss Trick for Low-Rank SELF Learning). Under Assm. 1, let $M, N \in \mathbb{R}^{n \times r}$ and $(A_k, B_k)$ be the $k$-th iterate of gradient descent on Eq. (12) from $A_0 = \sum_{i=1}^{n} \phi(x_i) \otimes M^i$ and $B_0 = \sum_{i=1}^{n} \psi(y_i) \otimes N^i$, with $M^i, N^i$ denoting the $i$-th rows of $M$ and $N$ respectively. Let $\hat{g}_k : \mathcal{X} \rightarrow \mathcal{H}_y$ be such that $\hat{g}_k(\cdot) = A_k B_k^* \phi(\cdot)$. Then, the predicted structured prediction estimator $\hat{f}_k = d \circ \hat{g}_k : \mathcal{X} \rightarrow \mathcal{Y}$ with decoding $d$ in Eq. (5) is such that
\[
\hat{f}_k(x) = \arg\min_{y \in \mathcal{Y}} \sum_{i=1}^{n} \alpha_i^{\text{tn}}(x) \ell(y, y_i)
\]
for any $x \in \mathcal{X}$, with $\alpha^{\text{tn}}(x) \in \mathbb{R}^n$ the output of Alg. 1 after $k$ iterations starting from $(M_0, N_0) = (M, N)$.
impossible to perform gradient descent in practice. In this sense, Thm. 2 can be interpreted as a representer theorem with respect to both inputs and outputs. The details of the proof are reported in Appendix A; the key aspect is to show that every iterate \((A_j, B_j)\) of gradient descent on Eq. (12) is of the form

\[ A_j = \sum_{i=1}^{n} \phi(x_i) \otimes M_i \]

and

\[ B_j = \sum_{i=1}^{n} \psi(y_i) \otimes N_i \]

for some matrices \(M, N \in \mathbb{R}^{n \times r}\). Hence, the products \(A_j^T A_j = M^T K_x M\) and \(B_j^T B_j = N^T K_y N\) – used in the optimization – are \(r \times r\) matrices that can be efficiently computed in practice, leading to Alg. 1.

We conclude this section by noting that, in contrast to trace norm regularization, not every MTL regularizer fits naturally within the SELF framework.

**SELF and other MTL Regularizer.** A well-established family of MTL methods consists in replacing the trace norm \(\|G\|_*\) with \(\text{tr}(GAG^*)\) in Eq. (11), where \(A \in \mathcal{H}_y \otimes \mathcal{H}_y\) is a positive definite linear operator enforcing specific relations on the tasks via a deformation of the metric of \(\mathcal{H}_y\) [see Micchelli and Pontil, 2005, Jacob et al., 2008, Alvarez et al., 2012, and references therein]. While in principle appealing also in surrogate settings, these approaches present critical computational and modelling challenges for the SELF framework: the change of metric induced by \(A\) has a disruptive effect on the loss trick. As a consequence, an equivalent of Thm. 2 does not hold in general (see Appendix A.3 for a detailed discussion).

### 4 Theoretical Analysis

In this section we study the generalization properties of low-rank SELF learning. Our analysis is indirect since we characterize the learning rates of the Ivanov estimator (in contrast to Tikhonov, see Eq. (11)), given by

\[ \hat{G} = \arg\min_{\|G\|_* \leq \gamma} \frac{1}{n} \sum_{i=1}^{n} \|G\phi(x_i) - \psi(y_i)\|_{\mathcal{H}_y}^2. \]  

(13)

Indeed, while Tikhonov regularization is typically more convenient from a computational perspective, Ivanov regularization often more amenable to theoretical analysis since it is naturally related to standard complexity measures for hypotheses spaces, such as Rademacher complexity, Covering Numbers or VC dimension [Shalev-Shwartz and Ben-David, 2014]. However, the two regularization strategies are equivalent in the following sense: for any \(\gamma\) there exists \(\lambda(\gamma)\) such that the minimizer of Eq. (11) (Tikhonov) is also a minimizer for Eq. (13) (Ivanov) with constraint \(\gamma\) (and vice-versa). This follows from a standard Lagrangian duality argument leveraging the convexity of the two problems [see e.g. Oneto et al., 2016, or Appendix E for more details]. Hence, while our results in the following are reported for the Ivanov estimator from Eq. (13), they apply equivalently to Tikhonov in Eq. (11).

We now proceed to present the main result of this section, proving excess risk bounds for the trace norm surrogate estimator. In the following we assume a reproducing kernel \(k_x\) on \(\mathcal{X}\) and \(k_y\) on \(\mathcal{Y}\) (according to Asm. 1) and denote \(m_x^2 = \sup_{x \in \mathcal{X}} k_x(x, x)\) and \(m_y^2 = \sup_{y \in \mathcal{Y}} k_y(y, y)\). We denote by \(C = \mathbb{E}_{x \sim \rho} \phi(x) \otimes \phi(x)\) the covariance operator over input data sampled from \(\rho\), and by \(\|C\|_{\text{op}}\) its operator norm, namely its largest singular value. Moreover, we make the following assumption.

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**Assumption 2.** There exists $G_* \in H_y \otimes H_x$ with finite trace norm, $\|G_*\|_* < +\infty$, such that $g_*(\cdot) = G_* \phi(\cdot)$ is a minimizer of the risk $\mathcal{R}$ in Eq. (2).

The assumption above requires the ideal solution of the surrogate problem to belong to the space of hypotheses of the learning algorithm. This is a standard requirement in statistical learning theory in order to characterize the excess risk bounds of an estimator [see e.g. Shalev-Shwartz and Ben-David, 2014].

**Theorem 3.** Under Asm. 2, let $Y$ be a compact set, let $(x_i, y_i)_{i=1}^n$ be a set of $n$ points sampled i.i.d. and let $\hat{g}(\cdot) = \hat{G}\phi(\cdot)$ with $\hat{G}$ the solution of Eq. (13) for $\gamma = \|G_*\|_*$. Then, for any $\delta > 0$

$$\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq (m_y + c) \sqrt{\frac{4 \log \frac{4}{\delta}}{n}} + O(n^{-1}),$$

with probability at least $1 - \delta$, where

$$c = 2m_x \|C\|_2^{1/2} \|G_*\|_*^2 + m_x \mathcal{R}(g_*) \|G_*\|_*,$$

with $\tau$ a constant not depending on $\delta, n$ or $G_*$. 

The proof is detailed in Appendix B. The two main ingredients are: i) the boundedness of the trace norm of $G_*$, which allows us to exploit the duality between trace and operator norms; ii) recent results on Bernstein’s inequalities for the operator norm of random operators between separable Hilbert spaces [Minsker, 2017].

We care to point out that previous results are available in the following settings: [Bach, 2008] shows the convergence in distribution for the trace norm estimator to the minimum risk and [Koltchinskii et al., 2011] shows excess risk bounds in high probability for an estimator which leverages previous knowledge on the distribution (e.g. matrix completion problem). Both [Bach, 2008] and [Koltchinskii et al., 2011] are devised for finite dimensional settings. To our knowledge, this is the first work proving excess risk bounds in high probability for trace norm regularized least squares. Note that the relevance of Thm. 3 is not limited to structured prediction but it can be also applied to problems such as collaborative filtering with attributes [Abernethy et al., 2009].

**Discussion.** We now discuss under which conditions trace norm (TN) regularization provides an advantage over standard the Hilbert-Schmidt (HS) one. We refer to Appendix B for a more in-depth discussion on the comparison between the two estimators, while addressing here the key points.

For the HS estimator, excess risk bounds can be derived by imposing the less restrictive assumption that $\|G_*\|_{HS} < +\infty$. A result analogous to Thm. 3 can be obtained (see Appendix B), with constant $c$

$$c = m_x (m_x + \|C\|_{op}^{1/2}) \|G_*\|_{HS}^2 + m_x \mathcal{R}(g_*) \|G_*\|_{HS}.$$

This constant is structurally similar to the one for TN (with $\| \cdot \|_{HS}$ appearing in place of $\| \cdot \|_*$), plus the additional term $m_x^2 \|G\|_{HS}^2$. 


We first note that if \( \|G\|_{HS} \ll \|G\|_{**} \), the bound offers no advantage with respect to the HS counterpart. Hence, we focus on the setting where \( \|G\|_{HS} \) and \( \|G\|_{**} \) are of the same order. This corresponds to the relevant scenario where the multiple outputs/tasks encoded by \( G \) are (almost) linearly dependent. In this case, the constant \( c \) associated to the TN estimator can potentially be significantly smaller than the one for HS: while for TN the term \( \|G\|_{2}^{2} \) is mitigated by \( \|C\|_{\max}^{1/2} \), for HS the corresponding term \( \|G\|_{HS} \) is multiplied by \( (mX + \|C\|_{\max}^{1/2}) \). Note that the operator norm is such that \( \|C\|_{\max}^{1/2} \leq mX \) but can potentially be significantly smaller than \( mX \). For instance, when \( X = \mathbb{R}^{d} \), \( kX \) is the linear kernel and training points are sampled uniformly on the unit sphere, we have \( mX = 1 \) while \( \|C\|_{\max}^{1/2} = \frac{1}{\sqrt{d}} \).

In summary, trace norm regularization allows to leverage structural properties of the data distribution provided that the output tasks are related. This effect can be interpreted as the process of “sharing” information among the otherwise independent learning problems. A similar result to Thm. 3 was proved in [Maurer and Pontil, 2013] for Lipschitz loss functions (and \( \mathcal{H}_{2} \) finite dimensional). We refer to such work for a more in-depth discussion on the implications of the link between trace norm regularization and operator norm of the covariance operator.

**Excess Risk Bounds for \( \hat{f} \).** By combining Thm. 3 with the comparison inequality for the SELF framework (see Thm. 1) we can immediately derive excess risk bounds for the structured prediction estimators \( \hat{f} = d \circ \hat{g} \).

**Corollary 4.** Under the same assumptions and notation of Thm. 3, let \( \ell \) be a SELF loss and \( \hat{f} = d \circ \hat{g} : \mathcal{X} \rightarrow \mathcal{Y} \). Then, for every \( \delta > 0 \), with probability not less than \( 1 - \delta \) it holds that

\[
\mathcal{E}(\hat{f}) - \mathcal{E}(f_{*}) \leq q_{\ell} \sqrt{\frac{4(m_{Y} + c)^{2} \log \frac{r}{\delta}}{n}} + O(n^{-\frac{1}{2}})
\]

where \( c \) and \( r \) are the same constants of Thm. 3 and \( q_{\ell} \) is as in Thm. 1.

The result above provides comparable learning rates to those of the original SELF estimator [Ciliberto et al., 2016]. However, since the constant \( c \) corresponds to the one from Thm. 3, whenever trace norm regularization provides an advantage with respect to standard Hilbert-Schmidt regularization on the surrogate problem, such improvement is directly inherited by \( \hat{f} \).

### 4.1 Multitask Learning

So far we have studied trace norm regularization when learning the multiple \( g_{t} \) in Eq. (10) within a vector-valued setting, namely where for any input sample \( x_{i} \) in training we observe all the corresponding outputs \( \psi_{t}(y_{i}) \). This choice was made mostly for notational purposes and the analysis can be extended to the more general setting of nonlinear multitask learning, where separate groups of surrogate outputs could be provided each with its own dataset. We give here a brief summary of this setting and our results within it, while postponing all details to Appendix C.

Let \( T \) be a positive integer. In typical multitask learning (MTL) settings the goal is to learn multiple functions \( f_{1}, \ldots, f_{T} : \mathcal{X} \rightarrow \mathcal{Y} \) jointly. While most previous MTL methods
considered how to enforce linear relations among tasks, [Ciliberto et al., 2017] proposed a generalization of SELF framework to address nonlinear multitask problems (NL-MTL). In this setting, relations are enforced by means of a constraint set \( C \subset \mathcal{Y}^T \) (e.g. a set of nonlinear constraints that \( f_1, \ldots, f_T \) need to satisfy simultaneously). The goal is to minimize the \textit{multi-task excess risk}

\[
\min_{f: \mathcal{X} \to C} \mathcal{E}_T(f), \quad \mathcal{E}_T(f) = \frac{1}{T} \sum_{t=1}^T \int_{\mathcal{X} \times \mathcal{Y}} \ell(f_t(x), y) d\rho_t(x, y),
\]

where the \( \rho_t \) are unknown probability distributions on \( \mathcal{X} \times \mathcal{Y} \), observed via finite samples \((x_{it}, y_{it})_{i=1}^{n_t}\), for \( t = 1, \ldots, T \). The NL-MTL framework interprets the nonlinear multitask problem as a structured prediction problem where the constraint set \( C \) represents the “structured” output. Assuming \( \ell \) to be SELF with space \( H_y \) and coding \( \psi \), the estimator \( \hat{f} : \mathcal{X} \to C \) then is obtained via the NL-MTL decoding map

\[
\hat{f}(x) = d_T(\hat{g}(x)) := \arg\min_{c \in C} \sum_{t=1}^T \langle \psi(c_t), V\hat{g}_t(x) \rangle,
\]

where each \( \hat{g}_t(\cdot) = G_t\phi(\cdot) : \mathcal{X} \to H_y \) is learned independently via surrogate ridge regression like in Eq. (6).

Similarly to the vector-valued case of Eq. (10), we can “aggregate” the operators \( G_t \in H_x \otimes H_y \) in a single operator \( \hat{G} \), which is then learned by trace norm regularization as in Eq. (11) (see Appendix C for a rigorous definition of \( \hat{G} \)). Then, a result analogous to Thm. 2 holds for the corresponding variational formulation of such problem, which guarantees the loss trick to hold as well (see Appendix A.2 for the details of the corresponding version of Alg. 1).

Also in this setting we study the theoretical properties of the low-rank structure prediction estimator obtained from the surrogate Ivanov regularization

\[
\hat{G} = \arg\min_{\|G\| \leq \gamma} \frac{1}{T} \sum_{t=1}^T \frac{1}{n_t} \sum_{i=1}^{n_t} \|G_t\phi(x_{it}) - \psi(y_{it})\|_{H_y}^2.
\]

We report the result characterizing the excess risk bounds for \( \hat{G} \) (see Thm. 7 for the formal version). Note that in this setting the surrogate risk \( \mathcal{R}_T \) of \( G \) corresponds to the average least-squares surrogate risks of the individual \( G_t \). In the following we denote by \( \bar{C} = \frac{1}{T} \sum_{t=1}^T C_t \) the average of the input covariance operators \( C_t = \mathbb{E}_{x \sim \rho_t} \phi(x) \otimes \phi(x) \) according to \( \rho_t \).

**Theorem 5** (Informal). Under Asm. 2, let \( \{x_{it}, y_{it}\}_{t=1}^n \) be independently sampled from \( \rho_t \) for \( t = 1, \ldots, T \). Let \( \tilde{g}(\cdot) = \hat{G}\phi(\cdot) \) with \( \hat{G} \) minimizer of Eq. (17). Then for every \( \delta > 0 \), with probability at least \( 1 - \delta \), it holds that

\[
\mathcal{R}_T(\tilde{g}) - \mathcal{R}_T(g_*) \leq \sqrt{\frac{2c'}{\delta n} \log \frac{T}{\delta}} + O((nT)^{-1}),
\]

where the constant \( c' \) depends on \( \|G_*\|, \|\bar{C}\|_{op}^2, \mathcal{R}_T(g_*) \) and \( r' \) is a constant independent of \( \delta, n, T, G_* \).
Here the constant $c'$ exhibits an analogous behavior to $c$ for Thm. 3 and can lead to significant benefits in the same regimes discussed for the vector-valued setting. Moreover, also in the NL-MTL setting we can leverage a comparison inequality similar to Thm. 1, with constant $q_{C,\ell,T}$ from [Thm. 5 Ciliberto et al., 2017]. As a consequence, we obtain the excess risk bound for our MTL estimator $\hat{f} = d_T \circ \hat{g}$ of the form
\[
\mathcal{E}(\hat{f}) - \mathcal{E}(f^*) \leq q_{C,\ell,T} \sqrt{c' \log \frac{T}{nT}} + O(n^{-\frac{1}{2}}).
\]

The constant $q_{C,\ell,T}$ encodes key structural properties of the constraint set $C$ and it was observed to potentially provide significant benefits over linear MTL methods (see Ex. 1 in the original NL-MTL paper). Since $q_{C,\ell,T}$ is appearing as a multiplicative factor with respect to $c'$, we could expect our low-rank estimator to provide even further benefits over standard NL-MTL by combining the advantages provided by the nonlinear relations between tasks and the low-rank relations among the surrogate outputs.

5 Experiments

We evaluated the empirical performance of the proposed method on ranking applications, specifically the pairwise ranking setting considered in [Duchi et al., 2010, Fürnkranz and Hüllermeier, 2003, Hüllermeier et al., 2008]. Denote by $D = \{d_1, \ldots, d_N\}$ the full set of documents (e.g. movies) that need to be ranked. Let $X$ be the space of queries (e.g. users) and assume that for each query $x \in X$, a subset of the set of the associated ratings $y = \{y_1, \ldots, y_N\}$ is given, representing how relevant each document is with respect to the query $x$. Here we assume each label $y_i \in \{0, \ldots, K\}$ with the relation $y_i > y_j$ implying that $d_i$ is more relevant than $d_j$ to $x$ and should be assigned a higher rank.

We are interested in learning a $f : X \to \{1, \ldots, N\}^N$, which assigns to a given query $x$ a rank (or ordering) of the $N$ object in $D$. We measure errors according to the (weighted) pairwise loss
\[
\ell(f(x), y) = \sum_{i=1}^{N} (y_i - y_j) \, \text{sign}(f_j(x) - f_i(x)),
\]
with $f_i(x)$ denoting the predicted rank for $d_i$. Following [Ciliberto et al., 2017], learning to rank with a pairwise loss can be naturally formulated as a nonlinear multitask problem and tackled via structured prediction. In particular we can model the relation between each pair of documents $(d_i, d_j)$ as a function (task) that can take values 1 or $-1$ depending on whether $d_i$ is more relevant than $d_j$ or vice-versa (or 0 in case they are equivalently relevant). Nonlinear constraints in the form of a constraint set $C$ need to be added to this setting in order to guarantee coherent predictions. This leads to a decoding procedure for Eq. (16) that amounts to solve a minimal feedback arc set problem on graphs [Slater, 1961].

We evaluated our low-rank SELF learning algorithm on the following datasets:
We compared our approach to a number of ranking methods: MART [Friedman, 2001], RankNet [Burges et al., 2005], RankBoost [Freund et al., 2003], AdaRank [Xu and Li, 2007], Coordinate Ascent [Metzler and Croft, 2007], LambdaMART [Wu et al., 2010], ListNet, and Random Forest. For all the above methods we used the implementation provided by RankLib library. We also compared with the SVMrank [Joachims, 2006] approach using the implementation made available online by the authors. Finally, we evaluated the performance of the original SELF approach in [Ciliberto et al., 2017] (SELF + \( \| \cdot \|_{HS} \)). For all methods we used a linear kernel on the input and for each dataset we performed parameter selection using 50% of the available ratings of each user for training, 20% for validation and the remaining for testing.

**Results.** Table 1 reports the average performance of the tested methods across five independent trials. Prediction errors are measured in terms of the pair-wise loss in Eq. (18), normalized between 0 and 1. A first observation is that the performance of both SELF approaches significantly outperform the competitors. This is in line with the observations in

|               | ml100k | jester1 | jester2 | jester3 | sushi |
|---------------|--------|---------|---------|---------|-------|
| MART          | 0.499  | 0.514   | 0.482   | 0.471   | 0.463 |
| RankNet       | 0.505  | 0.551   | 0.525   | 0.503   | 0.488 |
| RankBoost     | 0.504  | 0.532   | 0.505   | 0.487   | 0.479 |
| AdaRank       | 0.519  | 0.540   | 0.531   | 0.516   | 0.506 |
| Coordinate Ascent | 0.477 | 0.492   | 0.502   | 0.503   | 0.473 |
| LambdaMART    | 0.564  | 0.535   | 0.520   | 0.507   | 0.571 |
| ListNet       | 0.512  | 0.441   | 0.442   | 0.456   | 0.588 |
| Random Forests| 0.526  | 0.548   | 0.549   | 0.581   | 0.566 |
| SVMrank       | 0.513  | 0.507   | 0.506   | 0.514   | 0.541 |
| SELF + \( \| \cdot \|_{HS} \) | 0.312  | 0.386   | 0.366   | 0.375   | 0.391 |
| Ours) SELF + \( \| \cdot \|_{HS} \) | 0.156  | 0.247   | 0.340   | 0.343   | 0.313 |

Table 1: Ranking error of benchmark approaches and our proposed method on five ranking datasets.

- **Movielens.** We considered Movielens 100k (ml100k)\(^1\), which consists of ratings (1 to 5) provided by 943 users for a set of 1682 movies, with a total of 100,000 ratings available. Additional features for each movie, such as the year of release or its genre, are provided.

- **Jester.** The Jester\(^2\) datasets consist of user ratings of 100 jokes where ratings range from −10 to 10. Three datasets are available: *jester1* with 24,983 users, *jester2* with 23,500 users and *jester3* with 24,938.

- **Sushi.** The Sushi\(^3\) dataset consists of ratings provided by 5000 people on 100 different types of sushi. Ratings ranged from 1 to 5 and only 50,000 ratings are available. Additional features for users (e.g. gender, age) and sushi type (e.g. style, price) are provided.

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\(^1\)http://grouplens.org/datasets/movielens/

\(^2\)http://goldberg.berkeley.edu/jester-data/

\(^3\)http://www.kamishima.net/sushi/

\(^4\)https://sourceforge.net/p/lemur/wiki/RankLib/
[Ciliberto et al., 2017], where the nonlinear MTL approach based on the SELF framework already improved upon state of the art ranking methods. Moreover, our proposed algorithm, which combines ideas from structured prediction and multitask learning, achieves an even lower prediction error on all datasets. This supports the idea motivating this work that leveraging the low-rank relations can provide significant advantages in practice.

6 Conclusions

This work combines structured prediction methods based on surrogate approaches with multitask learning techniques. In particular, building on a previous framework for structured prediction we derived a trace norm regularization strategy that does not require explicit knowledge of the coding function. This led to a learning algorithm that can be efficiently applied in practice also when the surrogate space is large or infinite dimensional. We studied the generalization properties of the proposed estimator based on excess risk bounds for the surrogate learning problem. Our results on trace norm regularization with least-squares loss are, to our knowledge, novel and can be applied also to other settings such as collaborative filtering with side information. Experiments on ranking applications showed that leveraging the relations between surrogate outputs can be beneficial in practice.

A question opened by our study is whether other multitask regularizers could be similarly adopted. As mentioned in the paper, even well-established approaches, such as those based on incorporating in the regularizer prior knowledge of the similarity between tasks pairs, do not always extend to this setting. Further investigation in the future will be also devoted to consider alternative surrogate loss functions to the canonical least-squares loss, which could enforce desirable tasks relations between the surrogate outputs more explicitly.

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Appendix

The supplementary material is organized as follows:

- In Appendix A we show how the loss trick for both the vector-valued and multitask SELF estimator is derived.
- In Appendix B we carry out the theoretical analysis for trace norm estimator in the vector-valued setting.
- In Appendix C we prove the theoretical results characterizing the generalization properties of the SELF multitask estimator.
- In Appendix D we recall some results that are used in the proofs of previous sections.
- In Appendix E more details on the equivalence between Ivanov and Tikhonov regularization are provided.

A Loss Trick(s)

In this section we discuss some aspects related to the loss trick of the SELF framework when considering different vector-valued or MTL estimators.

A.1 Loss Tricks with Matrix Factorization

In this section we provide full details of the loss trick for trace norm regularization partly discussed in Section 3. To fix the setting, recall that we are interested in studying the following surrogate problem

$$
\min_{G \in \mathcal{H}_Y \otimes \mathcal{H}_X} \frac{1}{n} \sum_{i=1}^{n} \| G \phi(x_i) - \psi(y_i) \|_{\mathcal{H}_Y}^2 + \lambda \| G \|_*. 
$$

**Theorem 2** (Loss Trick for Low-Rank SELF Learning). Under Asm. 1, let $M, N \in \mathbb{R}^{n \times r}$ and $(A_k, B_k)$ be the $k$-th iterate of gradient descent on Eq. (12) from $A_0 = \sum_{i=1}^{n} \phi(x_i) \otimes M^i$ and $B_0 = \sum_{i=1}^{n} \psi(y_i) \otimes N^i$, with $M^i, N^i$ denoting the $i$-th rows of $M$ and $N$ respectively. Let $\hat{g}_k : \mathcal{X} \rightarrow \mathcal{H}_y$ be such that $\hat{g}_k(\cdot) = A_{k} B_{k}^* \phi(\cdot)$. Then, the structured prediction estimator $\hat{f}_k = d \circ \hat{g}_k : \mathcal{X} \rightarrow \mathcal{Y}$ with decoding $d$ in Eq. (5) is such that

$$
\hat{f}_k(x) = \arg\min_{y \in \mathcal{Y}} \sum_{i=1}^{n} \alpha_i^{tn}(x) \ell(y, y_i)
$$

for any $x \in \mathcal{X}$, with $\alpha_i^{tn}(x) \in \mathbb{R}$ the output of Alg. 1 after $k$ iterations starting from $(M_0, N_0) = (M, N)$.
Proof. We show the proof in the finite dimensional setting first and then note how it is valid in the infinite dimensional case as well. Assume $\mathcal{X} = \mathbb{R}^d$ and $\mathcal{H}_y = \mathbb{R}^T$. Let $\{(x_i, y_i)\}_{i=1}^n$ be the training set and denote by $X$ the $\mathbb{R}^{n \times d}$ matrix containing the training inputs $x_i$, $i = 1, \ldots, n$ and $Y$ the $\mathbb{R}^{n \times T}$ matrix whose rows are $\psi(y_i)$, $i = 1, \ldots, n$. Denote by $K_x$ the matrix $XX^\top$ and by $K_y$ the matrix $YY^\top$.

Using the variational form of trace norm, problem (19) can be rewritten as

$$
\min_{A \in \mathbb{R}^{d \times r}, B \in \mathbb{R}^{T \times r}} \frac{1}{n} \|Y - XAB^\top\|^2 + \lambda (\|A\|^2_{HS} + \|B\|^2_{HS}),
$$

where $r \in \mathbb{N}$ in a further hyperparameter of the problem. In the following we will absorb the factor $1/n$ in the hyperparameter $\lambda$.

We first show that starting gradient descent algorithm with $A_0 := X^\top M_0$ for some matrix $M_0 \in \mathbb{R}^{n \times r}$ and $B_0 := Y^\top N_0$ for some matrix $N_0 \in \mathbb{R}^{n \times r}$, then at every iteration $A_k := X^\top M_k$ and $B_k := Y^\top N_k$.

Let us set $\mathcal{L}(A, B) := \|Y - XAB^\top\|^2 + \lambda (\|A\|^2_{HS} + \|B\|^2_{HS})$; the gradients of $\mathcal{L}$ with respect to $A$ and $B$ are given by

1) $\nabla_A \mathcal{L}(A, B) = X^\top (XAB^\top - Y)B + \lambda A$

2) $\nabla_B \mathcal{L}(A, B) = (XAB^\top - Y)^\top XA + \lambda B$.

We show that $A_k := X^\top M_k$ and $B_k := Y^\top N_k$ by induction. Assume it is true for $k$ and show it holds for $k+1$; denoting by $\nu$ the stepsize, we have

$$
A_{k+1} = A_k - \nu \nabla_A \mathcal{L}(A_k, B_k) = A_k - \nu (X^\top (XA_kB_k^\top - Y)B_k + \lambda A_k)
$$

$$
= X^\top M_k - \nu (X^\top X X^\top M_k B_k^\top B_k - X^\top Y B_k) - \nu \lambda X^\top M_k
$$

$$
= X^\top ((1 - \nu\lambda) M_k - \nu (K_x M_k B_k^\top B_k - Y B_k))
$$

$$
= X^\top ((1 - \nu\lambda) M_k - \nu (K_x M_k N_k^\top K_y N_k - K_y N_k)),
$$

and hence $A_{k+1} = X^\top M_{k+1}$

$$
M_{k+1} = (1 - \nu\lambda) M_k - \nu (K_x M_k N_k^\top K_y N_k - K_y N_k).
$$

(21)

As for $B$, assume $B_k = Y^\top N_k$;

$$
B_{k+1} = B_k - \nu \nabla_B \mathcal{L}(A_k, B_k)
$$

$$
= B_k - \nu ((XA_k B_k^\top - Y)^\top X A_k + \lambda B_k)
$$

$$
= Y^\top N_k - \nu (Y^\top N_k A_k^\top X^\top X A_k - Y^\top X A_k) - \nu \lambda Y^\top N_k
$$

$$
= Y^\top ((1 - \nu\lambda) N_k - \nu (K_x N_k M_k^\top K_y M_k - K_y M_k))
$$

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and hence \( B_{k+1} = Y^\top N_{k+1} \) with
\[
N_{k+1} = (1 - \lambda \nu) N_k - \nu (N_k M_k^\top K_x K_x M_k - K_x M_k).
\] (22)

Then, denote by \( M \) and \( N \) the limits of \( M_k \) and \( N_k \). Given a new \( x \), the estimator is
\[
\hat{g}_k(x) = x X^\top M_k N_k^\top Y.
\]

Expanding the product we can rewrite
\[
\hat{g}_k(x) = \sum_{i=1}^n \alpha_i^{tn}(x) \psi(y_i), \quad \alpha^{tn}(x) = N_k M_k^\top X x^\top = N_k M_k^\top v_x,
\]
where \( v_x = X x^\top \in \mathbb{R}^n \). Let \( d \) be the decoding map defined by
\[
d(h) = \arg\min_{y \in Y} \langle \psi(y), V h \rangle.
\]

Then
\[
\hat{f}_k(x) = d \circ \hat{g}_k(x) = \{ \sum_{i=1}^n \alpha_i^{tn}(x) \langle \psi(y), V \psi(y_i) \rangle = \arg\min_{y \in Y} \sum_{i=1}^n \alpha_i^{tn}(x) \ell(y, y_i).
\]

Note that in order to obtain the estimator \( \hat{g}_k \), only the access to \( M_k \) and \( N_k \) is needed. Also, examining the updates for \( M_k \) and \( N_k \) outlined in (21) and (22) we note that the data are accessed through \( K_x \) and \( K_y \) only, which are kernels on input and output respectively. This leads to a direct extension of the argument in the infinite dimensional setting, where the RKHSs \( H_x \) and \( H_y \) on input and output spaces are infinite dimensional Hilbert spaces. \( \square \)

### A.2 Loss Trick in the Multitask Setting

We now turn to the **multitask** case.

We recall the surrogate problem with trace norm regularization, i.e.
\[
\min_{G \in \mathbb{R}^T \otimes \mathcal{H}_x} \frac{1}{T} \sum_{t=1}^T \frac{1}{n_t} \sum_{i=1}^{n_t} \| G_t \phi(x_{it}) - \psi(y_{it}) \|^2 + \lambda \| G \|_*.
\] (23)

**Proposition 6.** Let \( k : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) be a reproducing kernel with associated RKHS \( \mathcal{H}_x \). Let \( \hat{g} = \hat{G} \phi(\cdot) \) be the solution of problem (23), denote by \( \hat{g}_t, t = 1, \ldots, T \) its components. Then the loss trick applies to this setting, i.e. the estimator \( \hat{f} = d \circ \hat{g} \) with \( d_T \) as in Eq. (16), is equivalently written as
\[
\hat{f}(x) = \arg\min_{c \in \mathcal{C}} \sum_{i=1}^T \sum_{t=1}^{n_t} \alpha_{it}^{tn}(x) \ell(c_t, y_{it}),
\] (24)

for some coefficients \( \alpha_{it} \) which are derived in the proof below.
Proof. Assume \( X = \mathbb{R}^d \) and \( \mathcal{H}_y = \mathbb{R}^T \) for the sake of clarity, so that \( G\phi(x) = Gx \). For any \( t = 1, \ldots, T \), let \( \{(x_{it}, y_{it})\}_{i=1}^{n_t} \) be the training set for the \( t^{th} \) task.

Denote by \( X \in \mathbb{R}^{n \times d} \) the matrix containing the training inputs \( x_{it} \), and by \( Y \in \mathbb{R}^{n \times T} \) the matrix whose rows are \( \psi(y_{it}) \); denote by \( X_t \) the \( n_t \times d \) matrix containing training inputs of the \( t^{th} \) task and by \( Y_t \) the \( n_t \times 1 \) vector with entries \( \psi(y_{it}) \) \( i = 1, \ldots, n_t \). We rewrite (23) using the variational form of the trace norm:

\[
\min_{A \in \mathbb{R}^{d \times r}, B \in \mathbb{R}^{T \times r}} ||Q \odot (Y - XAB^\top)||^2 + \lambda(||A||^2_{\text{HS}} + ||B||^2_{\text{HS}}),
\]

where \( r \in \mathbb{N} \) is now a hyperparameter and \( Q \) is a mask which contains zeros in correspondence of missing data. The expression above is also equivalent to

\[
\min_{A \in \mathbb{R}^{d \times r}, B \in \mathbb{R}^{T \times r}} \frac{1}{T} \sum_{t=1}^{T} \left( \frac{1}{n_t} \|X_tA - Y_t\|^2 + \lambda(\|B_t\|^2_{\text{HS}} + ||A||^2_{\text{HS}}) \right),
\]

where \( B_t \) denotes the \( t^{th} \) row of \( B \), i.e. \( B_t \) is a \( 1 \times r \) vector. Thanks to this split, we can update \( B \) by updating its rows separately, via (we omit factors 2 which would come from derivatives)

\[
B_{t,k+1} = B_{t,k} - \nu(n_t^{-1}(B_{t,k}A_k^\top X_t^\top - Y_t^\top)X_tA_k + \lambda B_{t,k}).
\]

Initialising \( B_{t,0} = Y_t^\top N_{t,0} \) for some matrix \( N_{t,0} \in \mathbb{R}^{n_t \times r} \), gradient descent updates preserve the structure, and for each \( k \), \( B_{t,k} = Y_t^\top N_{t,k} \). Indeed,

\[
B_{t,k+1} = B_{t,k} - \nu(n_t^{-1}(B_{t,k}A_k^\top X_t^\top - Y_t^\top)X_tA_k + \lambda B_{t,k})
\]

\[
= Y_t^\top N_{t,k} - \nu(n_t^{-1}(Y_t^\top N_{t,k}A_k^\top X_t^\top - Y_t^\top)X_tA_k + \lambda Y_t^\top N_{t,k})
\]

\[
= Y_t^\top ((1 - \nu \lambda) N_{t,k} - \nu n_t^{-1}(N_{t,k}A_k^\top X_t^\top X_tA_k - X_tA_k))
\]

\[
= Y_t^\top N_{t,k+1}
\]

where

\[
N_{t,k+1} = (1 - \nu \lambda) N_{t,k} - \nu n_t^{-1}(N_{t,k}A_k^\top X_t^\top X_tA_k - X_tA_k).
\]

Let us now focus on updates of \( A \), and then combine the two. Set

\[
\mathcal{L}(A, B) := ||Q \odot (Y - XAB^\top)||^2 + \lambda(\|A\|^2_{\text{HS}} + ||B||^2_{\text{HS}});
\]

Note that the gradient with respect to \( A \) reads as \( \nabla_A \mathcal{L}(A, B) = X^\top (Q \odot (XAB^\top - Y))B + \lambda A \). Hence, initialising \( A_0 = X^\top M_0 \), each iterate \( A_k \) has the form \( X^\top M_k \) and it is possible to perform updates on \( M_k \) only as in the proof of Thm. 2, via

\[
M_{k+1} = (1 - \lambda \nu) M_k - ((Q \odot (XX^\top M_k B_k^\top - Y))B_k).
\]
Let us analyse the term \((Q \odot (XX^\top M_k B_k^\top - Y))B_k\): leveraging the structure of the mask,
\begin{equation}
(Q \odot (XX^\top M_k B_k^\top - Y))B_k = [S_1^\top, \ldots, S_T^\top]^\top
\end{equation}
where \(S_t\) is a \(n_t \times r\) matrix equal to
\[S_t = X_t X^\top M_k B_t^\top B_t k = X_t X^\top M_k N_t Y_t Y_t^\top N_t k.
\]
At convergence, we will have \(A = X^\top M\) and \(B_t = Y_t^\top N_t\) for \(t = 1, \ldots, T\). Hence, the \(t^\text{th}\)
component of the estimator is given by
\[
\hat{g}_t(x) = xA B_t^\top = x X^\top M N_t^\top Y_t = \sum_{i=1}^{n_t} \alpha_{it}^\text{tn}(x) \psi(y_{it}), \quad \alpha_{it}^\text{tn}(x) = N_t M^\top X x^\top.
\]
Then, the estimator \(\hat{f}_N\), with \(N = (n_1, \ldots, n_T)\) is given by
\[
\hat{f}_N(x) = \arg\min_{c \in \mathcal{C}} \sum_{t=1}^{T} \langle c_{t}, V \hat{g}_t(x) \rangle = \arg\min_{c \in \mathcal{C}} \sum_{t=1}^{T} \sum_{i=1}^{n_t} \alpha_{it}^\text{tn}(x) \langle c_{t}, V \psi(y_{it}) \rangle = \arg\min_{c \in \mathcal{C}} \sum_{t=1}^{T} \sum_{i=1}^{n_t} \alpha_{it}^\text{tn}(x) \ell(c_{t}, y_{it}),
\]
and hence the loss trick holds.

\[\text{A.3 \ Remark on the Lack of Loss Trick for Regularizers via Positive Semidefinite Operator}\]

Assume \(X = \mathbb{R}^d, \mathcal{H}_y = \mathbb{R}^T\) and let \(Y\) be the \(n \times T\) matrix containing \(\psi(y_{it})\) in its rows. Given \(A \in \mathbb{R}^{T \times T}\) symmetric positive definite, the surrogate problem with regularizer \(\text{tr}(GAG^\top)\) reads as
\[
\frac{1}{n} \|Y - XG\|^2 + \lambda \text{tr}(GAG^\top).
\]
We omit the factor \(1/n\) as it is does not affect what follows. The problem above has the following solution (see for instance [Alvarez et al., 2012])
\[
\text{vec}(G) = (I \otimes X^\top X + \lambda A \otimes I)^{-1} (I \otimes X^\top) \text{vec}(Y).
\]
This can be rewritten as
\[
\text{vec}(G) = (A^{-1/2} \otimes I)(A^{-1} \otimes X^\top X + \lambda I)^{-1}(A^{-1/2} \otimes X^\top) \text{vec}(Y)
\]
\[
= (A^{-1} \otimes X^\top)(A^{-1} \otimes K + \lambda I)^{-1} \text{vec}(Y),
\]
where \(K = XX^\top\) is the kernel matrix. Setting \(\text{vec}(M(Y)) = (A^{-1} \otimes K + \lambda M)^{-1} \text{vec}(Y)\),
\[
\text{vec}(G) = (A^{-1} \otimes X^\top) \text{vec}(M(Y)) = \text{vec}(X^\top M(Y) A^{-1}) = \text{vec}(X^\top M(Y) A^{-1}),
\]
since \(A\) is symmetric. Then \(G = X^\top M(Y) A^{-1}\). The decoding procedure yields
\[
\hat{f}(x) = d(\hat{g}(x)) = \arg\min_{y \in \mathcal{Y}} \langle Y, V \hat{g}(x) \rangle = \arg\min_{y \in \mathcal{Y}} \langle Y, VA^{-1} M(Y)^\top v_x \rangle,
\]
and due to the product \(VA^{-1}\) we cannot retrieve the loss function, i.e. the loss trick.

Now, let us distinguish the following cases
1. \(Y\) has finite cardinality;

2. \(Y\) has not finite cardinality, \(\mathcal{H}_y\) is infinite dimensional or \(\psi\) and \(V\) are unknown.

In the first case, let us set \(N = \{1, \ldots, |Y|\}\) and \(\mathcal{H}_y = \mathbb{R}^{|Y|}\). Let \(q : Y \rightarrow N\) be a one-to-one function and for \(y \in Y\) set \(Y = e_{q(y)}\) where \(e_i\) denoted the \(i^{th}\) element of the canonical basis of \(\mathbb{R}^{|Y|}\). Also, set \(V \in \mathbb{R}^{|Y| \times |Y|}\) the matrix with entries \(V_{ij} = \ell(q^{-1}(i), q^{-1}(j))\). Then, since \(A\) is a known matrix, \(\psi\) and \(V\) are defined as above, the estimator \(\hat{f}\) can be retrieved despite the lack of loss trick.

In the second case, it is not clear how to manage the operation \(VA^{-1}\) since \(V\) is unknown and also, both \(V\) and \(A\) are bounded operators from an infinite dimensional space to itself. While in the standard SELF framework, the infinite dimensionality is hidden in the loss trick, and there is no need to explicitly deal with infinite dimensional objects, here it appears to be necessary due to the action of \(A\).

B Theoretical Analysis

**Theorem 3.** Under Asm. 2, let \(Y\) be a compact set, let \((x_i, y_i)_{i=1}^n\) be a set of \(n\) points sampled i.i.d. and let \(\hat{g}(\cdot) = \hat{G}\psi(\cdot)\) with \(\hat{G}\) the solution of Eq. (13) for \(\gamma = \|G_s\|_*\). Then, for any \(\delta > 0\)

\[
R(\hat{g}) - R(g_\gamma) \leq (m_Y + c)\sqrt{\frac{4\log\frac{4}{\delta}}{n}} + O(n^{-1}),
\]

(14)

with probability at least \(1 - \delta\), where

\[
c = 2m_X\|C\|_{op}^{1/2}\|G_s\|_*^2 + m_XR(g_\gamma)\|G_s\|_*,
\]

(15)

with \(r\) a constant not depending on \(\delta, n\) or \(G_s\).

**Proof.** We split the error as follows:

\[
R(\hat{g}) - R(g_\gamma) \leq R(\hat{g}) - \hat{R}(g_\gamma) + \hat{R}(\hat{g}) - \hat{R}(g_\gamma)
\]

\[
+ \hat{R}(g_\gamma) - R(g_\gamma) + R(g_\gamma) - R(g_\gamma).
\]

Now, by definition of \(\hat{g}\) the term \(\hat{R}(\hat{g}) - \hat{R}(g_\gamma)\) is negative. Also, denoting by \(\rho_{\psi|\mathcal{X}}\) the
marginal on $\mathcal{X}$ of the probability measure $\rho_t$,

$$
\mathcal{R}(g_{\gamma^*}) - \mathcal{R}(g_{\gamma}) = \int_\mathcal{X} \|G_{\gamma^*}\phi(x) - G_{\gamma}\phi(x)\|_{L^2(\rho_t)}^2 \, d\rho_t(x) = \inf_{G \in \mathcal{H}_{\gamma}} \|G\phi(x) - G_{\gamma}\phi(x)\|_{L^2(\rho_t)}^2
$$

(27)

$$
\leq \left\|\left(\frac{\gamma}{\|G_{\gamma}\|_*}\right)G_{\gamma}\phi(x) - G_{\gamma}\phi(x)\right\|_{L^2(\rho_t)}^2 \leq \left(1 - \frac{\gamma}{\|G_{\gamma}\|_*}\right)^2 \|G_{\gamma}\|_{L^2(\rho_t)}^2
$$

(28)

$$
\leq \left(1 - \frac{\gamma}{\|G_{\gamma}\|_*}\right)^2 m^2\|G_{\gamma}\|_{HS}^2 \leq (\|G_{\gamma}\|_* - \gamma)^2 m^2.
$$

(29)

It remains to bound $R_1 := \mathcal{R}(\hat{g}) - \hat{\mathcal{R}}(\hat{g})$ and $R_2 := \hat{\mathcal{R}}(g_{\gamma^*}) - \mathcal{R}(G)$. Since

$$
R_1 + R_2 \leq 2 \sup_{G \in \mathcal{H}_{\gamma^*}} |\hat{\mathcal{R}}(G) - \mathcal{R}(G)|,
$$

we just have to bound the term on the right hand side.

Denote

$$
C = \mathbb{E}\phi(x) \otimes \phi(x), \quad \hat{C} = \frac{1}{n} \sum_{i=1}^{n} \phi(x_i) \otimes \phi(x_i)
$$

$$
Z = \mathbb{E}\psi(y) \otimes \phi(x), \quad \hat{Z} = \frac{1}{n} \sum_{i=1}^{n} \psi(y_i) \otimes \phi(x_i).
$$

For any operator $G$ in $\mathcal{H}_\gamma \otimes \mathcal{H}_\delta$, we have

$$
|\hat{\mathcal{R}}(G) - \mathcal{R}(G)| = \left|\frac{1}{n} \sum_{i=1}^{n} \|\psi(y_i) - G\phi(x_i)\|_{\mathcal{H}}^2 - \mathbb{E}\|\psi(y) - G\phi(x)\|_{\mathcal{H}}^2\right|
$$

$$
= \left|\frac{1}{n} \sum_{i=1}^{n} \left(\langle G^*G, \phi(x_i) \otimes \phi(x_i) \rangle_{HS} - 2 \langle G, \psi(y_i) \otimes \phi(x_i) \rangle_{HS} + \|\psi(y_i)\|_{\mathcal{H}}^2\right)\right|
$$

$$
- \mathbb{E}\left(\langle G^*G, \phi(x) \otimes \phi(x) \rangle_{HS} - 2 \langle G, \psi(y) \otimes \phi(x) \rangle_{HS} + \|\psi(y)\|_{\mathcal{H}}^2\right)\right|
$$

$$
= \left|\langle G^*G, \hat{C} - C \rangle_{HS} - 2 \langle G, \hat{Z} - Z \rangle_{HS} + \frac{1}{n} \sum_{i=1}^{n} \|\psi(y_i)\|_{\mathcal{H}}^2 - \mathbb{E}\|\psi(y)\|_{\mathcal{H}}^2\right|
$$

$$
\leq \|G\|_{HS}^2 \|C - \hat{C}\|_{op} + 2\|G\|_\ast \|Z - \hat{Z}\|_{op} + \mathbb{E}\|\psi(y)\|_{\mathcal{H}}^2 - \frac{1}{n} \sum_{i=1}^{n} \|\psi(y_i)\|_{\mathcal{H}}^2.
$$

In the last inequality we used that $\|G^*G\|_* = \|G^*G\|_{HS} = \|G\|_{HS}^2$ in the first part. In the following we bound $\|C - \hat{C}\|_{op}$ and $\|Z - \hat{Z}\|_{op}$, in two different steps.

**STEP 1** Let us start with $\|C - \hat{C}\|_{op}$. We leverage the result in [Minsker, 2017] on Bernstein’s inequality for self adjoint operators, which are recalled in Lemma 11 below. Let us set

$$
X_i := (\phi(x_i) \otimes \phi(x_i) - C)/n
$$
and note that $E(X_i) = 0$. Also, resolving the square we have that

$$E(X_i^2) = \frac{1}{n^2} E(\langle \phi(x_i), \phi(x_i) \rangle \phi(x_i) \otimes \phi(x_i) - 2\phi(x_i) \otimes \phi(x_i) C^2) = \frac{1}{n^2} E(m_i^2 \phi(x_i) \otimes \phi(x_i)) - C^2,$$

and hence (we assume $m_i \geq 1$)

$$\left\| \sum_{i=1}^{n} E X_i^2 \right\| \leq \frac{1}{n} \left( m_i^2 \left\| C \right\|_{\text{op}} + \left\| C \right\|_{\text{op}}^2 \right) \leq \frac{2m_i^2}{n} \left\| C \right\|_{\text{op}} =: \sigma^2,$$

Since $\left\| \phi(x_i) \right\| \leq m_i$ for any $i = 1, \ldots, n$, we get

$$\left\| X_i \right\| \leq \frac{m_i^2 + \left\| C \right\|_{\text{op}}}{n} \leq \frac{2m_i^2}{n} := U.$$

Set

$$\tilde{r}_1 := \frac{\text{tr} \left( \sum_{i=1}^{n} E X_i^2 \right)}{\left\| \sum_{i=1}^{n} E X_i^2 \right\|_{\text{op}}}.$$ 

Note that the quantity above is the effective rank of $\sum_{i=1}^{n} E X_i^2$. With $\sigma^2$ and $U$ as above, Lemma 11 yields

$$\left\| C - \hat{C} \right\|_{\text{op}} \leq \frac{4}{n} \left( \frac{m_i^2}{3} \ln \left( \frac{14\tilde{r}_1}{\delta} \right) \right) + \sqrt{\frac{4m_i^2\left\| C \right\|_{\text{op}}}{n} \ln \left( \frac{14\tilde{r}_1}{\delta} \right)}$$

with probability greater or equal to $1 - \delta$.

**STEP 2** As for $\left\| Z - \hat{Z} \right\|_{\text{op}}$ we proceed in a similar way: let $X_i := (\psi(y_i) \otimes \phi(x_i) - Z)/n$. Then,

$$\left\| X_i \right\| \leq \frac{m_y m_x + \left\| Z \right\|_{\text{op}}}{n} \leq \frac{2m_x m_y}{n}.$$ 

Also,

$$E X_i^* X_i = \frac{1}{n^2} E [\langle \phi(x_i) \otimes \psi(y_i) - Z^* \rangle (\psi(y_i) \otimes \phi(x_i) - Z)]$$

$$= \frac{1}{n^2} \left( E(\langle \psi(y_i), \psi(y_i) \rangle \phi(x_i) \otimes \phi(x_i)) - Z^* Z \right) \leq \frac{2}{n^2} E(\langle \psi(y_i), \psi(y_i) \rangle \phi(x_i) \otimes \phi(x_i)).$$

(30)
Then
\[ \| \sum_{i=1}^{n} E X_i^* X_i^* \|_{\text{op}} \leq \frac{2}{n} \| E(\langle \psi(y), \psi(y) \rangle \phi(x) \otimes \phi(x)) \|_{\text{op}}. \]

Applying Lemma 14, we obtain
\[ \| \sum_{i=1}^{n} E X_i^* X_i^* \|_{\text{op}} \leq \frac{2m^2}{n}(\| G_* \|_{\text{HS}}^2 \| C \|_{\text{op}} + R(g_*)). \]

Similarly,
\[ E X_i X_i^* = \frac{1}{n^2} E[(\psi(y_i) \otimes \phi(x_i) - Z)(\phi(x_i) \otimes \psi(y_i) - Z^*)] \]
\[ = \frac{1}{n^2} \left( E(\langle \phi(x_i), \phi(x_i) \rangle \psi(y_i) \otimes \psi(y_i)) - ZZ^* \right) \leq \frac{2}{n^2} E(\langle \phi(x_i), \phi(x_i) \rangle \psi(y_i) \otimes \psi(y_i)) \]
\[ \leq \frac{2}{n^2} m^2 E(\psi(y_i) \otimes \psi(y_i)). \]

and
\[ \| \sum_{i=1}^{n} E X_i X_i^* \|_{\text{op}} \leq \frac{2m^2}{n} \| E(\psi(y) \otimes \psi(y)) \|_{\text{op}}. \]

Applying Lemma 13, we conclude
\[ \| \sum_{i=1}^{n} E X_i X_i^* \|_{\text{op}} \leq \frac{2m^2}{n}(\| G_* \|_{\text{HS}}^2 \| C \|_{\text{op}} + R(g_*)). \]

Hence both \( \| \sum_{i=1}^{n} E X_i X_i^* \|_{\text{op}} \) and \( \| \sum_{i=1}^{n} E X_i^* X_i \|_{\text{op}} \) are bounded by \( \frac{2m^2}{n}(\| G_* \|_{\text{HS}}^2 \| C \|_{\text{op}} + R(g_*)). \)

Moreover, let
\[ \bar{r}_2 = \max \left( \frac{\text{tr}(\sum_{i=1}^{n} E X_i X_i^*)}{\| \sum_{i=1}^{n} E X_i X_i^* \|_{\text{op}}}, \frac{\text{tr}(\sum_{i=1}^{n} E X_i^* X_i)}{\| \sum_{i=1}^{n} E X_i^* X_i \|_{\text{op}}} \right), \]
which corresponds to the maximum between effective ranks of \( \sum_{i=1}^{n} E X_i X_i^* \) and \( \sum_{i=1}^{n} E X_i^* X_i \).

Bernstein’s inequality shown in [Minsker, 2017] (and recalled in Lemma 12) gives
\[ \| Z - \hat{Z} \|_{\text{op}} \leq \frac{4}{n} \left( \frac{m_s m_y}{3} \ln \left( \frac{28\bar{r}_2}{\delta} \right) \right) + \sqrt{\frac{2m^2}{n}(\| G_* \|_{\text{HS}}^2 \| C \|_{\text{op}} + R(g_*)) \ln \left( \frac{28\bar{r}_2}{\delta} \right)} \]
with probability greater or equal to \( 1 - \delta \). Splitting the second term we see that
\[ \| Z - \hat{Z} \|_{\text{op}} \leq \frac{4}{n} \left( \frac{m_s m_y}{3} \ln \left( \frac{28\bar{r}_2}{\delta} \right) \right) + \left( \| G \|_{\text{HS}} \| C \|_{\text{op}} m + m \sqrt{R(g_*)} \right) \sqrt{\frac{2}{n} \ln \left( \frac{28\bar{r}_2}{\delta} \right)}. \]
STEP 3. Finally, by Hoeffding inequality
\[
\left| \mathbb{E}\|\psi(y)\|^2_{\mathcal{H}_y} - \frac{1}{n} \sum_{i=1}^{n} \|\psi(y_i)\|^2_{\mathcal{H}_y} \right| \leq m_y \sqrt{\ln \left( \frac{2}{\delta} \right) \frac{1}{n}}
\]
with probability at least 1 − \( \delta \).

FINAL STEP. We have now all the bounds that we need. By taking \( r = \max(\bar{r}_1, \bar{r}_2) \) and performing an intersection bound on the three parts we conclude
\[
|\hat{\mathcal{R}}(G) - \mathcal{R}(G)| \leq \gamma^2 \left( \frac{A \sqrt{n}}{n} + \frac{B}{\sqrt{n}} \right) + \gamma \left( \frac{A' \sqrt{n}}{n} + \frac{B'}{\sqrt{n}} \right) + m_y \sqrt{\ln \left( \frac{2}{\delta} \right) \frac{1}{n}} \tag{32}
\]
with probability greater or equal than 1 − 3\( \delta \), with
\[
A = 4 \ln \left( \frac{28r \sqrt{m_y^2}}{\delta} \right) \sqrt{3} \quad B = (2 + \sqrt{2}) m_y \|C\|_{\bar{\mathcal{H}}_p} \sqrt{\ln \left( \frac{28r}{\delta} \right)} \\
A' = 4 \ln \left( \frac{28r \sqrt{m_y^* m_y}}{\delta} \right) \sqrt{3} \quad B' = m_y \sqrt{2 \mathcal{R}(g_*) \ln \left( \frac{28r}{\delta} \right)}.
\]
Combining with the approximation error in Eq. (27), we obtain
\[
\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq \gamma^2 \left( \frac{A \sqrt{n}}{n} + \frac{B}{\sqrt{n}} \right) + \gamma \left( \frac{A' \sqrt{n}}{n} + \frac{B'}{\sqrt{n}} \right) + \sqrt{\ln \left( \frac{2}{\delta} \right) \frac{m_y^2}{n}} + (\|G_*\|_* - \gamma)^2 m_y^2.
\]
In principle, starting from the bound above we should optimize with respect to \( \gamma \) to find the optimal value, which will be between 0 and \( \|G_*\|_* \). Here we consider the simpler case where \( \gamma = \|G_*\|_* \). Isolating the faster terms, the bound above becomes
\[
\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq \frac{\|G_*\|_*^2}{\sqrt{n}} \left( m_y \|C\|_{\bar{\mathcal{H}}_p} (2 + \sqrt{2}) + (\|G_*\|_* m_y \sqrt{2 \mathcal{R}(g_* \mathcal{R}(g_*))}) \sqrt{\ln \left( \frac{28r}{\delta} \right)} + m_y \sqrt{\ln \left( \frac{2}{\delta} \right) \frac{1}{n}} \right)
\]
Rearranging we get
\[
\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq \frac{\|G_*\|_*}{\sqrt{n}} \left[ \left( (\sqrt{2} + 1) m_y \|G_*\|_* \|C\|_{\bar{\mathcal{H}}_p} + m_y \sqrt{2 \mathcal{R}(g_* \mathcal{R}(g_*))} \right) \sqrt{\ln \left( \frac{28r}{\delta} \right)} \right] + m_y \sqrt{\ln \left( \frac{2}{\delta} \right) \frac{1}{n}} \tag{33}
\]
with probability greater or equal to 1 − 3\( \delta \). Bounding \( \ln \left( \frac{2}{\delta} \right) \) with \( \ln \left( \frac{28r}{\delta} \right) \) we get
\[
\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq (c + m_y) \sqrt{\ln \left( \frac{28r}{\delta} \right) \frac{1}{n}} + O(n^{-1})
\]
where \( c = (2 + \sqrt{2}) m_y \|G_*\|_* \|C\|_{\bar{\mathcal{H}}_p} + \sqrt{2} \|G_*\|_* m_y \mathcal{R}(g_*) \). In the main body of the paper we bound it as
\[
\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq (c + m_y) \sqrt{\frac{4 \ln \left( \frac{28r}{\delta} \right)}{n}} + O(n^{-1})
\]
with \( c = 2m_y \|G_*\|_* \|C\|_{\bar{\mathcal{H}}_p} + \|G_*\|_* m_y \mathcal{R}(g_*) \) to make it neater. \( \square \)
Comparison with Hilbert-Schmidt regularization. The goal of this remark is a comparison between the constants in the bound for the trace norm estimator and in the bound we would obtain with Hilbert-Schmidt estimator.

Bound for HS-regularization. We show here the bound obtained with Hilbert-Schmidt regularization. In this case, \( \mathcal{G}_\gamma := \{ g(\cdot) = G\phi(\cdot) \mid \| G \|_{\text{HS}} \leq \gamma \} \). Note that if \( G \) is a Hilbert-Schmidt operator, then \( G^*G \) is a trace norm operator. Therefore, the term \( \langle G^*G, \hat{C} - C \rangle_{\text{HS}} \) can be bounded as before:

\[
\| C - \hat{C} \|_{\text{op}} \leq \frac{4}{n} \left( \frac{m^2}{3} \ln \left( \frac{14r_1}{\delta} \right) \right) + \sqrt{\frac{4m^2\| C \|_{\text{op}}}{n} \ln \left( \frac{14r_1}{\delta} \right)}
\]

On the other hand, for the second term \( \langle G, \hat{Z} - Z \rangle_{\text{HS}} \), we have

\[
\left| \langle G, \hat{Z} - Z \rangle_{\text{HS}} \right| \leq \| G \|_{\text{HS}} \| \hat{Z} - Z \|_{\text{HS}}.
\]

Now, in order to bound \( \| \hat{Z} - Z \|_{\text{HS}} \), we note that \( \| Z \|_{\text{HS}}^2 \leq m^2 \mathbb{E} \| \psi(y) \|_{\text{HS}}^2 = m^2 \text{tr}(C_Y) \).

Proceeding in a similar way as in Lemma 2 in [Smales and Zhou, 2007], we obtain that \( \text{tr}(C_Y) \leq \mathcal{R}(g) + m^4 \| G \|_{\text{HS}}^4 \).

From Lemma 2 in [Smales and Zhou, 2007],

\[
\| \hat{Z} - Z \|_{\text{HS}} \leq \sqrt{\frac{2(m^2 \mathcal{R}(g) + m^4 \| G \|_{\text{HS}}^2)}{n}} \ln \left( \frac{2}{\delta} \right) + O(n^{-1}).
\]

Finally, no difference holds for the last term \( \| \mathbb{E}\| \psi(y) \|_{\text{HS}}^2 - \frac{1}{n} \sum_{i=1}^{n} \| \psi(y_i) \|_{\text{HS}}^2 \). Hence, combining the three parts and bounding \( \ln(\frac{2}{\delta}) \) with \( \ln(\frac{14r_1}{\delta}) \), we get

\[
\mathcal{R}(\hat{g}_{\text{HS}}) - \mathcal{R}(g) \leq \sqrt{\frac{m^4}{n}} \left( \| G \|_{\text{HS}} \| C \|_{\text{op}}^2 + m^2 \| G \|_{\text{HS}}^2 + m \sqrt{2 \mathcal{R}(g) + m} \right) \ln \left( \frac{14r_1}{\delta} \right) + O(n^{-1}).
\]

Note that this bound slightly refines the excess risk bounds for HS regularization provided in [Ciliberto et al., 2016].

Comparison and discussion. Let us compare the bound with HS regularization in Eq. (34) with the bound for the trace norm estimator that we derived in the proof of Thm. 3:

\[
\mathcal{R}(\hat{g}) - \mathcal{R}(g) \leq \sqrt{\frac{m^4}{n}} \left( \| G \|_{\text{HS}} \| C \|_{\text{op}}^2 + m^2 \sqrt{2 \mathcal{R}(g) + m} \right) \ln \left( \frac{28r_1}{\delta} \right) + O(n^{-1}).
\]

To make the comparison easier, we isolate the constants in the bounds:

HS: \( 2m^2 \| G \|_{\text{HS}}^2 \| C \|_{\text{op}}^2 + \sqrt{2}m^2 \| G \|_{\text{HS}}^2 + m \mathcal{R}(g) \| G \|_{\text{HS}} + m \) versus

TN: \( (2 + \sqrt{2})m^2 \| G \|_{\text{HS}}^2 \| C \|_{\text{op}}^2 + m \mathcal{R}(g) \| G \|_{\text{HS}} + m \).
We can summarize the cases as below.

- If \(\|G_*\|_{HS} \ll \|G_*\|_*\), then the TN bound gives no advantage over the HS one.
- Whenever \(\|G_*\|_{HS}\) and \(\|G_*\|_*\) are of the same order, our result shows an advantage in the constant of the bound: indeed, while in trace norm case, the norm \(\|G_*\|_*\) is mitigated by \(\|C\|_{\text{op}}\) in the HS case it is not, because of the extra term \(\|G_*\|_{HS}^2 m_x\).

Note that \(\|C\|_{\text{op}} \leq m_X\) and the gap between the two can be significant: for instance, if \(C\) is the covariance operator of a uniform distribution on a \(d\)-dimensional unit sphere, \(\|C\|_{\text{op}} = 1/d\) while \(m_X = 1\). Hence the entity of the improvement depends on how smaller \(\|C\|_{\text{op}}\) is with respect to \(\text{tr}(C)\).

The point above holds true when the other quantities \((m_Y, \|G\|_R(G_*))\) in the constant do not dominate. However, this is reasonable to expect:

- \(\mathcal{R}(g_*)\) is the minimum expected risk;
- \(m_x\) is 1 whenever we choose a normalized kernel on the input (Gaussian);
- \(m_Y\) is also typically 1: \(m_Y\) is such that \(\sup_{y \in Y} \|k_y(y, \cdot)\|_{\mathcal{H}_Y} \leq m_Y^2\) where \(h\) is a reproducing kernel on the output. Whenever \(Y\) is finite (and hence \(k_Y(y, y') = \delta_{y=y'}\)) or the loss is smooth (and hence \(h\) is the Abel kernel), \(m_Y = 1\).

C Theoretical Analysis: Multitask Case

We consider the general multitask learning case which allows a different loss function for each task: the goal is to minimize the multi-task excess risk

\[
\min_{f: \mathcal{X} \to \mathcal{C}} \mathcal{E}(f), \quad \mathcal{E}(f) = \frac{1}{T} \sum_{t=1}^{T} \int_{\mathcal{X} \times \mathbb{R}} \ell_t(f_t(x), y) d\rho_t(x, y),
\]

where the \(\rho_t\) are unknown probability distributions on \(\mathcal{X} \times \mathbb{R}\) that are observed via finite samples \((x_{it}, y_{it})_{i=1}^{n_t}\), for \(t = 1, \ldots, T\). Each \(\ell_t\) is required to satisfy the SELF assumption in Def. 1, i.e.

\[
\ell_t(y, y') = (\psi_t(y), V_t \psi_t(y')),
\]

and for \(t = 1, \ldots, T\) \(m_{y,t}\) is a constant such that \(\sup_{y \in Y} \|\psi_t(y)\| \leq m_{y,t}\). In this setting the surrogate problem corresponds to

\[
\min_{G: \mathcal{H}_x \to \mathcal{H}_Y^T} \mathcal{R}(G), \quad \mathcal{R}_T(G) := \frac{1}{T} \int_{\mathcal{X} \times \mathcal{Y}} \|\psi_t(y) - G_t \phi(x)\|_{\mathcal{H}_Y}^2 d\rho_t(x, y),
\]

and its solution is denoted with \(G_*\). Note that each \(G_t\) is an operator in \(\mathcal{H}_x \otimes \mathcal{H}_y\) and \(G\) denotes the operator from \(\mathcal{H}_x\) to \(\mathcal{H}_Y^T\) whose \(t\)-th component is \(G_t\), \(t = 1, \ldots, T\). Formally, \(G = \sum_{t=1}^{T} G_t \otimes e_t\), with \((e_t)_{t=1}^{T}\) the canonical basis of \(\mathbb{R}^T\). Since \(\|G\|_{HS}^2 = \sum_t \|G_t\|_{HS}^2\), in case of HS regularization the surrogate problem considers each task \(t\) separately.
Here we perform regularization with trace norm of the operator $G$. Setting $G_\gamma = \{ g(\cdot) = G \phi(\cdot) \mid G : \mathcal{H}_x \to \mathcal{H}_y^T \}$ is s.t. $\|G\|_* \leq \gamma$, we study the estimator $\hat{g}$ given by

$$
\hat{g} = \arg\min_{g \in G_\gamma} \frac{1}{T} \sum_{t=1}^T \frac{1}{n_t} \sum_{i=1}^{n_t} \|g_t(x_{it}) - \psi_t(y_{it})\|^2_{\mathcal{H}_y}.
$$ (35)

In the following we will consider $n_t = n$ for simplicity and denote $\mathcal{R}_T$ with $\mathcal{R}_s$ to avoid cumbersome notation. The estimator $\hat{g}$ satisfies the following excess risk bound:

**Theorem 7.** For $t = 1, \ldots, T$, let $(x_{it}, y_{it})_{i=1}^n$ be an iid sample of $\rho_t$ and $\hat{g}$ is the solution of Eq. (35) with $\gamma = \|G_*\|_*$. The section is devoted to the proof of this result, which is the formal version of theorem Thm. 5 in the main paper. We split the error as follows:

$$
\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq \mathcal{R}(\hat{g}) - \hat{\mathcal{R}}(\hat{g}) + \hat{\mathcal{R}}(\hat{g}) - \hat{\mathcal{R}}(g_*)
+ \hat{\mathcal{R}}(g_*) - \mathcal{R}(g_*) + \mathcal{R}(g_*) - \mathcal{R}(g_*).
$$

Now, by definition of $\hat{g}$ the term $\hat{\mathcal{R}}(\hat{g}) - \hat{\mathcal{R}}(g_*)$ is negative. Also, denoting by $\rho_{t|X}$ the marginal on $X$ of the probability measure $\rho_t$,

$$
\mathcal{R}(g_*) - \mathcal{R}(g_*) = \frac{1}{T} \sum_{t=1}^T \int_X \|G_{t*} \phi(x) - G_{t*} \phi(x)\|^2_{\mathcal{H}_y} d\rho_{t|X}(x)
\leq \frac{1}{T} \sum_{t=1}^T \|G_{t*} \phi(x) - G_{t*} \phi(x)\|^2_{L^2(\rho_{t|X})}
\leq \frac{1}{T} \sum_{t=1}^T \|G_{t*} \phi(x) - G_{t*} \phi(x)\|^2_{L^2(\rho_{t|X})}
\leq \left(1 - \frac{\gamma}{\|G_*\|_*} \right)^2 \frac{1}{T} \sum_{t=1}^T \|G_{t*} \phi\|^2_{L^2(\rho_{t|X})}
\leq \left(1 - \frac{\gamma}{\|G_*\|_*} \right)^2 \frac{m^2}{T} \|G_*\|^2_{\text{HS}} \leq \left(\|G_*\|_* - \gamma\right)^2 \frac{m^2}{T}.
$$
It remains to bound \( R_1 := \mathcal{R}(\hat{g}) - \hat{\mathcal{R}}(\hat{g}) \) and \( R_2 := \hat{\mathcal{R}}(g^*) - \mathcal{R}(g^*) \). Since
\[
R_1 + R_2 \leq 2 \sup_{G \in \hat{G}} |\hat{\mathcal{R}}(G) - \mathcal{R}(G)|,
\]

we just have to bound the term on the right hand side. In the following we assume \( n_t = n \) for \( t = 1, \ldots, T \) for clarity. Also, the notation \( \mathbb{E} u(x_t) \otimes v(y_t) \) is to be interpreted as \( \mathbb{E}_{(x_t) \sim \rho_t} u(x_t) \otimes v(y_t) \). For \( t = 1, \ldots, T \), denote
\[
C_t = \mathbb{E} \phi(x_t) \otimes \phi(x_t), \quad \hat{C}_t = \frac{1}{n} \sum_{i=1}^{n} \phi(x_{it}) \otimes \phi(x_{it})
\]
\[
Z_t = \mathbb{E} \psi(y_t) \otimes \phi(x_t), \quad \hat{Z}_t = \frac{1}{n} \sum_{i=1}^{n} \psi(y_{it}) \otimes \phi(x_{it}).
\]

For any operator \( G \), we have
\[
|\hat{\mathcal{R}}(G) - \mathcal{R}(G)| = \left| \frac{1}{T} \sum_{t=1}^{T} \frac{1}{n} \sum_{i=1}^{n} \| \psi(y_{it}) - G_t \phi(x_{it}) \|_{\mathcal{H}_y}^2 - \mathbb{E} \| \psi(y_t) - G_t \phi(x_t) \|_{\mathcal{H}_y}^2 \right|
\]
\[
= \left| \frac{1}{T} \sum_{t=1}^{T} \frac{1}{n} \sum_{i=1}^{n} \left( \langle G^*_t G_t, \phi(x_{it}) \otimes \phi(x_{it}) \rangle_{\mathcal{H}_S} - 2 \langle G_t, \psi(y_{it}) \otimes \phi(x_{it}) \rangle_{\mathcal{H}_S} + \| \psi(y_{it}) \|_{\mathcal{H}_y}^2 \right) \right|
\]
\[
= \left| \frac{1}{T} \sum_{t=1}^{T} \left( \langle G^*_t G_t, \hat{C}_t - C_t \rangle_{\mathcal{H}_S} - 2 \langle G_t, \hat{Z}_t - Z_t \rangle_{\mathcal{H}_S} + \frac{1}{n} \sum_{i=1}^{n} \| \psi(y_{it}) \|_{\mathcal{H}_y}^2 - \mathbb{E} \| \psi(y_t) \|_{\mathcal{H}_y}^2 \right) \right|
\] (36)

We analyse each term separately in the following lemmas.

**Lemma 8.** The first term in Eq. (39) satisfies the following inequality:
\[
\left| \frac{1}{T} \sum_{t=1}^{T} \langle G^*_t G_t, \hat{C}_t - C_t \rangle_{\mathcal{H}_S} \right| \leq \frac{1}{T} \frac{4 \| G \|_{\mathcal{H}_S}^2}{3^3} \left( \ln \left( \frac{T r_1}{\delta} \right) \right) + \frac{\| G \|_{\mathcal{H}_S}^2}{T} \sqrt{\frac{4m^2}{n} \max_{t} \| C_t \|_{\text{op}} \ln \left( \frac{T r_1}{\delta} \right)}
\]

with probability \( 1 - \delta \), where \( r_1 \) is a constant independent of \( n, T, G \) and which is given by the problem.

**Proof.**
\[
\frac{1}{T} \sum_{t=1}^{T} \langle G^*_t G_t, \hat{C}_t - C_t \rangle_{\mathcal{H}_S} = \frac{1}{T} \| \text{tr}(G^* C) \|_{\text{op}} \leq \frac{1}{T} \| G \| \| C_{\text{op}} \|.
\]
where \( \mathbf{G} = \sum_{t=1}^{T} (e_t \otimes e_t) \otimes (G_t^* G_t) \) and \( \mathbf{C} = \sum_{t=1}^{T} (e_t \otimes e_t) \otimes (\hat{C}_t - C_t) \). Now,

\[
\| \mathbf{G} \|_* = \sum_{t=1}^{T} \| G_t^* G_t \|_* = \sum_{t=1}^{T} \| G_t G_t^* \|_{\text{HS}} = \| \mathbf{G} \|_{\text{HS}}^2
\]

and

\[
\| \mathbf{C} \|_{\text{op}} = \max_{t=1,\ldots,T} \| C_t - \hat{C}_t \|_{\text{op}}.
\]

Using Lemma 11, we get

\[
\| C_t - \hat{C}_t \|_{\text{op}} \leq \frac{4}{n} \left( \frac{m^2}{3} \ln \left( \frac{14\tilde{r}_t}{\delta} \right) \right) + \sqrt{\frac{4m^2\| \mathbf{C}_t \|_{\text{op}} \ln \left( \frac{14\tilde{r}_t}{\delta} \right)}{n}}
\]

with probability greater than 1 - \( \delta \). Performing an intersection bound we have that for \( t = 1, \ldots, T \)

\[
\max_{t=1,\ldots,T} \| C_t - \hat{C}_t \|_{\text{op}} \leq \frac{4}{n} \left( \frac{m^2}{3} \ln \left( \frac{r_1}{\delta} \right) \right) + \sqrt{\frac{4m^2 \max_t \| C_t \|_{\text{op}} \ln \left( \frac{r_1}{\delta} \right)}{n}}
\]

with probability 1 - \( T\delta \), where \( r_1 = 14 \max_t \tilde{r}_t \). With some abuse of notation take \( \delta = \delta/T \) and we get

\[
\max_{t=1,\ldots,T} \| C_t - \hat{C}_t \|_{\text{op}} \leq \frac{4}{n} \left( \frac{m^2}{3} \ln \left( \frac{T r_1}{\delta} \right) \right) + \sqrt{\frac{4m^2 \max_t \| C_t \|_{\text{op}} \ln \left( \frac{T r_1}{\delta} \right)}{n}}
\]

with probability 1 - \( \delta \).

**Lemma 9.** The following bounds holds true:

\[
\frac{1}{T} \sum_{t=1}^{T} \langle G_t, \hat{Z}_t - Z_t \rangle \leq \frac{4\| \mathbf{G} \|_*}{nT} \left( \frac{k_1}{3} \ln \left( \frac{28\tilde{r}}{\delta} \right) \right) + \frac{m_* \| \mathbf{G} \|_*}{T \sqrt{n}} \left( \sqrt{2TR(G_*)} + m_* \| \mathbf{G} \|_{\text{op}} \| \sum_{t} C_t \|_{\text{op}} \right) \ln \left( \frac{r_2}{\delta} \right)
\]

with probability at least 1 - \( \delta \), where \( k_1 = m_* \max_t m_{x,t} \), and \( r_2 \) is independent of \( G_*, \delta, n \) and \( T \).

**Proof.** Let us start with the following bound

\[
\frac{1}{T} \sum_{t=1}^{T} \langle G_t, \hat{Z}_t - Z_t \rangle = \frac{1}{T} \text{tr}(G\mathbf{Z}) \leq \frac{1}{T} \| \mathbf{G} \|_* \| \mathbf{Z} \|_{\text{op}}
\]

where \( \mathbf{Z} = \sum_{t=1}^{T} (\hat{Z}_t - Z_t) \otimes e_t \). To bound \( \| \mathbf{Z} \|_{\text{op}} \) some extra work is needed. We aim to apply Lemma 12 again. Let us define

\[
X_{it} = \frac{1}{n} (\psi(y_{it}) \otimes \phi(x_{it}) - \mathbb{E}\psi(y_t) \otimes \phi(x_t)) \otimes e_t,
\]
so that \( \sum_{i,t} X_{it} = Z. \) Note that
\[
\|X_{it}\|_{\text{op}} \leq \max_{t} \frac{m_{x} m_{y,t}}{n} + \max_{t} \|Z_{t}\|_{\text{op}} \leq \frac{2 \max_{t} m_{x} m_{y,t}}{n} \text{ for any } i, t.
\]

In order to apply Lemma 12 we need to bound the following two quantities
\[
\| \sum_{i,t} E X_{it} X_{it}^{*} \|, \quad \| \sum_{i,t} E X_{it}^{*} X_{it} \|.
\]

Note that
\[
E X_{it} X_{it}^{*} = \frac{1}{n^2} (E(\psi(y_{it})^2 \phi(x_{it}) \otimes \phi(x_{it})) - Z_{t}Z_{t}^{*})
\]
and hence
\[
\| \sum_{i,t} E X_{it} X_{it}^{*} \|_{\text{op}} \leq \frac{2}{n} \| \sum_{t} E(\psi(y_{t})^2 \phi(x_{t}) \otimes \phi(x_{t})) \|_{\text{op}}.
\] (40)

A direct application of Lemma 16 yields
\[
\| \sum_{i,t} E X_{it} X_{it}^{*} \|_{\text{op}} \leq \frac{2 m_{x}^2}{n} (TR(G_{*}) + \| \sum_{t} C_{t} \|_{\text{op}} \| G \|_{\text{HS}}^2).
\]

Also,
\[
X_{it}^{*} X_{it} = \frac{1}{n^2} (k(x_{it}, x_{it}) \psi(y_{it})^2 - \|E(\psi(y_{t}) \otimes \phi(x_{t})) \|^2) e_{t} \otimes e_{t}
\]
and
\[
\sum_{i,t} E X_{it}^{*} X_{it} = \frac{1}{n} \sum_{t} \frac{1}{n} \sum_{i=1}^{n} (E k(x_{it}, x_{it}) \psi(y_{it})^2 - \|E(\psi(y_{t}) \otimes \phi(x_{t})) \|^2) e_{t} \otimes e_{t}
\]
\[
\leq \frac{1}{n} \sum_{t} (m_{x}^2 C_{Y,t} - \|E(\psi(y_{t}) \otimes \phi(x_{t})) \|^2) e_{t} \otimes e_{t}.
\]

Taking the operator norm, we obtain
\[
\| \sum_{i,t} E X_{it}^{*} X_{it} \|_{\text{op}} \leq \frac{2}{n} \max_{t} \left( m_{x}^2 \| C_{Y,t} \|_{\text{op}} \right) \leq \frac{2 m_{x}^2}{n} \| \sum_{t} C_{Y,t} \|_{\text{op}} \leq \frac{2 m_{x}^2}{n} (TR(G_{*}) + \| G_{*} \|_{\text{HS}}^2 \sum_{t} C_{t} \|_{\text{op}}).
\] (41)

where the last inequality follows by Lemma 15.
Both $\| \sum_{it} E X_{it} X_{it}^T \|_{op}$ and $\| \sum_{it} E X_{it} X_{it}^T \|_{op}$ are upper bounded by $\frac{2m^2}{n} (TR(G_*) + \|G_*\|_{HS}^2 \| \sum_t C_t \|_{op})$.

Then, by Lemma 12, we have

$$\|Z\|_{op} \leq \frac{4}{n} \left( \max_t m_t \ln \left( \frac{2\bar{r}}{\delta} \right) \right) + \sqrt{\frac{2m^2}{n} (TR(G_*) + \|G_*\|_{HS}^2 \| \sum_t C_t \|_{op}) \ln \left( \frac{2\bar{r}}{\delta} \right)},$$

where $\bar{r}$ is the effective rank of $Z$. Rearranging we get

$$\|Z\|_{op} \leq \frac{4}{n} \left( \frac{k_1}{3} \ln \left( \frac{28\bar{r}}{\delta} \right) \right) + m_x \sqrt{\frac{2TR(G_*)}{n} \ln \left( \frac{r_2}{\delta} \right)} + \|G_*\|_{op} \sqrt{\| \sum_t C_t \|_{op} \frac{2}{n} \ln \left( \frac{T_2}{\delta} \right)},$$

where $k_1 = m_x \max_t m_{y,t}$ and $r_2 = 28\bar{r}$.

**Lemma 10.** Recall that $\|\psi(y_{it})\|^2 \leq m^2_{y,t}$ for $i = 1, \ldots, n$, $t = 1, \ldots, T$.

$$\left| \frac{1}{T} \sum_{t=1}^T \frac{1}{n} \sum_{i=1}^n \|\psi(y_{it})\|_{H^t}^2 - E \|\psi(y_{it})\|_{H^t}^2 \right| \leq \sqrt{\left( \frac{1}{T} \sum_t m^2_{y,t} \right) \frac{1}{nT} \ln \left( \frac{2}{\delta} \right)}$$

with probability at least $1 - \delta$.

**Proof.** The bound follows by a direct application of Hoeffding inequality. \hfill \Box

We are now ready to prove theorem Thm. 7.

**Proof.** Recall that

$$\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq (\|G_*\|_* - \gamma)^2 \frac{m^2}{T} + 2 \sup_{G \in \mathcal{G}_r} \|\mathcal{R}(\hat{G}) - \mathcal{R}(G)\|.$$  

Recall that for any $G \in \mathcal{G}_r$, $\|G\|_* \leq \gamma$. Now, combining Eq. (39) and Lemma 8, Lemma 9 and 10, we get

$$\mathcal{R}(\hat{g}) - \mathcal{R}(g_*) \leq \left( (\|G_*\|_* - \gamma)^2 \frac{m^2}{T} + \gamma^2 \left( \frac{A}{n} + \frac{B}{\sqrt{n}} \right) + \gamma \left( \frac{A'}{n} + \frac{B'}{\sqrt{n}} \right) + \sqrt{\left( \frac{1}{T} \sum_t m^2_{y,t} \right) \frac{1}{nT} \ln \left( \frac{2}{\delta} \right)} \right),$$

where

$$A = \frac{4}{T} \left( \frac{m^2}{3} \ln \left( \frac{Tr_{\gamma}}{\delta} \right) \right) \quad B = \frac{1}{T} \sqrt{4m^2 \max_t \|C_t\|_{op} \ln \left( \frac{Tr_{\gamma}}{\delta} \right)} + \frac{1}{T} m_x \sqrt{2 \| \sum_t C_t \|_{op} \ln \left( \frac{r_2}{\delta} \right)},$$

$$A' = \frac{4}{T} \left( \frac{\max_t m_{x,t} m_{y,t}}{3} \ln \left( \frac{r_2}{\delta} \right) \right) \quad B' = \frac{1}{T} \sqrt{2TR(G_*) \ln \left( \frac{r_2}{\delta} \right)}.$$

Optimizing with respect to $\gamma$ we could find the optimal parameter and compute the corresponding bound. However, in the following we choose $\gamma = \|G_*\|_*$, so that the approximation...
error is zero. In the following we will bound $\max_t \|C_t\|_{op}$ with $\|\sum_t C_t\|_{op}$ and both the logarithm terms with $\ln(T/\delta)$ for a suitable $r$ (e.g. $\max(r_1, r_2)$). Isolating the faster term we obtain

$$
R(\hat{g}) - R(g^*) \leq \|G^*\|_2^2 m_x \left[ \sqrt{\frac{\|\sum_t C_t\|_{op} \left( 2 + \sqrt{2} \right)}{T \sqrt{n}}} + \frac{m_x \|G^*\|_s}{T} \sqrt{\frac{2T R(G^*)}{n}} \right] \ln \left( \frac{T}{\delta} \right) 
$$

$$
+ \sqrt{\left( \frac{1}{T} \sum_t m^2_{x,t} \right) \frac{1}{nT} \ln \left( \frac{2}{\delta} \right)} + O((nT)^{-1}).
$$

Denote by $\bar{C}$ the average of $C_1, \ldots, C_T$, i.e. $\frac{1}{T} \sum_t C_t$. Then,

$$
\frac{1}{T} T \|\sum_t C_t\|_{op} = \frac{1}{\sqrt{T}} \|\bar{C}\|_{op}.
$$

Rearranging the terms we get the final bound

$$
R(\hat{g}) - R(g^*) \leq \frac{1}{\sqrt{nT}} \left[ \|G^*\|_2^2 \|\bar{C}\|_{op} \frac{1}{\sqrt{nT}} \ln \left( \frac{2}{\delta} \right) + m_x \|G^*\|_s \sqrt{2T R(G^*)} \right] \ln \left( \frac{T}{\delta} \right) + O((nT)^{-1}),
$$

where $m_y = \sqrt{\frac{1}{T} \sum_t m^2_{y,t}}$. □

## D Auxiliary Lemmas

In this section we recall some auxiliary results that are used in the proofs of the work. Let us recall the definition of effective rank. Given an Hilbert space $H$ let $A : H \to H$, be a compact operator. The effective rank of $A$ is refined as

$$
r(A) = \frac{\text{tr} A}{\|A\|_{op}}.
$$

### Lemma 11

Let $X_1, \ldots, X_n \in \mathbb{C}^{d \times d}$ a sequence of independent self adjoint random matrices such that $\mathbb{E} X_i = 0$, for $i = 1, \ldots, n$ and $\sigma^2 \geq \|\sum_{i=1}^n \mathbb{E} X_i^2\|_{op}$. Assume that $\|X_i\| \leq U$ almost surely for all $1 \leq i \leq n$ and some positive $U \in \mathbb{R}$. Then, for any $t \geq \frac{1}{6}(U + \sqrt{U + 36\sigma^2})$,

$$
\mathbb{P}\left( \|\sum_{i=1}^n X_i\|_{op} > t \right) \leq 14 r(\sum_{i=1}^n \mathbb{E} X_i^2) \exp \left( - \frac{t^2/2}{\sigma^2 + tU/3} \right),
$$

where $r(\cdot)$ denotes the effective rank.
A similar results holds true for general matrices with no requirements on self adjointness:

**Lemma 12.** Let $X_1, \ldots, X_n \in \mathbb{C}^{d \times d}$ a sequence of independent random matrices such that $\mathbb{E}X_i = 0$, for $i = 1, \ldots, n$ and $\sigma^2 \geq \max(\|\sum_{i=1}^n \mathbb{E}X_i X_i^*\|_{\text{op}}, \|\sum_{i=1}^n \mathbb{E}X_i^* X_i\|_{\text{op}})$. Assume that $\|X_i\| \leq U$ almost surely for all $1 \leq i \leq n$ and some positive $U \in \mathbb{R}$. Then, for any $t \geq \frac{1}{2}(U + \sqrt{U} + 36\sigma^2)$,

$$
\mathbb{P}\left(\|\sum_{i=1}^n X_i\|_{\text{op}} > t\right) \leq 28\hat{d} \exp\left(-\frac{t^2}{\sigma^2 + tU/3}\right),
$$

(43)

where $\hat{d} = \max(r(\sum_{i=1}^n \mathbb{E}X_i X_i^*), r(\sum_{i=1}^n \mathbb{E}X_i^* X_i))$ and $r(\cdot)$ denotes the effective rank.

The lemma above holds true for Hilbert Schmidt operators between separable Hilbert spaces, as shown in section 3.2 in [Minsker, 2017].

**Lemma 13.** The following bound on the operator norm of the covariance operator on the output $\mathbb{E}\psi(y) \otimes \psi(y)$ holds true:

$$
\|\mathbb{E}\psi(y) \otimes \psi(y)\|_{\text{op}} \leq \|G_*\|_{\text{HS}} \|C\|_{\text{op}} + \mathcal{R}(g_*).
$$

Proof. Let us start for the identity below:

$$
\psi(y) \otimes \psi(y) = (\psi(y) - G_* \phi(x)) \otimes (\psi(y) - G_* \phi(x)) + G_* \phi(x) \otimes (\psi(y) - G_* \phi(x)) + \psi(y) \otimes G_* \phi(x).
$$

(44)

Taking the expectation on the right hand side we obtain

$$
\mathbb{E}((\psi(y) - G_* \phi(x)) \otimes (\psi(y) - G_* \phi(x))) + \mathbb{E}G_* \phi(x) \otimes (\psi(y) - G_* \phi(x)) + \mathbb{E}\psi(y) \otimes G_* \phi(x).
$$

Note that the second term is zero, since

$$
\mathbb{E}G_* \phi(x) \otimes (\psi(y) - G_* \phi(x)) = \int_{\mathcal{X} \times \mathcal{Y}} G_* \phi(x) \otimes (\psi(y) - G_* \phi(x)) d\rho(x, y)
$$

$$
= \int_{\mathcal{X}} G_* \phi(x) \left( \int_{\mathcal{Y}} \psi(y) d\rho(y \mid x) - G_* \phi(x) \right) d\rho_X
$$

and $G_* \phi(x) = \int_{\mathcal{Y}} \phi(y) d\rho(y \mid x)$. As for the last term, we have

$$
\mathbb{E}\psi(y) \otimes G_* \phi(x) = \int_{\mathcal{X}} \int_{\mathcal{Y}} \psi(y) d\rho(y \mid x) \otimes G_* \phi(x) d\rho_X = \int_{\mathcal{X}} G_* \phi(x) \otimes G_* \phi(x).
$$

Taking the operator norm we get

$$
\|\mathbb{E}\psi(y) \otimes \psi(y)\|_{\text{op}} \leq \|\mathbb{E}((\psi(y) - G_* \phi(x)) \otimes (\psi(y) - G_* \phi(x)))\|_{\text{op}} + \|G_* CG_*^*\|_{\text{HS}}
$$

$$
\leq \mathcal{R}(g_*) + \|G_* CG_*^*\|_{\text{HS}}^2 \leq \mathcal{R}(g_*) + \|G\|_{\text{HS}}^2 \|C\|_{\text{op}}.
$$
Lemma 14. The following bound holds true
\[ \|E(\langle \psi(y), \psi(y) \rangle \phi(x) \otimes \phi(x))\|_{op} \leq m_r^2 \|G_*\|_{HS}^2 \|C\|_{op} + \mathcal{R}(g_*). \]

Proof. Let us rewrite \( E(\langle \psi(y), \psi(y) \rangle \phi(x) \otimes \phi(x)) \) as follows
\[
\int_{\mathcal{X} \times \mathcal{Y}} \langle \psi(y), \psi(y) \rangle \phi(x) \otimes \phi(x) d\rho(x, y) = \int_{\mathcal{X}} \phi(x) \otimes \phi(x) \left( \int_{\mathcal{Y}} \langle \psi(y), \psi(y) \rangle d\rho(y | x) \right) d\rho_X(x).
\] (45)
The inner integral corresponds to \( E_{y \mid x} \text{tr}(\psi(y) \otimes \psi(y)) = \text{tr} E_{y \mid x} (\psi(y) \otimes \psi(y)) \). Writing \( \psi(y) \otimes \psi(y) \) as in Eq. (44) and integrating \( \rho(\cdot | x) \), we observe that
\[
\int_{\mathcal{Y}} \psi(y) \otimes \psi(y) d\rho(y | x) = \int_{\mathcal{Y}} (\psi(y) - G_\ast \phi(x)) \otimes (\psi(y) - G_\ast \phi(x)) d\rho(y | x)
+ G_\ast \phi(x) \otimes \left( \int_{\mathcal{Y}} \psi(y) d\rho(y | x) - G_\ast \phi(x) \right)
+ G_\ast \phi(x) \otimes \phi(x) G_\ast.
\]
Since \( \int_{\mathcal{Y}} \psi(y) d\rho(y | x) = G_\ast \phi(x) \), the second term on the right hand side is zero and hence
\[
\text{tr} E_{y \mid x} \psi(y) \otimes \psi(y) = \text{tr} E_{y \mid x} (\psi(y) - G_\ast \phi(x)) \otimes (\psi(y) - G_\ast \phi(x)) + \text{tr} G_\ast \phi(x) \otimes \phi(x) G_\ast.
\]
Substituting it on the right hand side of Eq. (45) and taking the operator norm and using the triangle inequality, we obtain
\[
\| \int_{\mathcal{X}} \phi(x) \otimes \phi(x) \left( \int_{\mathcal{Y}} \| \psi(y) - G_\ast \phi(x) \|_{H_\ast}^2 d\rho(y | x) \right) d\rho_X(x) \|_{op}
\leq m_r^2 \int_{\mathcal{X} \times \mathcal{Y}} \| \psi(y) - G_\ast \phi(x) \|_{H_\ast}^2 d\rho(y, x) = m_r^2 \mathcal{R}(g_*)
\] and
\[
\| \int_{\mathcal{X}} \phi(x) \otimes \phi(x) \text{tr}(G_\ast \phi(x) \otimes \phi(x) G_\ast) \|_{op} \leq \| C \|_{op} m_r^2 G_\ast \|_{HS}^2.
\]
Combining the parts together leads to the desired inequality
\[
\| E(\langle \psi(y), \psi(y) \rangle \phi(x) \otimes \phi(x)) \|_{op} \leq m_r^2 (\| G_\ast \|_{HS}^2 \| C \|_{op} + \mathcal{R}(g_*)).
\]
\[ \square \]

Lemma 15. Let \( C_{Y,t} \) denote the covariance on the output for the \( t \)th task, that is
\[ C_{Y,t} := \mathbb{E} \psi(y_t) \otimes \psi(y_t). \] (46)
Then the following inequality holds true
\[
\| \sum_t C_{Y,t} \|_{op} \leq \| G_\ast \|_{HS}^2 \sum_t \| C_t \|_{op} + TR(G_\ast).
\] (47)
Proof. Let us start from the identity below:
\[ \psi(y_t) \otimes \psi(y_t) = (\psi(y_t) - G_{ts} \phi(x_t)) \otimes (\psi(y_t) - G_{ts} \phi(x_t)) + G_{ts} \phi(x_t) \otimes (\psi(y_t) - G_{ts} \phi(x_t)) + G_{ts} \phi(x_t) \otimes (\psi(y_t) - G_{ts} \phi(x_t)). \]

Taking the expectation on the right hand side we obtain
\[ \mathbb{E}((\psi(y_t) - G_{ts} \phi(x_t)) \otimes (\psi(y_t) - G_{ts} \phi(x_t)) + \mathbb{E}G_{ts} \phi(x_t) \otimes (\psi(y_t) - G_{ts} \phi(x_t)) + \mathbb{E} \psi(y_t) \otimes G_{ts} \phi(x_t)). \]

As in Lemma 13, note that the second term is zero. As for the last term, we have
\[ \mathbb{E} \psi(y_t) \otimes G_{ts} \phi(x_t) = \int_X \int_X \mathbb{E}_t(y_t) d\rho_t(y_t) \otimes G_{ts} \phi(x_t) d\rho_t(x_t) = \int_X (G_{ts} \phi(x_t)) \otimes (G_{ts} \phi(x_t)) d\rho_t(x_t) \]
\[ = \int_X (G_{ts} \phi(x) \otimes (G_{ts} \phi(x)) \rho_t(x) = G_{ts} C_C G_{ts}. \]

Therefore, summing on \( t \) and taking the operator norm we get
\[ \| \sum_t C_{Y.t} \|_{op} \leq \| \sum_t \mathbb{E}((\psi(y_t) - G_{ts} \phi(x_t))^2)\|_{op} + \| G_{ts} C_{C} G_{ts} \|_{HS} \]
\[ \leq \sum_t \mathcal{R}(G_{ts}) + \| \sum_t G_{ts} C_{C} G_{ts} \|_{HS} \leq \sum_t \mathcal{R}(C_{ts}) + \| \sum_t G_{ts} \|_{op} \]
\[ \leq \sum_t \mathcal{R}(G_{ts}) + \sum_t \| G_{ts} \|_{op}^2 \sum_t C_{ts} C_{ts}^* \|_{HS} \leq \mathcal{R}(C_{ts}) + \| G_{ts} \|_{op} \sum_t C_{ts} C_{ts}^* \|_{HS}. \]

\[ \| \sum_t \mathbb{E}((\psi(y_t))^2 \phi(x_t) \otimes \phi(x_t)) \|_{op} \leq \mathbb{E}((\psi(y_t))^2 \|_{op}^2 + \mathcal{R}(g_\psi)). \]

Lemma 16. The following bound holds true
\[ \| \sum_t \mathbb{E}((\psi(y_t))^2 \phi(x_t) \otimes \phi(x_t)) \|_{op} \leq \mathbb{E}((\psi(y_t))^2 \|_{op}^2 + \mathcal{R}(g_\psi)). \]

Proof. It is a immediate variation of the proof of Lemma 14. \( \square \)

E. Equivalence between Tikhonov and Ivanov Problems for trace norm Regularization

In this section we provide more details regarding the relation between the Tikhonov regularization problem considered in Eq. (11) and the corresponding Ivanov problem in Eq. (13). As discussed in the paper this approach guarantees that theoretical results characterizing the excess risk of the Ivanov estimator extend automatically to the Tikhonov one.

Let \( (x_i, y_i)_{i=1}^n \) be a training set and consider \( \Phi : \mathcal{H}_x \rightarrow \mathbb{R}^n \) and \( \Psi : \mathcal{H}_y \rightarrow \mathbb{R}^n \) the operators
\[ \Phi = \sum_{i=1}^n e_i \otimes \phi(x_i) \quad \text{and} \quad \Psi = \sum_{i=1}^n e_i \otimes \psi(y_i) \]

with \( e_i \in \mathbb{R}^n \) the \( i \)-th element of the canonical basis in \( \mathbb{R}^n \). We can write the empirical surrogate risk in compact operatorial notation as

\[
\hat{R}(G) = \frac{1}{n} \sum_{i=1}^{n} \|G\phi(x_i) - \psi(y_i)\|_{\mathcal{H}_Y}^2 = \frac{1}{n} \|\Phi G^* - \Psi\|_{\mathcal{H}_Y \otimes \mathbb{R}^n}^2.
\]

**Proposition 17** (Representer Theorem for Trace Norm Regularization). Let \( \hat{G} \in \mathcal{H}_x \otimes \mathcal{H}_y \) be a minimizer of

\[
\min_{G \in \mathcal{H}_x \otimes \mathcal{H}_y} \hat{R}(G) + \lambda \|G\|_*.
\]

Then the range of \( \hat{G}^* \) is contained in the range of \( \Phi^* \), or equivalently

\[
\hat{G}(\Phi^\dagger \Phi) = \hat{G},
\]

where \( \Phi^\dagger \) denotes the pseudoinverse of \( \Phi \).

The proof of this result is essentially equivalent to the one in [Thm. 3 Abernethy et al., 2009]. We report it here for completeness.

**Proof.** For any \( G \in \mathcal{H}_x \otimes \mathcal{H}_y \), consider the factorization

\[
G = G_0 + G_\perp \quad \text{with} \quad G_0 = G(\Phi^\dagger \Phi) \quad \text{and} \quad G_\perp (I - (\Phi^\dagger \Phi)).
\]

Note that \( (\Phi^\dagger \Phi) \in \mathcal{H}_x \otimes \mathcal{H}_x \) corresponds to the orthogonal projector of \( \mathcal{H}_x \) onto the range of \( \Phi^* \) in \( \mathcal{H}_x \) (equivalently onto the span of \( \{\phi(x_i)\}_{i=1}^{n} \)). By construction, we have that \( \Phi G^* = \Phi G_0^* \). Hence \( \hat{R}(G) = \hat{R}(G_0) \). However, since \( (\Phi^\dagger \Phi) \) is an orthogonal projector, we have that

\[
\|G_0\|_* = \|G(\Phi^\dagger \Phi)\|_* \leq \|G\|_*,
\]

with equality holding if and only if \( G_0 = G \).

Now, if \( \hat{G} \) is a minimizer of the trace norm regularized ERM we have

\[
\hat{R}(\hat{G}_0) + \lambda \|\hat{G}_0\|_* \geq \hat{R}(\hat{G}) + \lambda \|\hat{G}\|_* = \hat{R}(\hat{G}_0) + \lambda \|\hat{G}\|_*,
\]

which implies \( \|\hat{G}_0\|_* \geq \|\hat{G}\|_* \).

We conclude that \( \hat{G} = \hat{G}_0 = \hat{G}(\Phi^\dagger \Phi) \). This corresponds to the range of \( G^* \) being contained in the range of \( \Phi \) as desired. \( \square \)

**Proposition 18.** The empirical risk minimization for \( \hat{R}(G) + \lambda \|G\|_* \) admits a unique minimizer.
Proof. According to Prop. 17, all minimizers of the trace norm regularized empirical risk minimization belong to the set

$$S = \{ G \in \mathcal{H}_y \otimes \mathcal{H}_x \mid G(\Phi^\dagger \Phi) = G \}.$$

Hence we can restrict to the optimization problem

$$\min_{G \in S} \hat{R}(G) + \lambda \|G\|_*.$$

Note that $S$ is identified by a linear relation and thus is a convex set and thus the problem above is a convex program. We now show that on $S$ the ERM objective functional is actually strongly convex for the case of the least-squares loss. To see this, let us consider the Hessian of $\hat{R}(\cdot)$. We have that, the gradient corresponds to

$$\nabla \hat{R}(G) = 2 \frac{n}{n} (G \Phi^* \Phi - \Psi^* \Phi),$$

and therefore the Hessian is the operator $\nabla^2 \hat{R}(G) : \mathcal{H}_y \otimes \mathcal{H}_x \to \mathcal{H}_y \otimes \mathcal{H}_x$ such that

$$\nabla^2 \hat{R}(G) H = 2 \frac{n}{n} H \Phi^* \Phi,$$

for any $H \in \mathcal{H}_y \otimes \mathcal{H}_x$ [see e.g. Kollo and von Rosen, 2006]. Now, we have that for any $H \in S$

$$\langle H, \nabla^2 \hat{R}(G) H \rangle_{\mathcal{H}_y \otimes \mathcal{H}_x} = 2 \frac{n}{n} \langle H, H \Phi^* \Phi \rangle_{\mathcal{H}_y \otimes \mathcal{H}_x} = 2 \frac{n}{n} \text{tr}(H^* H \Phi^* \Phi).$$

Now, let $r \leq n$ be the rank of $\Phi$ and consider the singular value decomposition of $\Phi = U \Sigma V^*$, with $U \in \mathbb{R}^{n \times r}$ a matrix with orthonormal columns $V \in \mathcal{H}_x \to \mathbb{R}^r$ a linear operator such that $V^* V = I \in \mathbb{R}^{r \times r}$ and $\Sigma \in \mathbb{R}^{r \times r}$ a diagonal matrix with all positive diagonal elements. Then,

$$\text{tr}(H^* H \Phi^* \Phi) = \text{tr}(H^* H V \Sigma^2 V^*) = \text{tr}(V^* H^* H V \Sigma^2) \geq \sigma_{min}^2 \|HV\|^2_{\mathcal{H}_y \otimes \mathbb{R}^r},$$

where $\sigma_{min}^2$ denotes the smallest singular value of $\Sigma$ (equivalently, $\sigma_{min}$ is the smallest singular value of $\Phi$ greater than zero).

Now, recall that $H \in S$. Therefore

$$H = H(\Phi^\dagger \Phi) = HVV^*,$$

which implies that

$$\|H\|^2_{\mathcal{H}_y \otimes \mathcal{H}_x} = \text{tr}(H^* H) = \text{tr}(VV^* H^* H VV^*) = \text{tr}(V^* H^* H V) = \|HV\|^2_{\mathcal{H}_y \otimes \mathbb{R}^r},$$

where we have used the orthonormality $V^* V = I \in \mathbb{R}^{r \times r}$.

We conclude that

$$\langle H, \nabla^2 \hat{R}(G) H \rangle_{\mathcal{H}_y \otimes \mathcal{H}_x} \geq \frac{2 \sigma_{min}^2}{n} \|H\|^2_{\mathcal{H}_y \otimes \mathcal{H}_x},$$

for any $H \in S$. Note that $\sigma_{min} > 0$ is greater than zero since it is the smallest singular value of $\Phi$ greater than zero and $\Phi$ has finite rank $r \leq n$. Hence, on $S$, the function $\hat{R}(G)$ is strongly convex. As a consequence also the objective functional $\hat{R}(G) + \lambda \|G\|_*$ is strongly convex and thus admits a unique minimizer, as desired. \qed
We conclude this section by reporting the result stating the equivalence between Ivanov and Tikhonov for trace norm regularization.

In the following we will denote by $G_\lambda$ the minimizer of the Tikhonov regularization problem corresponding to minimizing $\hat{R}(G) + \lambda \|G\|_*$ and by $G_\gamma^I$ the minimizer of the Ivanov regularization problem introduced in Eq. (13), namely

$$\min_{\|G\|_* \leq \gamma} \hat{R}(G).$$

We have the following.

**Theorem 19.** For any $\gamma > 0$ there exists $\lambda(\gamma)$ such that $G_{\lambda(\gamma)}$ is a minimizer of Eq. (13). Moreover, for any $\lambda > 0$ there exists a $\gamma = \gamma(\lambda) > 0$ such that $G_\lambda$ is a minimizer of Eq. (13).

**Proof.** We first consider the case where, given a $\gamma > 0$ we want to relate a solution of the Ivanov regularization problem to that of Tikhonov regularization. We will show that there exists $G_\gamma^I$ and $\lambda(\gamma)$ such that $G_\lambda = G_\gamma^I$. In particular we will show that such equality holds for $G_\gamma^I$ the solution of minimal trace norm in the set of solutions of the Ivanov problem.

Consider again the linear subspace

$$S = \left\{ G \in \mathcal{H}_y \otimes \mathcal{H}_x \mid \|G\|_* = \gamma \right\}.$$

We can restrict the original Ivanov problem to

$$\min_{G \in S} \hat{R}(G).$$

Note that the above is still a convex program and attains the same minimum value of the original Ivanov problem in $G_\gamma^I$.

Moreover, we can assume $\gamma = \|G_\gamma^I\|_*$ without loss of generality. Indeed, if $\gamma > \|G_\gamma^I\|_*$ we still have that $G_\gamma^I$ is a minimizer of $\hat{R}(G)$ over the smaller set of operators $\|G\|_* \leq \gamma' = \|G_\gamma^I\|_*$.

Now, consider the Lagrangian associated to this constrained problem problem, namely

$$L(G, \lambda, \nu) = \hat{R}(G) + \lambda(\|G\|_* - \gamma) + \nu (G - G(\Phi^\dagger \Phi)).$$

By Slater’s constraint qualification [see e.g. Sec. 5 in Boyd and Vandenberghe, 2004], we have that

$$\max_{\lambda \geq 0, \nu} \min_{G \in \mathcal{H}_y \otimes \mathcal{H}_x} L(G, \lambda, \nu) = \min_{G \in S} \hat{R}(G).$$

Denote by $(\lambda(\gamma), G_{\lambda(\gamma)}, \nu_\gamma)$ the pair form which the saddle point of $L(G, \lambda, \gamma)$ is attained. Note that since $\gamma$ is a constant

$$G_{\lambda(\gamma)} = \arg\min_{G \in \mathcal{H}_y \otimes \mathcal{H}_x} \hat{R}(G) + \lambda(\|G\|_* - \gamma) + \nu_\gamma (G - G(\Phi^\dagger \Phi)) = \arg\min_{G \in \mathcal{H}_y \otimes \mathcal{H}_x} \hat{R}(G) + \lambda(\gamma) \|G\|_*.$$
where we have made use of the representer theorem from Prop. 17, which guarantees any minimizer of \( \hat{R}(G) + \lambda(\gamma)\|G\|_* \) to belong to the set \( S \) and this satisfy \( G = G(\Phi^\dagger\Phi) \). Therefore, we have

\[
\hat{R}(G_{\lambda(\gamma)}) + \lambda(\gamma)\|G_{\lambda,\gamma}\|_* - \lambda(\gamma)\gamma = \hat{R}(G_{\gamma}^I),
\]

recalling that \( \gamma = \|G_{\gamma}^I\|_* \), this implies that

\[
\hat{R}(G_{\lambda,\gamma}) + \lambda(\gamma)\|G_{\lambda,\gamma}\|_* = \hat{R}(G_{\gamma}^I) + \lambda(\gamma)\|G_{\gamma}^I\|_*.
\]

Since by Prop. 18 the minimizer of \( \hat{R}(G) + \lambda\|G\|_* \) is unique, it follows that \( G_{\lambda,\gamma} = G_{\gamma}^I \) as desired.

The vice-versa is straightforward: let \( \lambda > 0 \) and \( G_\lambda \) be the minimizer of the Tikhonov problem. Then, for any \( G \in \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_X \)

\[
\hat{R}(G_\lambda) + \lambda\|G_\lambda\|_* \leq \hat{R}(G) + \lambda\|G\|_*.
\]

If \( \|G\|_* \leq \|G_\lambda\|_* \), the inequality above implies

\[
\hat{R}(G_\lambda) \leq \hat{R}(G),
\]

which implies that \( G_\lambda \) is a minimizer for the Ivanov problem with \( \gamma(\lambda) = \|G_\lambda\|_* \), namely \( G_\lambda = G_{\gamma(\lambda)}^I \) as desired.