On the Dualization of Operator-Valued Kernel Machines

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Abstract

Operator-Valued Kernels (OVKs) and Vector-Valued Reproducing Kernel Hilbert Spaces (vv-RKHSs) provide an elegant way to extend scalar kernel methods when the output space is a Hilbert space. First used in multi-task regression, this theoretical framework opens the door to various applications, ranging from structured output prediction to functional regression, thanks to its ability to deal with infinite dimensional output spaces. This work investigates how to use the duality principle to handle different families of loss functions, yet unexplored within vv-RKHSs. The difficulty of having infinite dimensional dual variables is overcome, either by means of a Double Representer Theorem when the loss depends on inner products solely, or by an in-depth analysis of the Fenchel-Legendre transform of integral losses. Experiments on structured prediction, function-to-function regression and structured representation learning with ε-insensitive and Huber losses illustrate the benefits of this framework.

1 Introduction

With the increasing availability of streaming and network data, learning from complex structured objects such as graphs and time series has attracted a great deal of attention in Machine Learning. For years, the development of approaches devoted to non-vectorial input data has been linked to the design of suited kernels (Gärtner, 2008), and the exploitation of the Reproducing Kernel Hilbert Space tools (Aronszajn, 1950; Hofmann et al., 2008). However, when dealing with complex output data, the original scalar-valued models such as Support Vector Machines (SVMs, Cortes and Vapnik (1995); Drucker et al. (1997)) are no more appropriate. While Structural SVM and variants cope with discrete structures (Joachims et al., 2009), Operator-Valued Kernels (OVKs) and Vector-Valued Reproducing Kernel Hilbert Spaces (vv-RKHSs, Micchelli and Pontil (2005); Carmeli et al. (2006, 2010)) provide a unique framework to handle both functional and structured outputs. Vv-RKHSs are classes of functions mapping an arbitrary input set $\mathcal{X}$ to some output Hilbert space $\mathcal{Y}$ (Senkene and Tempel’man, 1973; Caponnetto et al., 2008). First used in the finite dimensional case ($\mathcal{Y} = \mathbb{R}^p$) to solve multi-task regression (Micchelli and Pontil, 2005) and multiple class classification (Dinuzzo et al., 2011), OVK methods have then been exploited to handle outputs in an infinite dimensional Hilbert spaces. This ability has unlocked numerous applications, such as functional regression (Kadri et al., 2016), infinite quantile regression (Brault et al., 2019), structured prediction (Brouard et al., 2011; Kadri et al., 2013), or structured data representation learning (Laforgue et al., 2019).

However, these sophisticated schemes often come at the price of a simplistic loss function: the squared norm associated to the output space. In this work, we show that a careful use of the duality principle considerably broadens the range of loss functions for which OVK solutions are computable. Despite an extensive use within scalar kernel methods, very few attempts have been made to adapt duality to vv-RKHSs. In Brouard et al. (2016b), dualization is presented, but only used in the maximum margin regression scenario. In Sangnier et al. (2017), a wider class of loss functions is considered, the ε-insensitive losses, but only in the case of matrix-valued kernels (Álvarez et al., 2012), for which the dual problem is finite dimensional. For a general OVK, nonetheless, the dual problem is to be solved over $\mathcal{Y}^n$, which is intractable without additional work when $\mathcal{Y}$ is infinite dimensional. The present work aims at developing a comprehensive methodology to solve these dual problems in general Hilbert spaces for a wide range of losses. In particular, we define general conditions under which a Double Representer Theorem can be used, and analyze the family of integral losses.

The rest of the article is organized as follows. In Section 2, we introduce OVKs, and derive the gen-
eral formulation of dual problems for OVK machines. Section 3 is devoted to a specific, yet very common, case where the solution in the general output Hilbert space can be computed easily, with algorithms duly explicit for the $\varepsilon$-insensitive and Huber losses, while in Section 4 we analyze at length the case of integral losses. Numerical experiments are presented in Section 5, and technicalities postponed to the Appendix.

2 Learning in vv-RKHSs

In this section, we recall the notion of Operator-Valued Kernel (OVK), as well as some elements of the vv-RKHS learning theory. An OVK is defined as follows.

**Definition 1.** An OVK is an application $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathcal{L}(\mathcal{Y})$, that satisfies the following two properties:

1) $\forall (x, x') \in \mathcal{X} \times \mathcal{X}, \quad \mathcal{K}(x, x') = \mathcal{K}(x', x)^\#$,

with $A^\#$ the adjoint of any operator $A$, and $\mathcal{L}(E)$ the set of bounded linear operators of any vector space $E$. And $\forall n \in \mathbb{N}^*, \forall \{ (x_i, y_i) \}_{i=1}^n \in (\mathcal{X} \times \mathcal{Y})^n$,

2) $\sum_{i,j=1}^n \langle y_i, \mathcal{K}(x_i, x_j) y_j \rangle_{\mathcal{Y}} \geq 0$.

A simple example of OVK is the separable kernel.

**Definition 2.** $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathcal{L}(\mathcal{Y})$ is a separable kernel if there exist a scalar kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and a positive semi-definite operator $A$ on $\mathcal{Y}$ such that:

$\forall (x, x') \in \mathcal{X}^2, \quad \mathcal{K}(x, x') = k(x, x')A$.

Just as for standard scalar-valued kernels, an OVK can be uniquely associated to a functional space (its vv-RKHS), as detailed by the next definition.

**Definition 3.** Let $\mathcal{K}$ be an OVK, and for $x \in \mathcal{X}$, let $\mathcal{K}_x : y \mapsto \mathcal{K}_x y \in \mathcal{F}(\mathcal{X}, \mathcal{Y})$ the linear operator such that:

$\forall x' \in \mathcal{X}, \quad (\mathcal{K}_x y)(x') = \mathcal{K}(x, x')y$.

Then, there is a unique Hilbert space $\mathcal{H}_\mathcal{K} \subset \mathcal{F}(\mathcal{X}, \mathcal{Y})$ called the vv-RKHS associated to $\mathcal{K}$ such that $\forall x \in \mathcal{X}$:

- $\mathcal{K}_x$ spans the space $\mathcal{H}_\mathcal{K} (\forall y \in \mathcal{Y}, \forall x y \in \mathcal{H}_\mathcal{K})$
- $\mathcal{K}_x$ is bounded for the uniform norm
- $\forall f \in \mathcal{H}_\mathcal{K}, \quad f(x) = \mathcal{K}_x^\# f$ (reproducing property)

**Remark 1.** Let $k : \Theta \times \Theta \to \mathbb{R}$ be a (scalar) kernel, and $\mathcal{H}_k$ its associated RKHS. Then, choosing $\mathcal{Y} = \mathcal{H}_k$, the vv-RKHS associated to the identity decomposable OVK $\mathcal{K} = k_{\mathcal{X}} 1_{\mathcal{H}_\mathcal{K}}$ is isometric to the tensor product $\mathcal{H}_{\mathcal{X}} \otimes \mathcal{H}_k$, so that functions in $\mathcal{H}_\mathcal{K}$ may be seen as functions of two variables $(x, \theta)$ in the (scalar) RKHS associated to the kernel $k_{\mathcal{X}} \cdot k$ (Carmeli et al., 2010).

Given $\mathcal{S}_n = \{(x_i, y_i)\}_{i=1}^n \in (\mathcal{X} \times \mathcal{Y})^n$ a sample of $n$ i.i.d. realizations of a generic random variable $(X, Y)$, $\mathcal{K} : \mathcal{X} \times \mathcal{X} \to \mathcal{L}(\mathcal{Y})$ an OVK, $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ a loss function, and $\Lambda > 0$ a regularizer, the general form of an OVK learning problem is to find $\hat{h}$ that solves:

$$\min_{\hat{h} \in \mathcal{H}_\mathcal{K}} \frac{1}{n} \sum_{i=1}^n \ell(h(x_i), y_i) + \frac{\Lambda}{2} \|\hat{h}\|_{\mathcal{H}_\mathcal{K}}^2.$$  \hspace{1cm} (1)

A crucial tool in kernel methods is the Representer Theorem (e.g. Micchelli and Pontil (2005)), ensuring that $\hat{h}$ actually pertains to a reduced subspace of $\mathcal{H}_\mathcal{K}$.

**Theorem 1.** $\exists (\hat{\alpha}_i)_{i=1}^n \in \mathcal{Y}^n, \quad \hat{h} = \frac{1}{\Lambda n} \sum_{i=1}^n \mathcal{K}(:, x_i) \hat{\alpha}_i$.

Although Theorem 1 drastically downscales the search domain (from $\mathcal{H}_\mathcal{K}$ to $\mathcal{Y}^n$), it gives no information about the $(\hat{\alpha}_i)_{i=1}^n$. One way to gain insight about these coefficients is to perform Problem (1)’s dualization, with the notation $\ell_i : y \in \mathcal{Y} \mapsto \ell(y, y_i)$ for any $i \leq n$.

**Theorem 2.** The solution to Problem (1) is given by

$$\hat{h} = \frac{1}{\Lambda n} \sum_{i=1}^n \mathcal{K}(:, x_i) \hat{\alpha}_i,$$

with $(\hat{\alpha}_i)_{i=1}^n \in \mathcal{Y}^n$ the solutions to the dual problem

$$\min_{(\alpha_i)_{i=1}^n \in \mathcal{Y}^n} \sum_{i=1}^n \ell_i^* (-\alpha_i) + \frac{1}{2\Lambda n} \sum_{i,j=1}^n (\alpha_i, \mathcal{K}(x_i, x_j)\alpha_j)_{\mathcal{Y}},$$  \hspace{1cm} (2)

where $f^* : \alpha \in \mathcal{Y} \mapsto \sup_{y \in \mathcal{Y}} \langle \alpha, y \rangle_{\mathcal{Y}} - f(y)$ denotes the Ponchel-Legendre transform of a function $f : \mathcal{Y} \to \mathbb{R}$.

Refer to Appendix A.1 for Theorem 2’s proof, that can also be found in Brouard et al. (2016b). Compared to Theorem 1, dualization thus brings more information about the optimal coefficients (notice nonetheless that the Representer Theorem holds true for a much wider class of problems). As such, Problem (2) is however of little interest, as the optimization must be performed on the infinite dimensional space $\mathcal{Y}^n$, which is merely impossible. Depending on the loss, we propose two solutions: either using a Double Representer Theorem, or specific tools tailored to handle integral losses.

**Notation.** If $\mathcal{K}$ is identity decomposable, $K^X$ and $K^Y$ denote the input and output gram matrices. For any matrix $M$, $M_i$ represents its $i$th line, and $\|M\|_{p,q}$ its $p,q$ row wise mixed norm, i.e. the $\ell_p$ norm of its $\ell_q$ norms of its lines. Finally, $\chi_S$ is the characteristic function a set $S$, null on $S$ and equal to $+\infty$ otherwise, and $f \Box g$ the infimal convolution of $f$ and $g$ (Bauschke et al., 2011), i.e. $(f \Box g)(x) = \inf_y f(y) + g(x-y)$.

3 The Double Representer Theorem

In order to make Problem (2) solvable, we need some (mild) assumptions on the kernel and the loss function.
Here and throughout, $Y$ denotes span$(y_i, i \leq n)$.

**Assumption 1.** There exist $T \in \mathbb{N}^+$, and for all $t \leq T$ admissible scalar kernels $k_t : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and positive semi-definite operators $A_t \in \mathcal{L}(Y)$, for all $(x, x') \in \mathcal{X}^2$

$$K(x, x') = \sum_{t=1}^T k_t(x, x')A_t.$$ 

Under Assumption 1, $K_t^X$ and $K_t^Y$ denote the matrices such that $[K_t^X]_{ij} = k_t(x_i, x_j)$, $[K_t^Y]_{ij} = \langle y_i, A_t y_j \rangle_Y$. Notice that this assumption is by no means restrictive, since every shift-invariant OVK can be approximated arbitrarily closely by kernels satisfying Assumption 1.

**Assumption 2.** $\forall i, j \leq n$, $Y$ is invariant by $K(x_i, x_j)$.

Notice that if for all $t \leq T$, $A_t$ keeps $Y$ invariant, then Assumption 1 directly implies Assumption 2. The next two assumptions define admissible losses through conditions on their Fenchel-Legendre (FL) transforms.

**Assumption 3.** $\forall i \leq n$, $\forall (\alpha^Y, \alpha^\perp) \in Y \times Y^\perp$, 

$$\ell_i^*(\alpha^Y) \leq \ell_i^*(\alpha^Y + \alpha^\perp).$$ 

**Assumption 4.** $\forall i \leq n, \exists L_i : \mathbb{R}^{n} \to \mathbb{R}$ such that $\forall \omega = (\omega_j)_{j \leq n} \in \mathbb{R}^n,$

$$\ell_i^*\left(-\sum_{j=1}^n \omega_j y_j\right) = L_i(\omega, K^Y).$$

With these assumptions, Theorem 3 proves that the solutions lie in $Y^n$, ensuring their computability.

**Theorem 3.** Let $K$ be an OVK meeting Assumptions 1 and 2, and $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ be a loss function with Fenchel-Legendre transforms satisfying Assumptions 3 and 4. Then, the solution to Problem (1) is given by

$$\hat{h} = \frac{1}{\lambda} \sum_{i,j=1}^n \hat{\Omega}^{-1} \hat{K}(x_i, x_i) \hat{y}_j y_j,$$

with $\hat{\Omega} = [\hat{\omega}_{ij}] \in \mathbb{R}^{n \times n}$ the solution to the computable convex optimization problem

$$\min_{\Omega \in \mathbb{R}^{n \times n}} \sum_{i=1}^n L_i(\Omega, y_i) + \frac{1}{2\lambda n} \sum_{t=1}^T \text{Tr} \left( K_t^X \hat{\Omega} K_t^Y \hat{\Omega}^\top \right).$$

(4)

The reader may refer to Appendix A.2 for the proof. This theorem can be seen as a Double Representer Theorem, as both theorems share analogous proofs and consequences: a search domain reduction, respectively from $H_K$ to $\mathcal{Y}^n$, and $\mathcal{Y}$ to $\mathbb{R}^{n \times n}$. Before studying particular instances of Problem (4), Proposition 1 presents a non-exhaustive list of admissible losses.

**Proposition 1.** The following losses have Fenchel-Legendre transforms verifying Assumptions 3 and 4:

- $\ell_i(y) = f(\langle y, z_i \rangle), z_i \in Y$ and $f : \mathbb{R} \to \mathbb{R}$ convex. This encompasses maximum-margin regression, obtained with $z_i = y_i$ and $f(t) = \max(0, 1 - t)$.
- $\ell(y) = f(||y||), f : \mathbb{R}_+ \to \mathbb{R}$ convex increasing s.t. $t \to \frac{f(t)}{t}$ is continuous over $\mathbb{R}_+$. This includes all power functions $\frac{\lambda}{\eta}||y||^\eta$ for $\eta > 1$ and $\lambda > 0$.
- $\ell_i(y) = f(y - y_i), f^* \text{ verifying Assumptions 3-4.}$
- Any infimal convolution (Bauschke et al., 2011) of functions satisfying Assumptions 3 and 4. This encompasses $\epsilon$-insensitive losses (Sangnier et al., 2017), the Huber loss (Huber, 1964), and more generally all Moreau envelopes (Moreau, 1962).

Proposition 1’s proof is deferred to Appendix A.3. However, one can notice as of now that most losses that depend exclusively on norms and dot products satisfy Assumptions 3 and 4. For losses that leverage the functional nature of elements of $\mathcal{Y}$, specific tools must be used, that are detailed in Section 4. For now, we focus on particular instances of Problem (4) when $\ell$ is the $\epsilon$-insensitive square norm, or the Huber loss. To our knowledge, and despite their relatively natural resolution in our dualization framework, it is the first time these problems are addressed in the context of infinite dimensional output Hilbert spaces.

### 3.1 The $\epsilon$-Insensitive Ridge Regression

As a first go, we recall the important notion of $\epsilon$-insensitive losses. Following in the footsteps of Sangnier et al. (2017), we extend them in a natural way from $\mathbb{R}^p$ to any Hilbert space $\mathcal{Y}$. In order to avoid overwhelming notation, $\ell$ denotes here the loss taken with respect to one argument only (i.e. previously $\ell_i$).

**Definition 4.** Let $\ell : \mathcal{Y} \to \mathbb{R}$ be a convex loss, and $\epsilon > 0$. The $\epsilon$-insensitive version of $\ell$, denoted $\ell_\epsilon$, is defined by $\ell_\epsilon(y) = (\ell \square \chi_\epsilon)(y)$, or again:

$$\forall y \in \mathcal{Y}, \ell_\epsilon(y) = \begin{cases} 0 & \text{if } ||y||_\mathcal{Y} \leq \epsilon \\ \inf_{||d||_\mathcal{Y} \leq 1} \ell(y - \epsilon d) & \text{otherwise} \end{cases}$$

In other terms, $\ell_\epsilon(y)$ is the smallest value $\ell(z)$ attained by a point $z$ within the $\epsilon$-ball centered at $y$. Figure 5 gives an illustration of $\epsilon$-insensitive losses in one and two dimensions. Interestingly, and as detailed by Theorem 4, Problem 4 is the $\epsilon$-Insensitive Square norm and an identity decomposable kernel admits a very nice writing, allowing for an efficient resolution.
The Huber loss of parameter $\kappa$ is given by $\ell_{H,\kappa}(y) = (\kappa \cdot \| y \|_{1/2} - \frac{3}{2})$, or again:

$$\forall y \in \mathcal{Y}, \quad \ell_{H,\kappa}(y) = \begin{cases} \frac{3}{2} \| y \|_{Y} & \text{if } \| y \|_{Y} \leq \kappa \\ \kappa (\| y \|_{Y} - \frac{3}{2}) & \text{otherwise} \end{cases}$$

Definition 5. The Huber loss of parameter $\kappa$ is given by $\ell_{H,\kappa}(y) = (\kappa \cdot \| y \|_{1/2} - \frac{3}{2})$, or again:

$$\forall y \in \mathcal{Y}, \quad \ell_{H,\kappa}(y) = \begin{cases} \frac{3}{2} \| y \|_{Y} & \text{if } \| y \|_{Y} \leq \kappa \\ \kappa (\| y \|_{Y} - \frac{3}{2}) & \text{otherwise} \end{cases}$$

Due to its asymptotic behavior as $\| \cdot \|_{Y}$, the Huber loss is particularly useful when the training data is heavy tailed or contains outliers. Examples of the Huber loss in one and two dimensions are depicted in Figure 6. The following theorem explicits the dual problem for the Huber loss and identity decomposable kernels.

**Theorem 5.** For an OVK $K = k 1_{\mathcal{Y}}$, the solution to the Huber loss regression problem

$$\min_{h \in \mathcal{H}_K} \frac{1}{n} \sum_{i=1}^{n} \ell_{H,\kappa}(h(x_i) - y_i) + \frac{\Lambda}{2} \| h \|^2_{\mathcal{H}_K},$$

is given by (3), with $\hat{\Omega} = \hat{W} V^{-1}$, and $\hat{W}$ the solution to the constrained least squares problem

$$\min_{W \in \mathbb{R}^{n \times n}} \frac{1}{2} \| AW - B \|^2_{\text{Fro}},$$

s.t. $\| W \|_{2,1} \leq \kappa,$

with $V, A, B$ as in Theorem 4.

Theorem 5’s proof can be found in Appendix A.5. Again, the complex dual problem in $\mathbb{Y}^n$ boils down to a well known tractable one in $\mathbb{R}^{n \times n}$. Problem (8) can be solved by Projected Gradient Descent (PGD) for instance. See Algorithm 2, with $\gamma$ a predefined stepsize, and Proj the Projection operator such that $\text{Proj}(x, \tau) = \left(1 - \frac{\tau}{\| x \|_1} \right) x$. Analogously to Theorem 4, Problem (8) for a kernel fulfilling Assumption 1 is more complex to write, but not to solve. Refer to Appendix B.3 for a thorough analysis.

### 3.3 Applications

As evoked in the Introduction section, the ability to predict in infinite dimensional Hilbert spaces unlocks many applications, such as structured prediction and structured representation learning. In this section, we give a formal description of these tasks, and highlight the benefit of using the losses we have defined earlier.

**Structured Prediction.** Assume one is interested in learning a predictive decision rule $f$ from a set $\mathcal{X}$ to a complex structured space $\mathcal{Z}$. To bypass the absence of norm on $\mathcal{Z}$, one may design a (scalar) kernel $k$ on $\mathcal{Z}$, whose canonical feature map $\phi : z \mapsto k(\cdot, z)$ transforms any element of $\mathcal{Z}$ into an element of the (scalar) RKHS associated to $k$, denoted $\mathcal{Y} (= \mathcal{H}_K)$. One may then use the vv-RKHS theory to learn a predictive function $h$ from $\mathcal{X}$ to $\mathcal{Y}$, as in the previous sections:

$$h = \text{argmin}_{h \in \mathcal{H}_K} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x_i), \phi(z_i)) + \frac{\Lambda}{2} \| h \|^2_{\mathcal{H}_K}.$$
The whole procedure is depicted in Figure 1(a). While previous works are restricted to identity decomposable kernels with the standard Ridge regression (Brouard et al., 2016b), our general framework allows for many more losses and kernels. The use of an $\epsilon$-insensitive loss in Problem (9), in particular, seems all the more adequate as it is not the final task targeted, but rather a surrogate one. Indeed, inducing small mistakes, that does not harm the inverse problem, while improving generalization, sounds as a suitable compromise. The Huber loss, that does not penalize heavily big errors, benefits from the same type of arguments. We thus advocate to solve structured prediction in vv-RKHSs by using losses more sophisticated than the squared norm. Experimental results endorsing the soundness of our approach are collected in Section 5.

**Structured Representation Learning.** Extracting vectorial representations from structured inputs is another task that can be tackled through vv-RKHSs. When standard neural net functions are not able to produce reconstructions in the input space, because the latter is to complex for instance, it is still possible to embed the datapoints into a Hilbert space. Then, composing functions in vv-RKHSs results in a Kernel Autoencoder (KAE, Figure 1(b)) that outputs finite codes by minimizing the (regularized) discrepancy:

$$\frac{1}{2n}\sum_{i=1}^{n} \|\phi(x_i)-f_2 \circ f_1(\phi(x_i))\|^2_{\mathcal{Y}} + \Lambda\operatorname{Reg}(f_1, f_2). \quad \text{(10)}$$

Again, this criterion is not the real goal, but rather a proxy to make the internal representation meaningful. Therefore, all incentives to use $\epsilon$-insensitive losses or the Huber loss still apply. The inferred $\epsilon$ and Huber KAEs, obtained by changing the loss in Problem (10), are optimized following Algorithm 3. Each layer being fully characterized by the coefficients $\Phi_1$ and $\Phi_2$, the first ones, finite dimensional, are updated by Gradient Descent, while the second, infinite dimensional, are reparametrized into $W_2$ and updated through the BCD or PGD algorithms previously described depending on the chosen loss. Experiments attesting the benefit of these losses within KAEs are presented in Section 5.

**Algorithm 2** Projected Gradient Descent (PGD)

```plaintext```
input : Gram matrices $K^X$, $K^Y$, parameters $\Lambda$, $\kappa$
init : $\tilde{K} = \frac{1}{\sqrt{n}}K^X + I_n$, $K^Y = VV^T$, $W = 0_{\mathbb{R}^{n \times n}}$
while stopping criterion False do
  $W = W - \gamma(\tilde{K}W - V)$  // gradient step
  for row i from 1 to n do
    $W_i = \operatorname{Proj}(W_i, \kappa)$  // projection step
return $W$
```

4 Handling Integral Losses

When the loss $\ell$ does not depend directly upon the scalar product or the norm in $\mathcal{Y}$, it is impossible to verify the assumptions needed for a representer theorem. The dual problem is then seemingly intractable since no decomposition of the $(\alpha_i)_{i=1}^{n}$ on a finite basis can be exhibited. Moreover, the Fenchel-Legendre transforms $\ell_i^*$ may not be computable due to a lack of compatibility between $\ell_i$ and the scalar product in $\mathcal{Y}$.

Integral losses over function spaces stands as good examples of such a case. These losses, depicted in Equation (11), are key to solve function-to-function regression tasks (see Ramsay and Silverman (2007) for an
extensive description of challenges involving functional data analysis, as well as continuums of tasks (Braut et al., 2019). Such losses take the form

\[ l: L^2[\Theta, \mu] \times L^2[\Theta, \mu] \rightarrow \mathbb{R} \]

\[ (f, g) \mapsto \int_{\Theta} l_{\mu}(f(\theta), g(\theta))d\mu(\theta). \tag{11} \]

where \( \mu \) is a probability measure over some compact set \( \Theta \subset \mathbb{R} \), and \( l_{\mu}: \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R} \) is a family of loss functions indexed by \( \theta \in \Theta \), such that \( l \) is well defined. In our setting, \( \mathcal{Y} \) is a space of functions defined over \( \Theta \) which can be continuously embedded into \( L^2[\Theta, \mu] \) by means of an inclusion operator \( \mathcal{I} \). For all \( g \in L^2[\Theta, \mu] \), \( l_g \) relates to \( l(\cdot, g) \) and \( l_g = l_g \circ \mathcal{I} \) is the loss function at point \( g \) defined on \( \mathcal{Y} \). Given that \( (x_i, y_i)_{i=1}^n \in X \times L^2[\Theta, \mu] \) are i.i.d. samples, the problem within the empirical risk minimization framework reads

\[ \min_{h \in \mathcal{H}_\kappa} \frac{1}{n} \sum_{i=1}^n l_h(y_i, h(x_i)) + \frac{\lambda}{2} \| h \|^2_{\mathcal{H}_\kappa}. \tag{12} \]

Note that the \( (y_i)_{i=1}^n \) are functions which do not necessarily belong to \( \mathcal{Y} \), since \( \mathcal{Y} \) is the output space of the candidate functions within the vV-RKHS \( \mathcal{H}_\kappa \). Below we give a few examples of family of losses \((l_\theta)_{\theta \in \Theta}\) and emphasize on the usefulness of the associated Probability Programming Problem 2. Let \( \Theta \) be a compact subset of \( \mathbb{R} \) and \( k: \Theta \times \Theta \rightarrow \mathbb{R} \) be a positive definite kernel, associated to the RKHS \( \mathcal{H}_k \).

**Assumption 5.** The kernel \( k \) is continuous.

**Proposition 2.** Assume that Assumption 5 holds. Then \( \mathcal{H}_k \) is a subspace of \( L^2[\Theta, \mu] \) and the canonical inclusion \( \mathcal{I}_k: \mathcal{H}_k \rightarrow L^2[\Theta, \mu] \) is a bounded operator whose adjoint \( \mathcal{T}_k: L^2[\Theta, \mu] \rightarrow \mathcal{H}_k \) is given for all \( g \in L^2[\Theta, \mu] \) by \( T_k g = \frac{\lambda}{2} k(\cdot, \cdot)g(\cdot)d\mu \).

In particular, Proposition 2 ensures that for all \( (\alpha, g) \in \mathcal{H}_k \times L^2[\Theta, \mu] \), \( \langle \alpha, T_k g(\cdot) \rangle_{\mathcal{H}_k} = \langle \alpha, g \rangle_{L^2[\Theta, \mu]} \). Continuity of \( k \) also grants a spectral decomposition for its integral operator, as stated in Proposition 3.

**Proposition 3.** Assume that Assumption 5 hold. Denote by \( L_k = I_k T_k \). There exists an orthonormal basis \( (\psi_m)_{m=1}^\infty \) of \( L^2[\Theta, \mu] \) and some \( (\lambda_m)_{m=1}^\infty \in \mathbb{R}_+ \) ordered in a non-increasing fashion and converging to zero such that \( L_k = \sum_{m=1}^\infty \lambda_m \psi_m \otimes \psi_m \).

**Remark 2.** Even though each \( \psi_m \) is defined up to a null \( \mu \)-set, it is convenient to work with some \( \psi_m \) belonging to both \( \mathcal{H}_k \) and the equivalence class in \( L^2[\Theta, \mu] \) of \( \psi_m \), which is assumed afterwards.

**Assumption 6.** \( \mu \) is non-degenerate: \( \text{supp}(\mu) = \Theta \).

**Assumption 7.** The kernel \( k \) is universal, i.e. \( \mathcal{H}_k \) is dense in the set of continuous functions from \( \Theta \) to \( \mathbb{R} \).

**Proposition 4.** Under Assumptions 5-6, then \( T_k \) is surjective. Under Assumptions 5-7, \( T_k \) is bijective.

Lemma 1 below uses aforementioned assumptions to link the Fenchel-Legendre transforms of \( l_y \) and \( l_y^\ast \).

**Lemma 1.** Let \( l: L^2(\Theta, \mu) \times L^2(\Theta, \mu) \rightarrow \mathbb{R} \) be a continuous loss function. Under Assumptions 5-7, it holds

\[ \forall y \in L^2(\Theta, \mu), \quad l_y^\ast = l_y^\ast \circ T_k^{-1}. \tag{13} \]

**Proof.** (Sketch of) Use the fact that \( \langle \alpha, \xi \rangle_{\mathcal{H}_k} = \langle T_k^{-1} \alpha, \xi \rangle_{L^2[\Theta, \mu]} \), that \( \mathcal{H}_k \) is dense in \( L^2[\Theta, \mu] \) and the continuity of \( l_y \).

**Lemma 1** makes explicit the relationship between \( l_y^\ast \) and \( l_y^\ast \). It turns out that the scalar product in \( L^2[\Theta, \mu] \) is well suited to \( l_y \), so that \( l_y^\ast \) admits a simple expression, as stated by the theorem below.

**Theorem 1.**
Theorem 6. Let \( l_\theta : \mathbb{R} \times \mathbb{R} \to \mathbb{R} \) be a family of loss functions indexed by \( \theta \in \Theta \). Let \((y, g) \in L^2[\Theta, \mu] \times L^2[\Theta, \mu]\). If \( \int_{\Theta} \min \{0, l_{\theta, y}(g(\theta))\} d\mu(\theta) > -\infty \), then
\[
l'_{\theta}(g) = \int_{\Theta} l_{\theta, y}(g(\theta)) d\mu(\theta), \tag{14}\]
where \( \forall t \in \mathbb{R}, l'_{\theta,t} \) stands for \( l_{\theta,t}(\cdot)\).

Proof. (Sketch of) Use the fact that \( \sup \{ \int_{\Theta} \min \{0, l_{\theta, y}(g(\theta))\} d\mu(\theta) > -\infty \} \leq \sup \{ \int_{\Theta} l_{\theta, y}(g(\theta)) d\mu(\theta) \} \) in the definition of \( l'_{\theta} \), and that equality is attained when this integral has values in \( -\infty, +\infty \). \( \square \)

Remark 3. The instantiation of Equation (14) for specific loss functions gives:
- When \( l_\theta(s, t) = \frac{1}{2}(t - s)^2, (y, g) \in (L^2[\Theta, \mu])^2 \),
  \[
l'_{\theta}(g) = \frac{1}{2} \|y\|^2_{L^2[\Theta, \mu]} + \langle g, y \rangle_{L^2[\Theta, \mu]} \]
- When \( l_\theta(s, t) = \max(0, \theta(t - s), (\theta - 1)(t - s)) \), for all \( g \in L^2[\Theta, \mu] \), and \( y \) constant in \( L^2[\Theta, \mu] \),
  \[
l'_{\theta}(g) = \chi_{\theta - 1 \leq \cdot \leq \theta} + \frac{1}{\theta - 1} \int_{\Theta} g(\theta) d\mu(\theta) \]
where \( \chi_{\theta - 1 \leq \cdot \leq \theta} \) is to be understood in \( L^2[\Theta, \mu] \), that is up to a null \( \mu \)-set.
- When \( l_\theta(s, t) = \max(0, 1 - ts) \), for all \( g \in L^2[\Theta, \mu] \), and \( y \) constant in \( L^2[\Theta, \mu] \),
  \[
l'_{\theta}(g) = y \int_{\Theta} g(\theta) d\mu(\theta) + \chi_{\theta - 1 \leq \cdot \leq \theta} \langle g, y \rangle_{L^2[\Theta, \mu]} \]

The key idea of our approach is to find good candidates \( (\hat{g}_i)_{i=1}^n \in L^2[\Theta, \mu] \) such that \( (\alpha_i)_{i=1}^n = (T_k \hat{g}_i)_{i=1}^n \in H_k \) are close to the solution of the dual problem.

Theorem 7. Let \( K = k_X I_{H_k} \) be an OVK such that \( k \) verifies Assumptions 5 and 7. Assume also that Assumption 6 holds. The solution to Problem (12) is given by
\[
\hat{h} = \frac{1}{\lambda n} \sum_{i=1}^n k_X(\cdot, x_i) T_k \hat{g}_i
\]
with \((\hat{g}_i)_{i=1}^n \in (L^2[\Theta, \mu])^n\) minimizing
\[
\sum_{i=1}^n l'_{\theta}(g_i) + \frac{1}{2\lambda n} \sum_{i=1}^n \sum_{j=1}^n k_X(x_i, x_j) \langle g_i, L_k g_j \rangle \tag{15}\]

Proof. Use \( \alpha_i = T_k g_i \) for \( i \leq n \), and Equation (13). \( \square \)

Although Problem (15) phrases the optimization problem in a new space, it remains hard to solve since \( L^2[\Theta, \mu] \) is infinite dimensional. To circumvent this difficulty, the research of the \((g_i)_{i=1}^n\) will be performed in a finite dimensional subspace adapted to the problem, namely span\(\{\psi_m\}_{m=1}^M\), where \(\{\psi_m\}_{m=1}^M\) are the eigenvectors associated to the \( M \) largest eigenvalues of \( L_k \). Using the notation \( S = \text{diag}((\lambda_m)_{m=1}^M) \), an approximate dual problem reads:
\[
\min_{\beta \in \mathbb{R}^{n \times M}} \sum_{i=1}^n l'_{\theta}(g_i) - \sum_{m=1}^M \beta_m \psi_m + \frac{1}{2\lambda n} \text{Tr} \left( K X \beta S \beta^T \right) \tag{16}\]

Remark 4. The eigendecomposition of \( L_k \) is dependent both in \( k \) and \( \mu \), and can be approximately solved using the Galerkin method (Chatelin, 2011), or by solving a differential equation derived from the eigenvalue problem. However, given that the optimal kernel \( k \) is unknown, one can choose a Hilbertian basis \( \{\psi_m\}_{m=1}^\infty \) of \( L^2[\Theta, \mu] \) and a non-increasing sequence \( (\lambda_m)_{m=1}^\infty \in \mathbb{R}^+ \) to construct the kernel \( k \), which gives direct access to the eigendecomposition of \( T_k \).

Below are presented ways to solve Problem (16) in various scenarios of loss functions. In these applications, \( R \in \mathbb{R}^{n \times M} \) refers to the matrix such that \( \forall 1 \leq i \leq n, 1 \leq m \leq M, R_{im} = \langle \psi_m, y_i \rangle_{L^2[\Theta, \mu]} \).

Ridge Regression. When \( l_\theta(s, t) = \frac{1}{2}(t - s)^2 \), Problem (16) reads
\[
\min_{\beta \in \mathbb{R}^{n \times M}} \text{Tr} \left( \frac{1}{2} \beta \beta^T + \frac{1}{2\lambda n} K X \beta S \beta^T - \beta R^T \right) \tag{17}\]
so that it boils down to the minimization of a quadratic form. Setting the gradient to zero yields a solution \( \hat{\beta} = (I + \frac{1}{\lambda n} K X \otimes S)^{-1} R \), where \( K X \otimes S \) is the block operator matrix such that \( (K X \otimes S)_{ij} = k_X(x_i, x_j) S \). The inversion of this operator can be performed using its spectral decomposition, and \( \hat{\beta} \) coincides with the closed-form solution given in (Kadri et al., 2010).

Dealing with Lipschitz Losses. When \( (l_\theta)_{\theta \in \Theta} \) is a family of Lipschitz loss functions, \( l'_{\theta}(g) \) may take \( +\infty \) as value if \( g \) is not in the feasible set of the dual problem. This induces an additional difficulty to the resolution of Problem (16), since the finite dimensional space span\(\{\psi_m\}_{m=1}^M\) may not be stable with respect to the projection on the feasible set, which annihilates any hope for a vanilla proximal gradient descent. The design of appropriate optimization algorithms is out of the scope of this paper and left to future works.

Application to Huber Loss. Function-to-function regression has mainly been dealt with through the minimization of an empirical \( L^2 \) risk. However, in the spirit of Section 3.2, this task can be tackled using a Huber loss, which induces robustness. The approximate dual problem is then Problem (17) under the additional constraint that \( \|\beta\|_{2,\infty} \leq \kappa \), and it can be solved through PGD. Experimental results endorsing this approach are presented in section 5.
5 Numerical Experiments

Numerical experiments have been run in order to show the benefit of using more sophisticated loss than the standard squared norm in output Hilbert spaces, with focus on three applications: structured prediction, representation learning, and functional regression.

**Structured prediction.** We consider the problem of identifying metabolites based on their mass spectra (Brouard et al., 2016a). We investigate the advantages of substituting the Ridge Regression for the minimization of an ε-insensitive Ridge Regression or a Huber loss. Outputs are embedded in an infinite dimensional space through the use of the Gaussian kernel (with 0.72 bandwidth γ and 1ε − 6 regularizer λ). We compare the different algorithms performances on a set of 6974 mass spectra through the top-k accuracies for k = 1, 10, 20. As expected, a wide range of ε’s induce a substantial improvement compared to Ridge Regression (see Figure 3 and further figures in Appendix C). This improvement comes with a norm reduction until the collapsing point at ε = 1. The Huber results are gathered in Table 1, showing valuable gains for all κ’s.

| κ  | Top 1 | Top 10 | Top 20 | ||W||_{2,1} |
|----|-------|--------|--------|------------|
| 0.5 | 38.0  | 83.5   | 89.6   | 2789.6     |
| 1.0 | **38.9** | **83.8**   | **89.9**   | 5572.4     |
| 1.5 | 38.6  | 83.7   | 89.8   | 8231.9     |

Table 1: Huber test accuracies (%) with respect to κ

Figure 2: Test accuracy with respect to ε.

Figure 3: Test Mean Squared Error (MSE) w.r.t. ε.

**5 Conclusion**

This work presents an extended analysis of the duality principle in vv-RKHSs, allowing for the use of new loss functions. The particular case of convolved losses is tackled, offering novel ways to enforce sparsity and robustness. This opens an avenue for new applications on structured data (e.g. anomaly detection, robust prediction), whose generalization guarantees remain to be investigated.
Acknowledgment. This work has been funded by the Industrial Chair Data Science & Artificial Intelligence for Digitalized Industry & Services from Télécom Paris, Paris, France.

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A Technical Proofs

In this section are collected the technical proofs of the results stated in the core part of the article.

A.1 Proof of Theorem 2

First, notice that the primal problem

\[
\min_{h \in \mathcal{H}_K} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x_i), y_i) + \frac{\Lambda}{2} \|h\|^2_{\mathcal{H}_K}
\]

can be rewritten

\[
\min_{h \in \mathcal{H}_K} \sum_{i=1}^{n} \ell_i(u_i) + \frac{\Lambda n}{2} \|h\|^2_{\mathcal{H}_K},
\]

s.t. \( u_i = h(x_i) \quad \forall i \leq n. \)

Therefore, with the notation \( \mathbf{u} = (u_i)_{i \leq n} \) and \( \mathbf{\alpha} = (\alpha_i)_{i \leq n} \), the Lagrangian writes

\[
\mathcal{L}(h, \mathbf{u}, \mathbf{\alpha}) = \sum_{i=1}^{n} \ell_i(u_i) + \frac{\Lambda n}{2} \|h\|^2_{\mathcal{H}_K} + \sum_{i=1}^{n} \langle \alpha_i, u_i - h(x_i) \rangle_Y,
\]

\[
= \sum_{i=1}^{n} \ell_i(u_i) + \frac{\Lambda n}{2} \|h\|^2_{\mathcal{H}_K} + \sum_{i=1}^{n} \langle \alpha_i, u_i \rangle_Y - \sum_{i=1}^{n} \langle \mathcal{K}(\cdot, x_i)\alpha_i, h \rangle_{\mathcal{H}_K}.
\]

Differentiating with respect to \( h \) and using the definition of the Fenchel-Legendre transform, one gets

\[
g(\mathbf{\alpha}) = \inf_{h \in \mathcal{H}_K, \mathbf{u} \in Y^n} \mathcal{L}(h, \mathbf{u}, \mathbf{\alpha}),
\]

\[
= \sum_{i=1}^{n} \inf_{u_i \in Y} \{ \ell_i(u_i) + \langle \alpha_i, u_i \rangle_Y \} + \inf_{h \in \mathcal{H}_K} \left\{ \frac{\Lambda n}{2} \|h\|^2_{\mathcal{H}_K} - \sum_{i=1}^{n} \langle \mathcal{K}(\cdot, x_i)\alpha_i, h \rangle_{\mathcal{H}_K} \right\},
\]

\[
= \sum_{i=1}^{n} -\ell'_i(-\alpha_i) - \frac{1}{2\Lambda n} \sum_{i,j=1}^{n} \langle \alpha_i, \mathcal{K}(x_i, x_j)\alpha_j \rangle_Y,
\]

together with the equality \( \hat{h} = \frac{1}{\Lambda n} \sum_{i=1}^{n} \mathcal{K}(\cdot, x_i)\alpha_i \). The conclusion follows immediately. \( \square \)

A.2 Proof of Theorem 3

As a reminder, our goal is to compute the solutions to the following problem:

\[
\hat{h} \in \arg\min_{h \in \mathcal{H}_K} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x_i), y_i) + \frac{\Lambda}{2} \|h\|^2_{\mathcal{H}_K}.
\]

Using Theorem 2, one gets that \( \hat{h} = \frac{1}{\Lambda n} \sum_{i=1}^{n} \mathcal{K}(\cdot, x_i)\hat{\alpha}_i \), with the \( \hat{\alpha}_i \) satisfying:

\[
(\hat{\alpha}_i)_{i=1}^{n} \in \arg\min_{(\alpha_i)_{i=1}^{n} \in \mathbb{R}^n} \sum_{i=1}^{n} \ell'_i(-\alpha_i) + \frac{1}{2\Lambda n} \sum_{i,j=1}^{n} \langle \alpha_i, \mathcal{K}(x_i, x_j)\alpha_j \rangle_Y.
\]

However, this optimization problem cannot be solved in a straightforward manner, as \( Y \) is in general infinite dimensional. Nevertheless, it is possible to bypass this difficulty by noticing that the optimal \( \hat{\alpha}_i \) actually lie in \( Y^n \). Indeed, by virtue of Assumptions 2 and 3, for all for all \( (\alpha_Y^1)_{i \leq n}, (\alpha_Y^1)_{i \leq n} \in Y^n \times Y^{\perp n} \), it holds:

\[
\sum_{i=1}^{n} \ell'_i(-\alpha_Y^1) + \frac{1}{2\Lambda n} \sum_{i,j=1}^{n} \langle \alpha_Y^1, \mathcal{K}(x_i, x_j)\alpha_Y^1 \rangle_Y \leq \sum_{i=1}^{n} \ell'_i(-\alpha_Y^1 - \alpha_Y^1) + \frac{1}{2\Lambda n} \sum_{i,j=1}^{n} \langle \alpha_Y^1 + \alpha_Y^1, \mathcal{K}(x_i, x_j)(\alpha_Y^1 + \alpha_Y^1) \rangle_Y,
\]

\[
= \sum_{i=1}^{n} \ell'_i(-\alpha_Y^1 - \alpha_Y^1) + \frac{1}{2\Lambda n} \sum_{i,j=1}^{n} \langle \alpha_Y^1 + \alpha_Y^1, \mathcal{K}(x_i, x_j)(\alpha_Y^1 + \alpha_Y^1) \rangle_Y.
\]
The second term is quadratic in $\Omega$, and consequently convex. As for the computable quantities.

A.3 Proof of Proposition 1

The dual optimization problem thus rewrites:

$$
\min_{\Omega \in \mathbb{R}^{n \times n}} \sum_{i=1}^{n} L_i \left( (\omega_{ij})_{j \leq n}, K^{Y} \right) + \frac{1}{2 \lambda n} \sum_{i,j,k,l=1}^{n} \omega_{ik} \omega_{jl} \left( y_{kl} \sum_{t=1}^{T} k_t(x_i, x_j) A_t y_{il} \right)
$$

The second term is quadratic in $\Omega$, and consequently convex. As for the $L_i$’s, they are basically rewrites of the Fenchel-Legendre transforms $\ell^*_{i}$’s that ensure the computability of the problem (they only depend on $R^{Y}$, which is known). Regarding their convexity, we know by definition that the $\ell^*_{i}$’s are convex. Composing by a linear function preserving the convexity, we know that each $L_i$ is convex with respect to $\Omega_i$, and therefore with respect to $\Omega$.

Thus, we have first converted the infinite dimensional primal problem in $\mathcal{H}_K$ into an infinite dimensional dual problem in $\mathcal{Y}$, which in turn is reduced to a convex optimization procedure over $\mathbb{R}^{n \times n}$, that only involves computable quantities.

The proof technique is the same for all losses: first explicit the FL transforms $\ell^*_{i}$, then use simple arguments to verify Assumptions 3 and 4. For instance, any increasing function of $\|\alpha\|$ automatically satisfy the assumptions.

- Assume that $\ell$ is such that there is $f : \mathbb{R} \to \mathbb{R}$ convex, $\forall i \leq n, \exists z_i \in Y, \ell_i(y) = f(\langle y, z_i \rangle)$. Then $\ell^*_{i} : \mathcal{Y} \to \mathbb{R}$ writes $\ell^*_{i}(\alpha) = \sup_{y \in \mathcal{Y}} f(\langle \alpha, y \rangle)$. If $\alpha$ is not collinear to $z_i$, this quantity is obviously $+ \infty$. Otherwise, assume that $\alpha = \lambda z_i$. The FL transform rewrites: $\ell^*_{i}(\alpha) = \sup_{\lambda} \alpha \cdot \lambda - f(t) = f^*(\lambda) = f^*(\pm \|\alpha\|/\|z_i\|)$. Finally, $\ell^*_{i}(\alpha) = \chi_{\text{span}(z_i)}(\alpha) + f^*(\pm \|\alpha\|/\|z_i\|)$. If $\alpha \neq Y$, then a fortiori $\alpha \notin \text{span}(z_i)$, so $\ell^*_{i}(\alpha^{Y} + \alpha^{-}) = + \infty \geq \ell^*_{i}(\alpha^{Y})$ for all $(\alpha^{Y}, \alpha^{-}) \in Y \times Y^\perp$. For all $i \leq n$, $\ell^*_{i}$ satisfies Assumption 3. As for Assumption 4, if $\alpha = \sum_{i=1}^{n} c_i y_{i}$, then $\chi_{\text{span}(z_i)}(\alpha)$ only depends on the $(c_i)_{i \leq n}$. Indeed, assume that $z_i \in Y$ writes $\sum c_i b_j y_{j}$. Then $\chi_{\text{span}(z_i)}(\alpha)$ is equal to 0 if there exists $\lambda \in \mathbb{R}$ such that $c_j = \lambda b_j$ for all $j \leq n$, and to $+ \infty$ otherwise. The second term of $\ell^*_{i}$ depending only on $\|\alpha\|$, it directly satisfies Assumption 4. This concludes the proof.

- Assume that $\ell$ is such that there is $f : \mathbb{R}_+ \to \mathbb{R}$ convex increasing, with $f'(\alpha)$ continuous over $\mathbb{R}_+$, $\ell(y) = f(\|y\|)$. Although this loss may seem useless at the first sight since $\ell$ does not depend on $y_i$, it should not be forgotten that the composition with $y \mapsto y - y_i$ does not affect the validation of Assumptions 3 and
4 (see below). One has: $\ell^*(\alpha) = \sup_{y \in \mathcal{Y}} \langle \alpha, y \rangle - f(||y||)$, differentiating w.r.t. $y$, one gets: $\alpha = \frac{f'(||y||)}{||y||} y$, which is always well define as $t \mapsto \frac{f'(t)}{t}$ is continuous over $\mathbb{R}_+$. Reverting the equality, it holds: $y = \frac{\ell^*(\alpha)}{\alpha}$, and $\ell^*(\alpha) = ||\alpha||f'^{-1}(||\alpha||) - f \circ f'^{-1}(||\alpha||)$. This expression depending only on $||\alpha||$, Assumption 4 is automatically satisfied. Let us now investigate the monotonicity of $\ell^*$ w.r.t. $||\alpha||$. Let $g : \mathbb{R}_+ \to \mathbb{R}$ such that $g(t) = tf'^{-1}(t) - f \circ f'^{-1}(t)$. Then $g'(t) = f'^{-1}(t) \geq 0$. Indeed, as $f' : \mathbb{R}_+ \to \mathbb{R}_+$ is always positive due to the monotonicity of $f$, so is $f'^{-1}$. This final remark guarantees that $\ell^*$ is increasing with $||\alpha||$. It is then direct that $\ell^*$ fulfills Assumption 3.

- Assume that $\ell(y) = \lambda ||y||$. It is well known that $\ell^*(\alpha) = \chi_{\mathcal{B}_s}(\alpha)$. The latter being an increasing function of $||\alpha||$, it directly fulfills Assumptions 3 and 4.

- Assume that $\ell(y) = \chi_{\mathcal{B}_s}(y)$. It is well known that $\ell^*(\alpha) = \lambda ||\alpha||$. The usual arguments on the monotonicity of $\ell^*$ w.r.t. $||\alpha||$ permit to conclude.

- Assume that $\ell(y) = \lambda ||y|| \log(||y||)$. It can be shown that $\ell^*(\alpha) = \lambda e^{\frac{||\alpha||}{\alpha}} - 1$. The same arguments as above apply.

- Assume that $\ell(y) = \lambda(\exp(||y||) - 1)$. It can be shown that $\ell^*(\alpha) = \lambda \{ ||\alpha|| \geq \lambda \} \cdot (||\alpha|| \log (\frac{||\alpha||}{\alpha}) + \lambda)$. Again, the FL transform is an increasing function of $||\alpha||$: it satisfies Assumptions 3 and 4.

- Assume that $\ell_i(y) = f(y - y_i)$, with $f$ such that $f^*$ fulfills Assumptions 3 and 4. Then $\ell^*_i(\alpha) = \sup_{y \in \mathcal{Y}} \langle \alpha, y \rangle - f(y - y_i) = f^*(\alpha) + \langle \alpha, y_i \rangle$. If $f^*$ satisfies Assumptions 3 and 4, then so does $\ell^*_i$. This remark is very important, as it gives more sense to loss function based on $\ell_i$ only, since they can be applied to $y - y_i$ now.

- Assume that there exists $f, g$ satisfying Assumptions 3 and 4 such that $\ell_i(y) = (f \Box g)(y)$, where $\Box$ denotes the infimal convolution, i.e. $(f \Box g)(y) = \inf_x f(x) + g(y - x)$. Standard arguments about FL transforms state that $(f \Box g)^* = f^* + g^*$, so that if both $f$ and $g$ satisfy Assumptions 3 and 4, so does $f \Box g$. This last example allows to deal with $\epsilon$-insensitive losses for instance (convolution of a loss and $\chi_{\mathcal{B}_s}$), the Huber loss (convolution of $||.||$ and $||.||^2$), or more generally all Moreau envelopes (convolution of a loss and $\frac{1}{2}||.||^2$).

\[ \square \]

A.4 Proof of Theorem 4

Applying Theorem 2 together with the Fenchel-Legendre transforms detailed in the proof of Proposition 1, a dual to Problem (5) is:

\[
\min_{\alpha_i \in \mathcal{Y}_n} \frac{1}{2} \sum_{i=1}^n \alpha_i y_i^2 - \sum_{i=1}^n \langle \alpha_i, y_i \rangle y_i + \epsilon \sum_{i=1}^n \alpha_i ||y|| + \frac{1}{2\Lambda n} n \sum_{i,j=1}^n \langle \alpha_i, K(x_i, x_j) \alpha_j \rangle_y,
\]

\[
\min_{\alpha_i \in \mathcal{Y}_n} \frac{1}{2} \sum_{i,j=1}^n \langle \alpha_i, \delta_{ij} y + \frac{1}{\Lambda n} K(x_i, x_j) \alpha_j \rangle_y - \sum_{i=1}^n \langle \alpha_i, y_i \rangle y_i + \epsilon \sum_{i=1}^n \alpha_i ||y||.
\]

By virtue of Theorem 3, we known that the optimal $(\alpha_i)_{i=1}^n \in \mathcal{Y}_n$ are in $\mathcal{Y}_n$. After the reparametrization $\alpha_i = \sum_{j=1}^{n} \omega_{ij} y_j$, the problem rewrites:

\[
\min_{\Omega \in \mathbb{R}^{n \times n}} \frac{1}{2} \text{Tr} \left( \hat{K} \Omega K^T \Omega^T \right) - \text{Tr} \left( K^T \Omega \right) + \epsilon \sum_{i=1}^n \sqrt{\text{Tr} \left[ \Omega K^T \Omega^T \right]}_i,
\]

with $\Omega$, $\hat{K}$, $K$ the $n \times n$ matrices such that $[\Omega]_{i,j} = \omega_{i,j}$, $\hat{K} = \frac{1}{\Lambda n} K^X + I_n$, and $[K^T]_{i,j} = \langle y_i, y_j \rangle_y$.

Now, let $K^Y = U \Sigma U^T = (U \Sigma^{1/2}) (U \Sigma^{1/2})^T = V V^T$ be the SVD of $K^Y$, and let $W = \Omega V$. Notice that $K^Y$ is positive semi-definite, and can be made positive definite if necessary, so that $V$ is full rank, and optimizing w.r.t. $W$ is strictly equivalent to minimizing w.r.t. $\Omega$. With this change of variable, Problem (18) rewrites:

\[
\min_{W \in \mathbb{R}^{n \times n}} \frac{1}{2} \text{Tr} \left( \hat{K} W W^T \right) - \text{Tr} \left( V^T W \right) + \epsilon ||W||_{2,1},
\]
with $\|W\|_{2,1} = \sum_i \|W_{i,}\|_2$ the row-wise $\ell_{2,1}$ mixed norm of matrix $W$. With $\tilde{K} = A^T A$ the SVD of $\tilde{K}$, and $B$ such that $A^T B = V$, one can add the constant term $\frac{1}{2} \text{Tr}(A^{-1}VV^T A^{-1}) = \frac{1}{2} \text{Tr}(BB^T)$ to the objective without changing Problem (19). One finally gets the Multi-Task Lasso problem:

$$\min_{W \in \mathbb{R}^{n \times n}} \frac{1}{2} \|AW - B\|_{\text{Fro}}^2 + \epsilon \|W\|_{2,1}.$$ 

\[\square\]

### A.5 Proof of Theorem 5

Basic manipulations give the Fenchel-Legendre transforms of the Huber loss:

\[
\left( y \mapsto \ell_{H,\kappa}(y - y_i) \right)^\ast (\alpha) = \left( \kappa \cdot \| y \| \ominus \frac{1}{2} \| \cdot \|_2^2 \right)^\ast (\alpha) + \langle \alpha, y_i \rangle_{\mathcal{Y}},
\]

\[
= (\kappa \cdot \| y \|)^\ast (\alpha) + \left( \frac{1}{2} \| \cdot \|_2^2 \right)^\ast (\alpha) + \langle \alpha, y_i \rangle_{\mathcal{Y}},
\]

\[
= \chi_{\mathcal{H}_k}(\alpha) + \frac{1}{2} \| \alpha \|_2^2 + \langle \alpha, y_i \rangle_{\mathcal{Y}}.
\]

The rest of the proof is similar to that of Theorem 4, except that the $\ell_{2,1}$ mixed norm $\|W\|_{2,1}$ is replaced by constraints on the norms of $W$’s lines. \[\square\]

### A.6 Proof of Lemma 1

Define $l_y: g \in L^2[\Theta, \mu] \mapsto \int_\Theta \ell_\theta(g(\theta), y(\theta))d\mu(\theta)$ so that $\ell_y = l_y \circ I_k$. Let $\alpha \in \mathcal{H}_k$. Using the bijectivity of $T_k$, one gets:

\[
(l_y \circ I_k)^\ast (\alpha) = \sup_{\xi \in \mathcal{H}_k} \langle \alpha, \xi \rangle_{\mathcal{H}_k} - l_y \circ I_k(\xi)
\]

\[
= \sup_{\xi \in \mathcal{H}_k} \langle T_k(T_k)^{-1}(\alpha), \xi \rangle_{\mathcal{H}_k} - l_y \circ I_k(\xi)
\]

\[
= \sup_{\xi \in \mathcal{H}_k} \langle (T_k)^{-1}(\alpha), I_k(\xi) \rangle_{L^2[\Theta, \mu]} - l_y \circ I_k(\xi).
\]

Since $\xi \mapsto \langle (T_k)^{-1}(\alpha), I_k(\xi) \rangle_{L^2[\Theta, \mu]} - l_y \circ I_k(\xi)$ is continuous, and $\mathcal{H}_k$ is dense in $L^2[\Theta, \mu]$ (Carmeli et al., 2010), it holds that

\[
\sup_{\xi \in \mathcal{H}_k} \langle (T_k)^{-1}(\alpha), I_k(\xi) \rangle_{L^2[\Theta, \mu]} - l_y \circ I_k(\xi) = \sup_{f \in L^2[\Theta, \mu]} \langle (T_k)^{-1} f, \xi \rangle_{L^2[\Theta, \mu]} - l_y(f)
\]

which gives $(l_y \circ I_k)^\ast = l_y^\ast \circ (T_k)^{-1}$.

### A.7 Proof of Theorem 6

Recall that $l_y: g \in L^2[\Theta, \mu] \mapsto \int_\Theta \ell_\theta(g(\theta), y(\theta))d\mu(\theta)$. Let $f \in L^2[\Theta, \mu]$. $l_y^\ast(f) = \sup_{g \in L^2[\Theta, \mu]} \langle f, g \rangle_{L^2[\Theta, \mu]} - l_y(g)$

\[
= \sup_{g \in L^2[\Theta, \mu]} \int_\Theta f(\theta)g(\theta)d\mu(\theta) - \int_\Theta l_\theta(g(\theta), y(\theta))d\mu(\theta)
\]

\[
= \sup_{g \in L^2[\Theta, \mu]} \int_\Theta f(\theta)g(\theta) - l_\theta(g(\theta), y(\theta))d\mu(\theta)
\]

\[
\leq \int_\Theta \sup_{t \in \Theta} f(\theta) - l_\theta(t, y(\theta))d\mu(\theta)
\]

\[
\leq \int_\Theta l_y^\ast(t, y(\theta))(f(\theta))d\mu(\theta)
\]

where $\forall s \in \mathbb{R}$, $l_y^\ast(s)$ stands for $l_y(\cdot, s)^\ast$. Since $\int_\Theta \min(0, l_y^\ast(t, y(\theta))(f(\theta)))d\mu(\theta) > -\infty$, it holds that $\int_\Theta l_y^\ast(t, y(\theta))(f(\theta))d\mu(\theta) \in ]-\infty, +\infty]$ is well defined, and equality is attained.
B On Variants of Dual Problems

In this section, we investigate variants of the dual problems established in Theorems 4 and 5. Appendices B.1 and B.3 focus on the case where \( \mathcal{K} \) is not identity decomposable but only satisfies Assumption 1, respectively for the \( \epsilon \)-insensitive Ridge regression and the Huber loss regression. Appendix B.2 highlights that the standard Ridge regression is naturally recovered by the \( \epsilon \)-insensitive Ridge when \( \epsilon = 0 \).

B.1 \( \epsilon \)-Ridge Regression Problems under Assumption 1

When \( \mathcal{K} \) is not identity decomposable, Problem (4) cannot be simplified as Problem (6). Nonetheless, it admits a simple resolution, as detailed in the following lines. After the \( \Omega \) reparametrization, the problem writes

\[
\min_{\Omega \in \mathbb{R}^{n \times n}} \frac{1}{2} \text{Tr}(\Omega Y^T Y) - \text{Tr}(K Y) + \epsilon n \sum_{i=1}^{n} \sqrt{[\Omega K Y]_{i,i}} + \frac{1}{2 \lambda n} \sum_{t=1}^{T} \text{Tr}(K_t^X \Omega K_t^Y Y),
\]

with \( K^Y = V V^T, W = \Omega V, \hat{K}^Y = V^{-1} K^Y (V^T)^{-1} \). Due to the different quadratic terms, this problem cannot be summed up as a Multi-Task Lasso like Problem (6). However, it may still be solved, e.g. by proximal gradient descent. Indeed, the gradient of the smooth term (i.e. all but the \( \ell_{2,1} \) mixed norm) reads

\[
W + \frac{1}{\lambda n} \sum_{t=1}^{T} K_t^X W \hat{K}_t^Y - V,
\]

while the proximal operator of the \( \ell_{2,1} \) mixed norm is

\[
\text{prox}_{\epsilon \cdot \| \cdot \|_{2,1}}(W) = \left( \text{prox}_{\epsilon \cdot \| \cdot \|_2}(W_i) \right) = \left( 1 - \frac{\epsilon}{\| W_i \|_2} \right) W_i = \left( \text{BST}(W_i, \epsilon) \right).
\]

Hence, even in the more involved case of an OVK satisfying Assumption 1, we have designed an efficient algorithm to compute the solutions to the dual problem.

B.2 Recovering Standard Ridge Regressions when \( \epsilon = 0 \)

In this subsection, we emphasize on the fact that the solution to Problem (6) for \( \epsilon = 0 \) is exactly that of the standard Ridge regression. Indeed, coming back to Problem (18) and differentiating with respect to \( \Omega \), one gets:

\[
\hat{K} \hat{\Omega} K - K = 0 \iff \hat{\Omega} = \hat{K}^{-1},
\]

which is exactly the standard kernel Ridge regression solution, see e.g. Brouard et al. (2016b).

B.3 Huber Regression Problems under Assumption 1

When \( \mathcal{K} \) is not identity decomposable, but only satisfies Assumption 1, Problem (8) rewrites

\[
\min_{W \in \mathbb{R}^{n \times n}} \frac{1}{2} \text{Tr}(W W^T) + \frac{1}{2 \lambda n} \sum_{t=1}^{T} \text{Tr}(K_t^X W \hat{K}_t^Y Y) - \text{Tr}(V^T W),
\]

\[\text{s.t.} \quad \| W_i \|_2 \leq \kappa \quad \forall i \leq n, \]

The gradient term is again given by Equation (20), while the projection is similar. The only change thus occurs in the gradient step of Algorithm 2, with a replacement by the above formula.
C Additional Figures

Figure 5: Standard and $\epsilon$-version of the square loss in 1 (left) and 2 (right) dimensions, $\epsilon = 1.5$.

Figure 6: Standard square loss and Huber loss in 1 (left) and 2 (right) dimensions, $\kappa = 0.8$. 
Figure 7: \( \epsilon \)-Insensitive Output Kernel Regression Results

(a) Top-1 Accuracy, linear scale

(b) Top-1 Accuracy, logarithmic scale

(c) Top-10/20 Accuracy, linear scale

(d) Top-10/20 Accuracy, logarithmic scale