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Input Output Kernel Regression: Supervised and Semi-Supervised Structured Output Prediction with Operator-Valued Kernels

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Abstract

In this paper, we introduce a novel approach, called Input Output Kernel Regression (IOKR), for learning mappings between structured inputs and structured outputs. The approach belongs to the family of Output Kernel Regression methods devoted to regression in feature space endowed with some output kernel. In order to take into account structure in input data and benefit from kernels in the input space as well, we use the Reproducing Kernel Hilbert Space theory for vector-valued functions. We first recall the ridge solution for supervised learning and then study the regularized hinge loss-based solution used in Maximum Margin Regression. Both models are also developed in the context of semi-supervised setting. In addition we derive an extension of Generalized Cross Validation for model selection in the case of the least-square model. Finally we show the versatility of the IOKR framework on two different problems: link prediction seen as a structured output problem and multi-task regression seen as a multiple and interdependent output problem. Eventually, we present a set of detailed numerical results that shows the relevance of the method on these two tasks.

Keywords: structured output prediction, output kernel regression, vector-valued RKHS, operator-valued kernel, semi-supervised learning

1. Introduction

Many real world applications involve objects with an explicit or implicit discrete structure. Texts, images and videos in document processing and retrieval as well as genes and proteins in computational biology are all examples of implicit structured data that we may want to use as inputs or outputs in a prediction system. Besides these structured objects, structured output prediction can also concern multiple outputs linked by some relationship that is relevant to take into account. Surprisingly, although a lot of attention has been paid to learning from structured inputs for now two decades, this problem, often referred as *structured output learning*, has emerged relatively recently as a field of interest in statistical learning. In the literature, structured output prediction has been addressed from two main angles. A first angle consists in *discriminative learning algorithms* that provide predictions by maximizing a scoring function over the output space. Conditional Random Fields (Lafferty et al., 2001) and their extension to kernels (Lafferty et al., 2004) were first proposed for discriminative modeling of graph-structured data and sequence labeling. Other discriminative learning algorithms based on maximum margin such as structured SVM (Tsochantaridis et al., 2004, 2005), Maximum Margin Markov Networks (M^3N) (Taskar et al., 2004) or Maximum Margin Regression (Szedmak et al., 2005) have then been developed and thoroughly studied. A common approach to those methods consists in defining a linear scoring function based on the image of an input-output pair by a joint feature map. Both methods, either based on Conditional Random Fields or maximum-margin techniques, are costly to train and generally assume that the output set \mathcal{Y} is discrete. Keeping the idea of a joint feature map over inputs and outputs, a generative method called Joint Kernel Support Estimation has been recently proposed (Lampert and Blaschko, 2009). In this approach, a one-class SVM is used to learn the support of the joint-probability density $p(x, y)$. More recently, another angle to structured output prediction, that we called *Output Kernel Regression* (OKR), has emerged around the idea of using the kernel trick in the output space and making predictions in a feature space associated to the output kernel. As a first example, the seminal work of Kernel Dependency Estimation (KDE) was based on the definition of an input kernel as well as an output kernel. After a first version using kernel PCA to define a finite-dimensional output feature space (Weston et al., 2003), a more general KDE framework consisting in learning a linear function from the input feature space to the output feature space was proposed by Cortes et al. (2005). In this setting, predictions in the original output space are retrieved by solving a pre-image problem. Interestingly, the idea of Output Kernel Regression can be implemented without defining an input kernel as it is shown with Output Kernel Tree-based methods (Geurts et al., 2006, 2007a,b). In these approaches, a regression tree whose outputs are linear combinations of the training outputs in the output feature space is built using the kernel trick in the output space: the loss function which is locally minimized during the construction only involves inner products between training outputs. These methods are not limited to discrete output sets and they do not require expensive computations to make a prediction nor to train the model. Combined in ensembles such as random forests and boosting, they exhibit excellent performances. However these tree-based approaches suffer from two drawbacks: trees do not take into account structured input data except by using a flat description of them and the associated (greedy) building algorithm cannot be easily extended to semi-supervised learning.

In this work, we therefore propose to extend the methodology of Output Kernel Regression to another large family of nonparametric regression tools that allows to tackle structured data in the input space as well as in the output space. Moreover we will show that this new family of tools is useful in a semi-supervised context. Called Input Output Kernel Regression, this novel family for structured output prediction from structured inputs relies on Reproducing Kernel Hilbert Spaces (RKHS) for vector-valued functions with the following specification: the output vector belongs to some output feature space associated to a chosen output kernel, as introduced in the works of Brouard et al. (2011) and Brouard (2013). Let us recall that in the case of scalar-valued functions, the RKHS theory offers a flexible framework for penalized regression as witnessed by the abundant literature on the subject (Wahba, 1990; Pearce and Wand, 2006). A penalized regression problem is seen as a minimization problem in a functional space built on an input scalar-valued kernel. Depending the nature of the prediction problem, appropriate penalties can be defined and representer theorem can be proven, facilitating the minimization problem to be further solved. In the RKHS theory, regularization constraint on the geometry of the probability distribution of labeled and unlabeled data can also be added to perform semi-supervised regression (Belkin et al., 2006). When functions are vector-valued, the adequate RKHS theory makes use of operator-valued kernels (Pedrick, 1957; Senkane and Tempel'man, 1973; Micchelli and Pontil, 2005). Operator-valued kernels have already been proposed to solve problems of multi-task regression (Evgeniou et al., 2005; Baldassarre et al., 2012), structured classification (Dinuzzo et al., 2011), vector autoregression (Lim et al., 2013) as well as functional regression (Kadri et al., 2010). The originality of this work is to consider that the output space is a feature space associated to a chosen output kernel. This new approach not only enhances setting of pattern recognition tasks by requiring to pay attention on both input and output sets but also opens new perspectives in machine learning. It encompasses in a unique framework kernel-based regression tools devoted to structured inputs as well as structured outputs.

1.1 Related Works

In Brouard et al. (2011), the vector-valued RKHS theory was used to address the output kernel regression problem in the semi-supervised setting. This approach was applied to the link prediction problem. By working in the framework of RKHS theory for vector-valued functions, we extended the manifold regularization framework introduced by Belkin et al. (2006) to functions with values in a Hilbert space. We have also shown that the first step of KDE (Cortes et al., 2005) is a special case of IOKR using a particular operator-valued kernel.

Kadri et al. (2013) studied a formulation of KDE using operator-valued kernels. The first step of this approach is identical to the IOKR framework developed in Brouard et al. (2011) and Brouard (2013). The second step consists in extending the pre-image step of KDE using the vector-valued RKHS theory. They also proposed two covariance-based operator-valued kernels and showed that using these operator-valued kernels allow to express the pre-image problem using only input and output Gram matrices.

In parallel of Brouard et al. (2011), Minh and Sindhvani (2011) generalized the manifold regularization framework proposed by Belkin et al. (2006) for semi-supervised learning to vector-valued functions.

1.2 Contributions

We introduce Input Output Kernel Regression (IOKR), a novel class of penalized regression problems based on the definition of an output scalar-valued kernel and an input operator-valued kernel. This article is an extended version of Brouard et al. (2011), that addresses more generally the problem of structured output prediction. In this work, we present several novel contributions regarding the RKHS theory for functions with values in a Hilbert space. We present the representer theorem for vector-valued functions in the semi-supervised setting. Based on this representer theorem, we study two particular models obtained using two different loss functions: the *IOKR-ridge* model introduced in Brouard et al. (2011) and a new model called *IOKR-margin*. This model extends the Maximum Margin Regression (MMR) framework introduced by Szedmak et al. (2005) to operator-valued kernels and to the semi-supervised setting. In this paper, we also put the reformulation of Kernel Dependency Estimation proposed by Cortes et al. (2005) into perspective in the Output Kernel Regression framework. We present the solutions corresponding to decomposable kernels. In the case of the least-squared loss function, we describe a new tool for model selection, which was first introduced in Brouard (2013). The selection of the hyperparameters is done by estimating the averaged error obtained with leave-one-out cross-validation as a closed-form solution. We show the versatility of the IOKR framework on two different problems: link prediction and multi-task regression. Finally, we present numerical results obtained with IOKR on these two tasks.

1.3 Organization of the Paper

This paper is organized as follows. In Section 2, we introduce the Input Output Kernel Regression approach and show how it can be used to solve structured output prediction problems. In Section 3 we describe the RKHS theory devoted to vector-valued function and present our contributions to this theory in the supervised and semi-supervised settings. We also present in this section models based on decomposable operator-valued kernels. We then show in Section 4 that, in the case of the least-squares loss function, the leave-one-out criterion can be estimated by a closed-form solution. In Section 5, we describe how Input Output Kernel Regression (IOKR) can be used to solve two structured prediction problems, which are link prediction and multi-task learning. In Section 6, we present the results obtained with IOKR on these two problems.

The notations used in this paper are summarized in Table 1.

2. From Output Kernel Regression to Input Output Kernel Regression

We consider the general regression task consisting in learning a mapping between an input set \mathcal{X} and an output set \mathcal{Y} . We assume that both \mathcal{X} and \mathcal{Y} are sample spaces and that $\mathcal{S}_n = \{(x_i, y_i), i = 1 \dots n\}$ is an i.i.d. sample drawn from the joint probability law \mathcal{P} defined on $\mathcal{X} \times \mathcal{Y}$. Outputs are supposed to be structured, for example objects such as sequences,

Meaning	Symbol
number of labeled examples	ℓ
number of unlabeled examples	n
input set	\mathcal{X}
set of labeled examples	\mathcal{X}_ℓ
union of the labeled and unlabeled sets	$\mathcal{X}_{\ell+n}$
output set	\mathcal{Y}
input scalar kernel	$\kappa_x : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$
output scalar kernel	$\kappa_y : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$
input feature space	\mathcal{F}_x
output feature space	\mathcal{F}_y
input feature map	$\varphi_x : \mathcal{X} \rightarrow \mathcal{F}_x$
output feature map	$\varphi_y : \mathcal{Y} \rightarrow \mathcal{F}_y$
set of bounded operators from an Hilbert space \mathcal{F} to itself	$\mathcal{B}(\mathcal{F})$
set of bounded operators from \mathcal{F} to an Hilbert space \mathcal{G}	$\mathcal{B}(\mathcal{F}, \mathcal{G})$
operator-valued kernel	$\mathcal{K}_x : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{B}(\mathcal{F}_y)$
reproducing kernel Hilbert space of \mathcal{K}_x	$\mathcal{H}, \mathcal{H}_{\mathcal{K}_x}$
canonical feature map of \mathcal{K}_x	$\phi_x : \mathcal{X} \rightarrow \mathcal{B}(\mathcal{F}_y, \mathcal{H})$
gram matrix of \mathcal{K}_x on \mathcal{X}_ℓ and $\mathcal{X}_{\ell+n}$	$\mathbf{K}_{X_\ell}, \mathbf{K}_{X_{\ell+n}}$
gram matrix of κ_x on \mathcal{X}_ℓ and $\mathcal{X}_{\ell+n}$	$K_{X_\ell}, K_{X_{\ell+n}}$
gram matrix of κ_y on \mathcal{Y}_ℓ	K_{Y_ℓ}
graph Laplacian	L
matrix vectorization	vec
Kronecker product	\otimes
Hadamard product (element-wise product)	\circ

Table 1: Notations used in this paper

graphs, nodes in a graph, or simply vectors of interdependent variables. It is realistic to assume that one can build a similarity $\kappa_y : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ between the elements of the output set \mathcal{Y} , such that κ_y takes into account the inherent structure of the elements of \mathcal{Y} and has the properties of a positive definite kernel. Then, due to the Moore-Aronszajn theorem (Aronszajn, 1950), there exists a Hilbert space \mathcal{F}_y , called a *feature space*, and a corresponding function $\varphi_y : \mathcal{Y} \rightarrow \mathcal{F}_y$, called a *feature map* such that:

$$\forall (y, y') \in \mathcal{Y} \times \mathcal{Y}, \kappa_y(y, y') = \langle \varphi_y(y), \varphi_y(y') \rangle_{\mathcal{F}_y}.$$

The regression problem between \mathcal{X} and \mathcal{Y} can be decomposed into two tasks (see Figure 1):

- the first task is to learn a function h from the set \mathcal{X} to the Hilbert space \mathcal{F}_y
- the second one is to define or learn a function f from \mathcal{F}_y to \mathcal{Y} to provide an output in the set \mathcal{Y} .

We call the first task, *Output Kernel Regression* (OKR), referring to previous works based on Output Kernel Trees (OK3) (Geurts et al., 2006, 2007a) and the second task, a

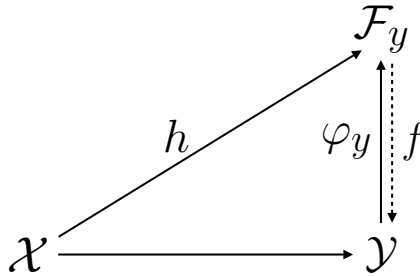


Figure 1: Schema of the Output Kernel Regression approach.

pre-image problem. In this paper, we develop a general theoretical and practical framework for the OKR task, allowing to deal with structured inputs as well as structured outputs. To illustrate our approach, we have chosen two structured output learning tasks which do not require to solve a pre-image problem. One is *multi-task regression* for which the dimension of the output feature space is finite, and the other one is *link prediction* for which prediction in the original set \mathcal{Y} is not required. However, the approach we propose can be combined with pre-image solvers now available on the shelves. The interested reader may want to refer to Honeine and Richard (2011) or Kadri et al. (2013) to benefit from existing pre-image algorithms to solve structured output learning tasks.

In this work, we propose to build a family of models and learning algorithms devoted to *Output Kernel Regression* that present two additional properties compared to OK3-based methods: namely, models are able to take into account structure in input data and can be learned within the framework of penalized regression, enjoying various penalties including smoothness penalties for semi-supervised learning. To achieve this goal, we choose to use kernels both in the input and output spaces. As the models have values in a feature space and not in \mathbb{R} , we turn to the vector-valued reproducing kernel Hilbert spaces theory (Pedrick, 1957; Senkne and Tempel'man, 1973; Burbea and Masani, 1984) to provide a general framework for penalized regression of nonparametric vector-valued functions. In that theory, the values of kernels are operators on the output vectors which belong to some Hilbert space. Introduced in machine learning by the seminal work of Micchelli and Pontil (2005) to solve multi-task regression problems, operator-valued kernels (OVK) have then been studied under the angle of their universality (Caponnetto et al. (2008); Carmeli et al. (2010)) and developed in different contexts such as structured classification (Dinuzzo et al., 2011), functional regression (Kadri et al., 2010), link prediction (Brouard et al., 2011) or semi-supervised learning (Minh and Sindhwani, 2011; Brouard et al., 2011). With operator-valued kernels, models of the following form can be constructed:

$$\forall x \in \mathcal{X}, h(x) = \sum_{i=1}^n \mathcal{K}_x(x, x_i) \mathbf{c}_i, \quad \mathbf{c}_i \in \mathcal{F}_y, x_i \in \mathcal{X}, \quad (1)$$

extending nicely the usual kernel-based models devoted to real-valued functions.

In the case of IOKR, the output Hilbert space \mathcal{F}_y is defined as a feature space related to a given output kernel. Note that there exists different pairs (feature space, feature map) associated with a given kernel κ_y . Let us take for instance the polynomial kernel

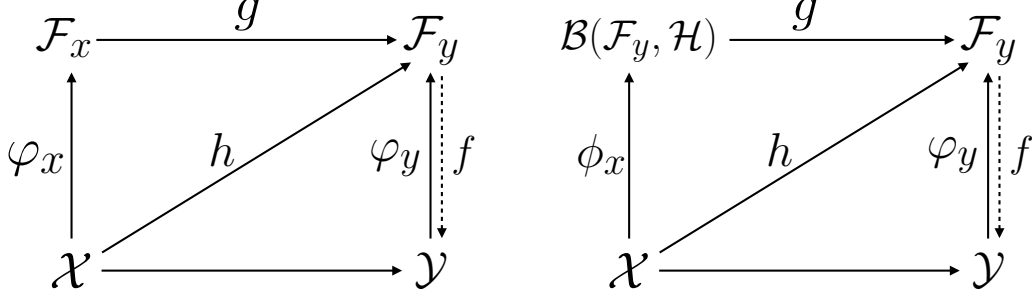


Figure 2: Diagrams describing Kernel Dependency Estimation (KDE) on the left and Input Output Kernel Regression (IOKR) on the right.

$\kappa_y(y, y') = (y^T y' + c)^p$: we can choose the finite feature space defined by the different monomes of the coordinates of a vector \mathbf{y} or we can choose the RKHS associated with the polynomial kernel. This choice will open doors to different output feature spaces \mathcal{F}_y , leading to different definitions of the input operator-valued kernel \mathcal{K}_x and thus to different learning problems. Omitting the choice of the feature map associated to \mathcal{F}_y , we therefore need to define a triplet $(\kappa_y, \mathcal{F}_y, \mathcal{K}_x)$ as a pre-requisite to solve the structured output learning task. By explicitly requiring to define an output kernel we emphasize the fact that an input operator-valued kernel cannot be defined without calling into question the output space, \mathcal{F}_y , and therefore, the output kernel κ_y . We will show in Section 6 that the same structured output prediction problem can be solved in different ways using different values for the triplet $(\kappa_y, \mathcal{F}_y, \mathcal{K}_x)$.

Interestingly, IOKR generalizes Kernel Dependency Estimation (KDE), a problem that was introduced in Weston et al. (2003) and was reformulated in a more general way by Cortes et al. (2005). If we call \mathcal{F}_x a feature space associated to a scalar input kernel $\kappa_x : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ and $\varphi_x : \mathcal{X} \rightarrow \mathcal{F}_x$ a corresponding feature map, KDE uses Kernel Ridge regression to learn a function h from \mathcal{X} to \mathcal{F}_y by building a function g from \mathcal{F}_x to \mathcal{F}_y and composing it with the feature map φ_x (see Figure 2). The function h is modeled as a linear function: $h(x) = W\varphi_x(x)$, where W is a linear operator from \mathcal{F}_x to \mathcal{F}_y . The second phase consists in computing the pre-image of the obtained prediction.

In the case of IOKR, we build models of the general form introduced in Equation (1). Denoting ϕ_x the canonical feature map associated to the OVK \mathcal{K}_x , which is defined as: $\phi_x(x) = \mathcal{K}_x(\cdot, x)$, we can draw the chart depicted in Figure 2 on the right. The function ϕ_x maps inputs from \mathcal{X} to $\mathcal{B}(\mathcal{F}_y, \mathcal{H})$. Indeed the value $\phi_x(x)y = \mathcal{K}_x(\cdot, x)y$ is a function of the RKHS \mathcal{H} for all y in \mathcal{F}_y . The model h is seen as the composition of a function g from $\mathcal{B}(\mathcal{F}_y, \mathcal{H})$ to the output feature space \mathcal{F}_y with the input feature map ϕ_x .

We can therefore see on Figure 2 how IOKR extends KDE. In Brouard et al. (2011), we have shown that we retrieve the model used in KDE when considering the following operator-valued kernel:

$$\mathcal{K}_x(x, x') = \kappa_x(x, x')I, \quad (2)$$

where I is the identity operator from \mathcal{F}_y to \mathcal{F}_y . Unlike KDE, that learns independently each component of the vectors $\varphi_y(y)$, IOKR takes into account the structure existing between these components.

The next section is devoted to the RKHS theory for vector-valued functions and to our contributions to this theory in the supervised and semi-supervised settings.

3. Operator-Valued Kernel Regression

In the following, we briefly recall the main elements of the RKHS theory devoted to vector-valued functions (Senkane and Tempel'man, 1973; Micchelli and Pontil, 2005) and then present our contributions to this theory.

Let \mathcal{X} be a set and \mathcal{F}_y a Hilbert space. In this section, no assumption is needed about the existence of an output kernel κ_y . We note $\tilde{\mathbf{y}}$ the vectors in \mathcal{F}_y . Given two Hilbert spaces \mathcal{F} and \mathcal{G} , we note $\mathcal{B}(\mathcal{F}, \mathcal{G})$ the set of bounded operators from \mathcal{F} to \mathcal{G} and $\mathcal{B}(\mathcal{F})$ the set of bounded operators from \mathcal{F} to itself. Given an operator A , A^* denotes the adjoint of A .

Definition 1 *An operator-valued kernel on $\mathcal{X} \times \mathcal{X}$ is a function $\mathcal{K}_x : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{B}(\mathcal{F}_y)$ that verifies the two following conditions:*

- $\forall (x, x') \in \mathcal{X} \times \mathcal{X}, \mathcal{K}_x(x, x') = \mathcal{K}_x(x', x)^*$,
- $\forall m \in \mathbb{N}, \forall \mathcal{S}_m = \{(x_i, \tilde{\mathbf{y}}_i)\}_{i=1}^m \subseteq \mathcal{X} \times \mathcal{F}_y, \sum_{i,j=1}^m \langle \tilde{\mathbf{y}}_i, \mathcal{K}_x(x_i, x_j) \tilde{\mathbf{y}}_j \rangle_{\mathcal{F}_y} \geq 0$.

The following theorem shows that given any operator-valued kernel, it is possible to build a reproducing kernel Hilbert space associated to this kernel.

Theorem 2 (Senkane and Tempel'man (1973); Micchelli and Pontil (2005))

Given an operator-valued kernel $\mathcal{K}_x : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{B}(\mathcal{F}_y)$, there is a unique Hilbert space $\mathcal{H}_{\mathcal{K}_x}$ of functions $h : \mathcal{X} \rightarrow \mathcal{F}_y$ which satisfies the following reproducing property:

$$\forall h \in \mathcal{H}_{\mathcal{K}_x}, \forall x \in \mathcal{X}, h(x) = \mathcal{K}_x(x, \cdot)h,$$

where $\mathcal{K}_x(x, \cdot)$ is an operator in $\mathcal{B}(\mathcal{H}_{\mathcal{K}_x}, \mathcal{F}_y)$.

As a consequence, $\forall x \in \mathcal{X}, \forall \tilde{\mathbf{y}} \in \mathcal{F}_y, \forall h \in \mathcal{H}_{\mathcal{K}_x}, \langle \mathcal{K}_x(\cdot, x) \tilde{\mathbf{y}}, h \rangle_{\mathcal{H}_{\mathcal{K}_x}} = \langle \tilde{\mathbf{y}}, h(x) \rangle_{\mathcal{F}_y}$.

The Hilbert space $\mathcal{H}_{\mathcal{K}_x}$ is called the reproducing kernel Hilbert space associated to the kernel \mathcal{K}_x . This RKHS can be built by taking the closure of $\text{span}\{\mathcal{K}_x(\cdot, x)\alpha \mid x \in \mathcal{X}, \alpha \in \mathcal{F}_y\}$. The scalar product on $\mathcal{H}_{\mathcal{K}_x}$ between two functions $f = \sum_{i=1}^n \mathcal{K}_x(\cdot, x_i)\alpha_i$ and $g = \sum_{j=1}^m \mathcal{K}_x(\cdot, t_j)\beta_j$, $x_i, t_j \in \mathcal{X}, \alpha_i, \beta_j \in \mathcal{F}_y$, is defined as:

$$\langle f, g \rangle_{\mathcal{H}_{\mathcal{K}_x}} = \sum_{i=1}^n \sum_{j=1}^m \langle \alpha_i, \mathcal{K}_x(x_i, t_j) \beta_j \rangle_{\mathcal{F}_y}.$$

The corresponding norm $\|\cdot\|_{\mathcal{H}_{\mathcal{K}_x}}$ is defined by $\|f\|_{\mathcal{H}_{\mathcal{K}_x}}^2 = \langle f, f \rangle_{\mathcal{H}_{\mathcal{K}_x}}$. For sake of simplicity we replace the notation $\mathcal{H}_{\mathcal{K}_x}$ by \mathcal{H} in the rest of the paper.

As for scalar-valued functions, one of the most appealing feature of RKHS is to provide a theoretical framework for regularization with the representer theorems.

3.1 Regularization in Vector-Valued RKHS

Based on the RKHS theory for vector-valued functions, Micchelli and Pontil (2005) have proved a representer theorem for convex loss functions in the supervised case.

We note $S_\ell = \{(x_i, \tilde{\mathbf{y}}_i)\}_{i=1}^\ell \subseteq \mathcal{X} \times \mathcal{F}_y$ the set of labeled examples and \mathcal{H} the RKHS with reproducing kernel $\mathcal{K}_x : \mathcal{X} \times \mathcal{X} \rightarrow \mathcal{B}(\mathcal{F}_y)$.

Theorem 3 (Micchelli and Pontil (2005)) *Let \mathcal{L} be a convex loss function, and $\lambda_1 > 0$ a regularization parameter. The minimizer of the following optimization problem:*

$$\operatorname{argmin}_{h \in \mathcal{H}} \mathcal{J}(h) = \sum_{i=1}^{\ell} \mathcal{L}(h(x_i), \tilde{\mathbf{y}}_i) + \lambda_1 \|h\|_{\mathcal{H}}^2 ,$$

admits an expansion:

$$\hat{h}(\cdot) = \sum_{j=1}^{\ell} \mathcal{K}_x(\cdot, x_j) \mathbf{c}_j ,$$

where the coefficients $\mathbf{c}_j, j = 1, \dots, \ell$ are vectors in the Hilbert space \mathcal{F}_y .

In the following, we plug the expansion form of the minimizer into the optimization problem and consider the problem of finding the coefficients \mathbf{c}_j for two different loss functions: the least-squares loss and the hinge loss.

3.1.1 PENALIZED LEAST SQUARES

Considering the least-squares loss function for regularization of vector-valued functions, the minimization problem becomes:

$$\operatorname{argmin}_{h \in \mathcal{H}} \mathcal{J}(h) = \sum_{i=1}^{\ell} \|h(x_i) - \tilde{\mathbf{y}}_i\|_{\mathcal{F}_y}^2 + \lambda_1 \|h\|_{\mathcal{H}}^2 . \quad (3)$$

Theorem 4 (Micchelli and Pontil (2005)) *Let $\mathbf{c}_j \in \mathcal{F}_y, j = 1, \dots, \ell$, be the coefficients of the expansion admitted by the minimizer \hat{h} of the optimization problem in Equation (3). The vectors $\mathbf{c}_j \in \mathcal{F}_y$ satisfy the equations:*

$$\sum_{i=1}^{\ell} (\mathcal{K}_x(x_j, x_i) + \lambda_1 \delta_{ij}) \mathbf{c}_i = \tilde{\mathbf{y}}_j ,$$

where δ is the Kronecker symbol: $\delta_{ii} = 1$ and $\forall j \neq i, \delta_{ij} = 0$.

Let $\mathbf{c} = (\mathbf{c}_j)_{j=1}^\ell \in \mathcal{F}_y^\ell$ and $\tilde{\mathbf{y}} = (\tilde{\mathbf{y}}_j)_{j=1}^\ell \in \mathcal{F}_y^\ell$. This system of equations can be equivalently written (Micchelli and Pontil, 2005):

$$(S_{X_\ell} S_{X_\ell}^* + \lambda_1 I) \mathbf{c} = \tilde{\mathbf{y}},$$

where I denotes the identity operator from \mathcal{F}_y^ℓ to \mathcal{F}_y^ℓ and $S_{X_\ell} : \mathcal{H} \rightarrow \mathcal{F}_y^\ell$ is the sampling operator defined for every $h \in \mathcal{H}$ by: $S_{X_\ell} h = (h(x_i))_{i=1}^\ell$. The expression of its adjoint $S_{X_\ell}^* : \mathcal{F}_y^\ell \rightarrow \mathcal{H}$ of S_{X_ℓ} for every $\mathbf{c} \in \mathcal{F}_y^\ell$ is given by: $S_{X_\ell}^* \mathbf{c} = \sum_{i=1}^\ell \mathcal{K}_x(\cdot, x_i) \mathbf{c}_i$. Therefore the solution of the optimization problem in Equation (3) writes as:

$$h_{\text{ridge}}(x) = \mathcal{K}_x(x, \cdot) S_{X_\ell}^* (S_{X_\ell} S_{X_\ell}^* + \lambda_1 I)^{-1} \tilde{\mathbf{y}}.$$

3.1.2 MAXIMUM MARGIN REGRESSION

Szedmak et al. (2005) formulated a Support Vector Machine algorithm with vector output, called Maximum Margin Regression (MMR). The optimization problem of MMR in the supervised setting is the following:

$$\operatorname{argmin}_h \mathcal{J}(h) = \sum_{i=1}^{\ell} \max(0, 1 - \langle \tilde{\mathbf{y}}_i, h(x_i) \rangle_{\mathcal{F}_y}) + \lambda_1 \|h\|_{\mathcal{H}}^2. \quad (4)$$

In Szedmak et al. (2005), the function h was modeled as: $h(x) = W\varphi_x(x) + b$, where φ_x is a feature map associated to a scalar-valued kernel. In this subsection, we extend this maximum margin based regression framework to the context of the vector-valued RKHS theory by searching h in the RKHS \mathcal{H} associated to \mathcal{K}_x .

Similarly to SVM, the MMR problem (4) can be expressed according to a primal formulation that involves the optimization of $h \in \mathcal{H}$ and slack variables $\xi_i \in \mathbb{R}$, $i = 1, \dots, \ell$, as well as its dual formulation which is expressed according to the Lagrangian parameters $\boldsymbol{\alpha} = [\alpha_1, \dots, \alpha_\ell]^T \in \mathbb{R}^\ell$. The latter leads to solve a quadratic program, for which efficient solvers exist. Both formulations are given below.

The primal form of the MMR optimization problem can be written as:

$$\begin{aligned} \min_{h \in \mathcal{H}, \{\xi_i \in \mathbb{R}\}_{i=1}^{\ell}} \quad & \lambda_1 \|h\|_{\mathcal{H}}^2 + \sum_{i=1}^{\ell} \xi_i \\ \text{s.t.} \quad & \langle \tilde{\mathbf{y}}_i, h(x_i) \rangle_{\mathcal{F}_y} \geq 1 - \xi_i, i = 1, \dots, \ell \\ & \xi_i \geq 0, i = 1, \dots, \ell. \end{aligned}$$

The Lagrangian of the above problem is given by:

$$\mathcal{L}_a(h, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\eta}) = \lambda_1 \|h\|_{\mathcal{H}}^2 + \sum_{i=1}^{\ell} \xi_i - \sum_{i=1}^{\ell} \alpha_i (\langle \mathcal{K}_x(\cdot, x_i) \tilde{\mathbf{y}}_i, h \rangle_{\mathcal{H}} - 1 + \xi_i) - \sum_{i=1}^{\ell} \eta_i \xi_i,$$

with α_i and η_i being Lagrange multipliers. By differentiating the Lagrangian with respect to ξ_i and h and setting the derivatives to zero, the dual form of the optimization problem can be expressed as:

$$\begin{aligned} \min_{\boldsymbol{\alpha} \in \mathbb{R}^\ell} \quad & \frac{1}{4\lambda_1} \sum_{i,j=1}^{\ell} \alpha_i \alpha_j \langle \tilde{\mathbf{y}}_i, \mathcal{K}_x(x_i, x_j) \tilde{\mathbf{y}}_j \rangle_{\mathcal{F}_y} - \sum_{i=1}^{\ell} \alpha_i \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq 1, i = 1, \dots, \ell \end{aligned} \quad (5)$$

and the solution \hat{h} can be written as: $\hat{h}(\cdot) = \frac{1}{2\lambda_1} \sum_{j=1}^{\ell} \alpha_j \mathcal{K}_x(\cdot, x_j) \tilde{\mathbf{y}}_j$. Note that, similarly to KDE, we retrieve the original MMR solution when using the following operator-valued kernel: $\mathcal{K}_x(x, x') = \kappa_x(x, x') I$.

In Appendix B, we derive the dual optimization problem for a general convex loss function using the Fenchel duality.

3.2 Extension to Semi-Supervised Learning

In the case of real-valued functions, Belkin et al. (2006) have introduced a novel framework, called *manifold regularization*. This approach is based on the assumption that the data lie in a low-dimensional manifold. Belkin et al. (2006) have proved a representer theorem devoted to semi-supervised learning by adding a new regularization term which exploits the information of the geometric structure. This regularization term forces the target function h to be smooth with respect to the underlying manifold. In general, the geometry of this manifold is not known but it can be approximated by a graph. In this graph, nodes correspond to labeled and unlabeled data and edges reflect the local similarities between data in the input space. For example, this graph can be built using k -nearest neighbors. The representer theorem of Belkin et al. (2006) has been extended to the case of vector-valued functions in Brouard et al. (2011) and Minh and Sindhwani (2011). In the following, we present this theorem and derive the solutions for the least-squares loss function and maximum margin regression.

Let \mathcal{L} be a convex loss function. Given a set of ℓ labeled examples $\{(x_i, \tilde{\mathbf{y}}_i)\}_{i=1}^{\ell} \subseteq \mathcal{X} \times \mathcal{F}_y$ and an additional set of n unlabeled examples $\{x_i\}_{i=\ell+1}^{\ell+n} \subseteq \mathcal{X}$, we consider the following optimization problem:

$$\operatorname{argmin}_{h \in \mathcal{H}} \mathcal{J}(h) = \sum_{i=1}^{\ell} \mathcal{L}(h(x_i), \tilde{\mathbf{y}}_i) + \lambda_1 \|h\|_{\mathcal{H}}^2 + \lambda_2 \sum_{i,j=1}^{\ell+n} W_{ij} \|h(x_i) - h(x_j)\|_{\mathcal{F}_y}^2, \quad (6)$$

where $\lambda_1, \lambda_2 > 0$ are two regularization hyperparameters and W is the adjacency matrix of a graph built from labeled and unlabeled data. This matrix measures the similarity between objects in the input space. We assume that the values of W are non-negative. This optimization problem can be rewritten as:

$$\operatorname{argmin}_{h \in \mathcal{H}} \mathcal{J}(h) = \sum_{i=1}^{\ell} \mathcal{L}(h(x_i), \tilde{\mathbf{y}}_i) + \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h(x_i), h(x_j) \rangle_{\mathcal{F}_y},$$

where L is the graph Laplacian given by $L = D - W$, and D is the diagonal matrix of general term $D_{ii} = \sum_{j=1}^{\ell+n} W_{ij}$. Instead of the graph Laplacian, other matrices, such as iterated Laplacians or diffusion kernels (Kondor and Lafferty, 2002), can also be used.

Theorem 5 (Brouard et al. (2011); Minh and Sindhwani (2011)) *The minimizer of the optimization problem in Equation (6) admits an expansion:*

$$\hat{h}(\cdot) = \sum_{j=1}^{\ell+n} \mathcal{K}_x(\cdot, x_j) \mathbf{c}_j,$$

for some vectors $\mathbf{c}_j \in \mathcal{F}_y, j = 1, \dots, \ell + n$.

This theorem extends the representer theorem proposed by Belkin et al. (2006) to vector-valued functions. Besides, it also extends Theorem 3 to the semi-supervised framework.

3.2.1 SEMI-SUPERVISED PENALIZED LEAST-SQUARES

Considering the least-squares cost, the optimization problem becomes:

$$\operatorname{argmin}_{h \in \mathcal{H}} \mathcal{J}(h) = \sum_{i=1}^{\ell} \|h(x_i) - \tilde{\mathbf{y}}_i\|_{\mathcal{F}_y}^2 + \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h(x_i), h(x_j) \rangle_{\mathcal{F}_y}. \quad (7)$$

Theorem 6 (Brouard et al. (2011); Minh and Sindhwani (2011)) *The coefficients $\mathbf{c}_j \in \mathcal{F}_y, j = 1, \dots, \ell + n$ of the expansion admitted by the minimizer \hat{h} of the optimization problem (7) satisfy this equation:*

$$J_j \sum_{i=1}^{\ell+n} \mathcal{K}_x(x_j, x_i) \mathbf{c}_i + \lambda_1 \mathbf{c}_j + 2\lambda_2 \sum_{i=1}^{\ell+n} L_{ij} \sum_{m=1}^{\ell+n} \mathcal{K}_x(x_i, x_m) \mathbf{c}_m = J_j \tilde{\mathbf{y}}_j,$$

where $J_j \in \mathcal{B}(\mathcal{F}_y)$ is the identity operator if $j \leq \ell$ and the null operator if $\ell < j \leq (\ell + n)$.

For the proofs of Theorems 5 and 6, the reader can refer to the proofs given in the supplementary materials of Brouard et al. (2011) or Minh and Sindhwani (2011).

As in the supervised setting, the solution of the optimization problem (7) can be expressed using the sampling operator:

$$h_{\text{ridge}}(x) = \mathcal{K}_x(x, \cdot) S_{X_{\ell+n}}^* (J J^* S_{X_{\ell+n}} S_{X_{\ell+n}}^* + \lambda_1 I + 2\lambda_2 M S_{X_{\ell+n}} S_{X_{\ell+n}}^*)^{-1} J \tilde{\mathbf{y}},$$

where the operator $J \in \mathcal{B}(\mathcal{F}_y^\ell, \mathcal{F}_y^{\ell+n})$ is defined for every $\mathbf{c} = (\mathbf{c}_j)_{j=1}^{\ell+n} \in \mathcal{F}_y^\ell$ as: $J\mathbf{c} = (\mathbf{c}_1, \dots, \mathbf{c}_\ell, \mathbf{0}, \dots, \mathbf{0})$. Its adjoint is defined as: $J^*(\mathbf{c}_j)_{j=1}^{\ell+n} = (\mathbf{c}_j)_{j=1}^\ell$. M is an operator in $\mathcal{B}(\mathcal{F}_y^{\ell+n})$ and each $M_{ij}, i, j \in \mathbb{N}^{\ell+n}$ is an operator in $\mathcal{B}(\mathcal{F}_y)$ equal to $L_{ij}I$.

3.2.2 SEMI-SUPERVISED MAXIMUM MARGIN REGRESSION

The optimization problem in the semi-supervised case using the hinge loss is the following:

$$\operatorname{argmin}_{h \in \mathcal{H}} \mathcal{J}(h) = \sum_{i=1}^{\ell} \max(0, 1 - \langle \tilde{\mathbf{y}}_i, h(x_i) \rangle_{\mathcal{F}_y}) + \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h(x_i), h(x_j) \rangle_{\mathcal{F}_y}. \quad (8)$$

Theorem 7 *The solution of the optimization problem (8) is given by*

$$h(\cdot) = \frac{1}{2} B^{-1} \left(\sum_{i=1}^{\ell} \alpha_i \mathcal{K}_x(\cdot, x_i) \tilde{\mathbf{y}}_i \right),$$

where $B = \lambda_1 I + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \mathcal{K}_x(\cdot, x_i) \mathcal{K}_x(x_j, \cdot)$ is an operator from \mathcal{H} to \mathcal{H} , and α is the solution of

$$\begin{aligned} \min_{\alpha \in \mathbb{R}^\ell} \quad & \frac{1}{4} \sum_{i,j=1}^{\ell} \alpha_i \alpha_j \langle \mathcal{K}_x(\cdot, x_i) \tilde{\mathbf{y}}_i, B^{-1} \mathcal{K}_x(\cdot, x_j) \tilde{\mathbf{y}}_j \rangle_{\mathcal{H}} - \sum_{i=1}^{\ell} \alpha_i \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq 1, i = 1, \dots, \ell. \end{aligned} \quad (9)$$

The proof of this theorem is detailed in Appendix A.

3.3 Solutions when $\mathcal{F}_y = \mathbb{R}^d$

In this subsection we consider that the dimension of \mathcal{F}_y is finite and equal to d . We first introduce the following notations:

- $\tilde{Y}_\ell = (\tilde{y}_1, \dots, \tilde{y}_\ell)$ is a matrix of size $d \times \ell$,
- $C_\ell = (\mathbf{c}_1, \dots, \mathbf{c}_\ell)$, $C_{\ell+n} = (\mathbf{c}_1, \dots, \mathbf{c}_{\ell+n})$,
- $\mathcal{K}_{X_\ell}^x = (\mathcal{K}_x(x_1, x), \dots, \mathcal{K}_x(x_\ell, x))^T$, $\mathcal{K}_{X_{\ell+n}}^x = (\mathcal{K}_x(x_1, x), \dots, \mathcal{K}_x(x_{\ell+n}, x))^T$,
- \mathbf{K}_{X_ℓ} is a $\ell \times \ell$ block matrix, where each block is a $d \times d$ matrix. The (j, k) -th block of \mathbf{K}_{X_ℓ} is equal to $\mathcal{K}_x(x_j, x_k)$,
- $\mathbf{K}_{X_{\ell+n}}$ is a $(\ell + n) \times (\ell + n)$ block matrix such that the (j, k) -th block of $\mathbf{K}_{X_{\ell+n}}$ is equal to $\mathcal{K}_x(x_j, x_k)$,
- $I_{\ell d}$ and $I_{(\ell+n)d}$ are identity matrices of size $(\ell d) \times (\ell d)$ and $(\ell + n)d \times (\ell + n)d$,
- $J = (I_\ell, 0)$ is a $\ell \times (\ell + n)$ matrix that contains an identity matrix of size $\ell \times \ell$ on the left hand side and a zero matrix of size $\ell \times n$ on the right hand side,
- \otimes denotes the Kronecker product and $\text{vec}(A)$ denotes the vectorization of a matrix A , formed by stacking the columns of A into a single column vector.

In the supervised setting, the solutions for the least-squares loss and MMR can be rewritten as $h(x) = (\mathcal{K}_{X_\ell}^x)^T C_\ell$, where C_ℓ is given by:

$$\begin{aligned} C_{\ell_{ridge}} &= (\lambda_1 I_{\ell d} + \mathbf{K}_{X_\ell})^{-1} \text{vec}(\tilde{Y}_\ell), \\ C_{\ell_{mmr}} &= \frac{1}{2\lambda_1} \text{vec}(\tilde{Y}_\ell \text{diag}(\boldsymbol{\alpha})). \end{aligned}$$

In the semi-supervised setting, these solutions can be written as $h(x) = (\mathcal{K}_{X_{\ell+n}}^x)^T C_{\ell+n}$ where:

$$\begin{aligned} C_{\ell+n_{ridge}} &= (\lambda_1 I_{(\ell+n)d} + ((J^T J + 2\lambda_2 L) \otimes I_d) \mathbf{K}_{X_{\ell+n}})^{-1} \text{vec}(\tilde{Y}_\ell J), \\ C_{\ell+n_{mmr}} &= (2\lambda_1 I_{(\ell+n)d} + 4\lambda_2 (L \otimes I_d) \mathbf{K}_{X_{\ell+n}})^{-1} \text{vec}(\tilde{Y}_\ell \text{diag}(\boldsymbol{\alpha}) J). \end{aligned}$$

For MMR, the vector $\boldsymbol{\alpha}$ is obtained by solving the following optimization problem:

$$\begin{aligned} \min_{\boldsymbol{\alpha} \in \mathbb{R}^\ell} \quad & \frac{1}{4} \text{vec} \left(\tilde{Y}_\ell \text{diag}(\boldsymbol{\alpha}) J \right)^T \\ & \left(\lambda_1 I_{(\ell+n)d} + 2\lambda_2 \mathbf{K}_{X_{\ell+n}} (L \otimes I_d) \right)^{-1} \mathbf{K}_{X_{\ell+n}} \text{vec} \left(\tilde{Y}_\ell \text{diag}(\boldsymbol{\alpha}) J \right) - \boldsymbol{\alpha}^T \mathbf{1} \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq 1, i = 1, \dots, \ell. \end{aligned} \tag{10}$$

In the case of IOKR, \mathcal{F}_y is the feature space of some output kernel. Its dimension may therefore be infinite depending of which kernel is used. In this case, explicit feature vectors can be defined using the eigendecomposition of the output kernel matrix on the labeled data.

3.4 Models for General Decomposable Kernels

In the remainder of this section we propose to derive models based on a simple but powerful family of operator-valued kernels (OVK) based on scalar-valued kernels, called *decomposable kernels* or *separable kernels* (Álvarez et al., 2012; Baldassarre et al., 2012). They correspond to the simplest generalization of scalar kernels to operator-valued kernels. Decomposable kernels were first defined to deal with multi-task regression (Evgeniou et al., 2005; Micchelli and Pontil, 2005) and later, with structured multi-class classification (Dinuzzo et al., 2011). Other kernels (Caponnetto et al., 2008; Álvarez et al., 2012) have also been proposed: for instance, Lim et al. (2013) introduced a Hadamard kernel based on the Hadamard product of decomposable kernels and transformable kernels to deal with nonlinear vector autoregressive models. Caponnetto et al. (2008) proved that they are universal, meaning that an operator-valued regressor built on them is a universal approximator in \mathcal{F}_y .

Proposition 8 *The class of decomposable operator-valued kernels is composed of kernels of the form:*

$$\begin{aligned} \mathcal{K}_x : \mathcal{X} \times \mathcal{X} &\rightarrow \mathcal{B}(\mathcal{F}_y) \\ (x, x') &\mapsto \kappa_x(x, x') A \end{aligned}$$

where $\kappa_x : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a scalar-valued input kernel and $A \in \mathcal{B}(\mathcal{F}_y)$ is a positive semidefinite operator.

In the multi-task learning framework, $\mathcal{F}_y = \mathbb{R}^d$ is a finite dimensional output space and the matrix A encodes the existing relations among the d different tasks. This matrix can be estimated from labeled data or being learned simultaneously with the matrix C (Dinuzzo et al., 2011).

In the following we assume that the dimension of \mathcal{F}_y is finite and equal to d : $\mathcal{F}_y = \mathbb{R}^d$.

3.4.1 PENALIZED LEAST-SQUARES REGRESSION

In this section, we will use the following notations: \mathcal{F}_x and the function $\varphi_x : \mathcal{X} \rightarrow \mathcal{F}_x$ correspond respectively to the feature space and the feature map associated to the input scalar kernel κ_x . We note $\boldsymbol{\kappa}_{X_\ell}^x = (\kappa_x(x_1, x), \dots, \kappa_x(x_\ell, x))^T$ the vector of length ℓ containing the kernel values between the labeled examples and x and $\boldsymbol{\kappa}_{X_{\ell+n}}^x = (\kappa_x(x_1, x), \dots, \kappa_x(x_{\ell+n}, x))^T$. Let K_{X_ℓ} and $K_{X_{\ell+n}}$ be respectively the Gram matrices of κ_x over the sets \mathcal{X}_ℓ and $\mathcal{X}_{\ell+n}$. I_ℓ denotes the identity matrix of size ℓ .

The minimizer h of the optimization problem for the penalized least-squares cost in the supervised setting (3) using a decomposable OVK can be expressed as:

$$\begin{aligned} \forall x \in \mathcal{X}, h(x) &= A \sum_{i=1}^{\ell} \kappa_x(x, x_i) \mathbf{c}_i = A C_\ell \boldsymbol{\kappa}_{X_\ell}^x = ((\boldsymbol{\kappa}_{X_\ell}^x)^T \otimes A) \text{vec}(C_\ell) \\ &= ((\boldsymbol{\kappa}_{X_\ell}^x)^T \otimes A) (\lambda_1 I_{\ell d} + K_{X_\ell} \otimes A)^{-1} \text{vec}(\tilde{Y}_\ell). \end{aligned} \quad (11)$$

Therefore, the computation of the solution h requires to compute the inverse of a matrix of size $\ell d \times \ell d$. A being a real symmetric matrix, we can write the eigendecomposition of A :

$$A = E \Gamma E^T = \sum_{i=1}^d \gamma_i \mathbf{e}_i \mathbf{e}_i^T,$$

where $E = (\mathbf{e}_1, \dots, \mathbf{e}_d)$ is a $d \times d$ matrix and Γ is a diagonal matrix containing the eigenvalues of A : $\Gamma = \text{diag}(\gamma_1, \dots, \gamma_d)$. Using the eigendecomposition of A , we can prove that the solution $\hat{h}(x)$ can be obtained by solving d independent problems.

Proposition 9 *The minimizer of the optimization problem for the supervised penalized least squares cost (3) in the case of a decomposable operator-valued kernel can be expressed as:*

$$\forall x \in \mathcal{X}, h_{\text{ridge}}(x) = \sum_{j=1}^d \gamma_j \mathbf{e}_j \mathbf{e}_j^T \tilde{Y}_\ell (\lambda_1 I_\ell + \gamma_j K_{X_\ell})^{-1} \boldsymbol{\kappa}_{X_\ell}^x, \quad (12)$$

and in the semi-supervised setting (7), it writes as

$$\forall x \in \mathcal{X}, h_{\text{ridge}}(x) = \sum_{j=1}^d \gamma_j \mathbf{e}_j \mathbf{e}_j^T \tilde{Y}_\ell J (\lambda_1 I_{\ell+n} + \gamma_j K_{X_{\ell+n}} (J^T J + 2\lambda_2 L))^{-1} \boldsymbol{\kappa}_{X_{\ell+n}}^x.$$

We observe that, in the supervised setting, the complexity to solve Equation (11) is equal to $O((\ell d)^3)$, while the complexity for solving Equation (12) is $O(d^3 + \ell^3)$.

3.4.2 MAXIMUM MARGIN REGRESSION

Proposition 10 *Given $\mathcal{K}_x(x, x') = \kappa_x(x, x') A$, the dual formulation of the MMR optimization problem (4) in the supervised setting becomes:*

$$\begin{aligned} \min_{\boldsymbol{\alpha} \in \mathbb{R}^\ell} \quad & \frac{1}{4\lambda_1} \boldsymbol{\alpha}^T (\tilde{Y}_\ell^T A \tilde{Y}_\ell \circ K_{X_\ell}) \boldsymbol{\alpha} - \boldsymbol{\alpha}^T \mathbf{1} \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq 1, i = 1, \dots, \ell \end{aligned}$$

where \circ denotes the Hadamard product, and the solution is given by:

$$h_{\text{mmr}}(x) = \frac{1}{2\lambda_1} A \tilde{Y}_\ell \text{diag}(\boldsymbol{\alpha}) \boldsymbol{\kappa}_{X_\ell}^x.$$

In the semi-supervised MMR minimization problem (8), it writes as:

$$\begin{aligned} \min_{\boldsymbol{\alpha} \in \mathbb{R}^\ell} \quad & \frac{1}{2} \boldsymbol{\alpha}^T \left(\sum_{i=1}^d \gamma_i \tilde{Y}_\ell^T \mathbf{e}_i \mathbf{e}_i^T \tilde{Y}_\ell \circ J (2\lambda_1 I_{\ell+n} + 4\lambda_2 \gamma_i K_{X_{\ell+n}} L) \right)^{-1} K_{X_{\ell+n}} J^T \boldsymbol{\alpha} - \boldsymbol{\alpha}^T \mathbf{1} \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq 1, i = 1, \dots, \ell. \end{aligned}$$

The corresponding solution is:

$$h_{\text{mmr}}(x) = \frac{1}{2} \sum_{j=1}^d \gamma_j \mathbf{e}_j \mathbf{e}_j^T \tilde{Y}_\ell \text{diag}(\boldsymbol{\alpha}) J (\lambda_1 I_{\ell+n} + 2\gamma_j \lambda_2 K_{X_{\ell+n}} L)^{-1} \boldsymbol{\kappa}_{X_{\ell+n}}^x.$$

Proofs of Propositions 9 and 10 are given in Appendix A.

4. Model Selection

Real-valued kernel-based models enjoy a closed-form solution for the estimate of the leave-one-out criterion in the case of kernel ridge regression (Golub et al., 1979; Rifkin and Lippert, 2007). In order to select the hyperparameters of OVK-based models with a least-squares loss presented below, we develop a closed-form solution for the leave-one-out estimate of the sum of square errors. This solution extends Allen's predicted residual sum of squares (PRESS) statistics (Allen, 1974) to vector-valued functions. This result was first presented in french in the PhD thesis of Brouard (2013) in the case of decomposable kernels. In the following, we will use the notations used by Rifkin and Lippert (2007). We assume in this section that the dimension of \mathcal{F}_y is finite.

Let $\mathcal{S} = \{(x_1, \tilde{\mathbf{y}}_1), \dots, (x_\ell, \tilde{\mathbf{y}}_\ell)\}$ be the training set composed of ℓ labeled points. We define \mathcal{S}^i , $1 \leq i \leq \ell$, as the labeled data set with the i^{th} point removed:

$$\mathcal{S}^i = \{(x_1, \tilde{\mathbf{y}}_1), \dots, (x_{i-1}, \tilde{\mathbf{y}}_{i-1}), (x_{i+1}, \tilde{\mathbf{y}}_{i+1}), \dots, (x_\ell, \tilde{\mathbf{y}}_\ell)\}.$$

In this section, $h_{\mathcal{S}}$ denotes the function obtained when the regression problem is trained on the entire training set \mathcal{S} and we note $h_{\mathcal{S}^i}(x_i)$ the i^{th} leave-one-out value, that is the value at the point x_i of the function obtained when the training set is \mathcal{S}^i . The PRESS criterion corresponds to the sum of the ℓ leave-one-out square errors:

$$PRESS = \sum_{i=1}^{\ell} \|\tilde{\mathbf{y}}_i - h_{\mathcal{S}^i}(x_i)\|_{\mathcal{F}_y}^2.$$

As for scalar-valued functions, we show that it is possible to compute this criterion without evaluating explicitly $h_{\mathcal{S}^i}(x_i)$ for $i = 1, \dots, \ell$ and for each value of the grid of parameters.

Assuming we know $h_{\mathcal{S}^i}$, we define the matrix $\tilde{Y}_\ell^i = (\tilde{\mathbf{y}}_1^i, \dots, \tilde{\mathbf{y}}_\ell^i)$, where the vector $\tilde{\mathbf{y}}_j^i$ is given by:

$$\tilde{\mathbf{y}}_j^i = \begin{cases} \tilde{\mathbf{y}}_j & \text{if } j \neq i, \\ h_{\mathcal{S}^i}(x_i) & \text{if } j = i. \end{cases}$$

In the following, we show that when using \tilde{Y}_ℓ^i instead of \tilde{Y}_ℓ , the optimal solution corresponds to $h_{\mathcal{S}^i}$:

$$\begin{aligned} & \sum_{j=1}^{\ell} \|\tilde{\mathbf{y}}_j^i - h_{\mathcal{S}}(x_j)\|_{\mathcal{F}_y}^2 + \lambda_1 \|h_{\mathcal{S}}\|_{\mathcal{H}}^2 + \lambda_2 \sum_{j,k=1}^{\ell+n} W_{jk} \|h_{\mathcal{S}}(x_j) - h_{\mathcal{S}}(x_k)\|_{\mathcal{F}_y}^2 \\ & \geq \sum_{j \neq i} \|\tilde{\mathbf{y}}_j^i - h_{\mathcal{S}}(x_j)\|_{\mathcal{F}_y}^2 + \lambda_1 \|h_{\mathcal{S}}\|_{\mathcal{H}}^2 + \lambda_2 \sum_{j,k=1}^{\ell+n} W_{jk} \|h_{\mathcal{S}}(x_j) - h_{\mathcal{S}}(x_k)\|_{\mathcal{F}_y}^2 \\ & \geq \sum_{j \neq i} \|\tilde{\mathbf{y}}_j^i - h_{\mathcal{S}^i}(x_j)\|_{\mathcal{F}_y}^2 + \lambda_1 \|h_{\mathcal{S}^i}\|_{\mathcal{H}}^2 + \lambda_2 \sum_{j,k=1}^{\ell+n} W_{jk} \|h_{\mathcal{S}^i}(x_j) - h_{\mathcal{S}^i}(x_k)\|_{\mathcal{F}_y}^2 \\ & \geq \sum_{j=1}^{\ell} \|\tilde{\mathbf{y}}_j^i - h_{\mathcal{S}^i}(x_j)\|_{\mathcal{F}_y}^2 + \lambda_1 \|h_{\mathcal{S}^i}\|_{\mathcal{H}}^2 + \lambda_2 \sum_{j,k=1}^{\ell+n} W_{jk} \|h_{\mathcal{S}^i}(x_j) - h_{\mathcal{S}^i}(x_k)\|_{\mathcal{F}_y}^2. \end{aligned}$$

The second inequality comes from the fact that $h_{\mathcal{S}^i}$ is defined as the minimizer of the optimization problem when the i^{th} point is removed from the training set. As $h_{\mathcal{S}^i}$ is the optimal solution when \tilde{Y}_ℓ is replaced with \tilde{Y}_ℓ^i , it can be written as:

$$\forall i = 1, \dots, \ell, \quad h_{\mathcal{S}^i}(x_i) = (\mathbf{K}_{X_{\ell+n}}^{x_i})^T B \text{vec}(\tilde{Y}_\ell^i) = (KB)_{i,\cdot} \text{vec}(\tilde{Y}_\ell^i),$$

where $K = \mathbf{K}_{X_{\ell \times (\ell+n)}}$ is the input gram matrix between the sets \mathcal{X}_ℓ and $\mathcal{X}_{\ell+n}$ and $B = (\lambda_1 I_{(\ell+n)d} + ((J^T J + 2\lambda_2 L) \otimes I_d) \mathbf{K}_{X_{\ell+n}})^{-1} (J^T \otimes I_d)$. $(KB)_{i,\cdot}$ corresponds to the i^{th} row of the matrix KB and $(KB)_{i,j}$ is the value of the matrix corresponding to the row i and the column j .

We can then derive an expression of $h_{\mathcal{S}^i}$ by computing the difference between $h_{\mathcal{S}^i}(x_i)$ and $h_{\mathcal{S}}(x_i)$:

$$\begin{aligned} h_{\mathcal{S}^i}(x_i) - h_{\mathcal{S}}(x_i) &= (KB)_{i,\cdot} \text{vec}(\tilde{Y}_\ell^i - \tilde{Y}_\ell) \\ &= \sum_{k=1}^{\ell} (KB)_{i,k} (\tilde{\mathbf{y}}_k^i - \tilde{\mathbf{y}}_k) \\ &= (KB)_{i,i} (h_{\mathcal{S}^i}(x_i) - \tilde{\mathbf{y}}_i), \end{aligned}$$

which leads to

$$\begin{aligned} (I_d - (KB)_{i,i}) h_{\mathcal{S}^i}(x_i) &= h_{\mathcal{S}}(x_i) - (KB)_{i,i} \tilde{\mathbf{y}}_i \\ \Rightarrow (I_d - (KB)_{i,i}) h_{\mathcal{S}^i}(x_i) &= (KB)_{i,\cdot} \text{vec}(\tilde{Y}_\ell) - (KB)_{i,i} \tilde{\mathbf{y}}_i \\ \Rightarrow h_{\mathcal{S}^i}(x_i) &= (I_d - (KB)_{i,i})^{-1} \left((KB)_{i,\cdot} \text{vec}(\tilde{Y}_\ell) - (KB)_{i,i} \tilde{\mathbf{y}}_i \right). \end{aligned}$$

Let $L_{oo} = (h_{\mathcal{S}^1}(x_1), \dots, h_{\mathcal{S}^\ell}(x_\ell))$ be the matrix containing the leave-one-out vector values over the training set. The equation above can be rewritten as:

$$\text{vec}(L_{oo}) = (I_{\ell d} - \text{diag}_b(KB))^{-1} (KB - \text{diag}_b(KB)) \text{vec}(\tilde{Y}_\ell),$$

where diag_b corresponds to the block diagonal of a matrix.

The Allen's PRESS statistic can be expressed as:

$$\begin{aligned} PRESS &= \|\text{vec}(\tilde{Y}_\ell) - \text{vec}(L_{oo})\|^2 \\ &= \|(I_{\ell d} - \text{diag}_b(KB))^{-1} (I_{\ell d} - \text{diag}_b(KB) - KB + \text{diag}_b(KB)) \text{vec}(\tilde{Y}_\ell)\|^2 \\ &= \|(I_{\ell d} - \text{diag}_b(KB))^{-1} (I_{\ell d} - KB) \text{vec}(\tilde{Y}_\ell)\|^2. \end{aligned}$$

This closed-form expression allows to evaluate the PRESS criterion without having to solve ℓ problems involving the inversion of a matrix of size $(\ell + n - 1)d$.

5. Input Output Kernel Regression

We now have all the needed tools to approximate vector-valued functions. In this section, we go back to IOKR and consider that \mathcal{F}_y is the feature space associated to some output kernel $\kappa_y : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$, and that vectors $\tilde{\mathbf{y}}_i$ now correspond to output feature vectors $\varphi_y(y_i)$. Several feature spaces can be defined, including the unique RKHS associated to the kernel

κ_y . This choice has direct consequences on the choice of the input operator-valued kernel \mathcal{K}_x . Depending on the application, we might be interested for instance on choosing \mathcal{F}_y as a functional space to get integral operators or as the finite-dimensional Euclidean space \mathbb{R}^d to get matrices. It is important to notice that this reflects a radically new approach in machine learning where we usually focus on the choice of the input feature space and do not discuss a lot the output space. Moreover, the choice of a given triplet $(\kappa_y, \mathcal{F}_y, \mathcal{K}_x)$ has a great impact of the learning task both in terms of complexity in time and potentially of performance. In the following, we explain how Input Output Kernel Regression can be used to solve link prediction and multi-task problems.

5.1 Link Prediction

Link prediction is a challenging machine learning problem that has been defined recently in social networks as well as biological networks. Let us formulate this problem using the previous notations: $\mathcal{X} = \mathcal{Y} = \mathcal{U}$ is the set of candidate nodes we are interested in. We want to estimate some relation between these nodes, for example a social relationship between persons or some physical interaction between molecules. During the training phase we are given $\mathcal{G}_\ell = (\mathcal{U}_\ell, A_\ell)$, a non oriented graph defined by the subset $\mathcal{U}_\ell \subseteq \mathcal{U}$ and the adjacency matrix A_ℓ of size $\ell \times \ell$. Supervised link prediction is usually addressed by learning a binary pairwise classifier $f : \mathcal{U} \times \mathcal{U} \rightarrow \{0, 1\}$ that predicts if there exists a link between two objects or not, from the training information \mathcal{G}_ℓ . One way to solve this learning task is to build a pairwise classifier. However, the link prediction problem can also be formalized as an output kernel regression task (Geurts et al., 2007a; Brouard et al., 2011).

The OKR framework for link prediction is based on the assumption that an approximation of the output kernel κ_y will provide valuable information about the proximity of the objects of \mathcal{U} as nodes in the unknown graph defined on \mathcal{U} . Given that assumption, a classifier f_θ is defined from the approximation $\widehat{\kappa}_y$ by thresholding its output values:

$$f_\theta(u, u') = \text{sgn}(\widehat{\kappa}_y(u, u') - \theta).$$

An approximation of the target output kernel κ_y is built from the scalar product between the outputs of a single variable function $h : \mathcal{U} \rightarrow \mathcal{F}_y$: $\widehat{\kappa}_y(u, u') = \langle h(u), h(u') \rangle_{\mathcal{F}_y}$. Using the kernel trick in the output space therefore allows to reduce the problem of learning a pairwise classifier to the problem of learning a single variable function with output values in a Hilbert space (the output feature space \mathcal{F}_y).

In the case of IOKR, the function h is learnt in an appropriate RKHS by using the operator-valued kernel regression approach presented in Section 3. In the following, we describe the output kernel and the input operator-valued kernel that we propose to use for solving the link prediction problem with IOKR.

Regarding the output kernel, we do not have a kernel κ_y defined on $\mathcal{U} \times \mathcal{U}$ in the link prediction problem but we can define a Gram matrix K_{Y_ℓ} on the training set \mathcal{U}_ℓ . Here, we define K_{Y_ℓ} from the known adjacency matrix A_ℓ of the training graph such that it encodes the proximities in the graph between the labeled nodes. For instance, we can choose the diffusion kernel matrix (Kondor and Lafferty, 2002), which is defined as:

$$K_{Y_\ell} = \exp(-\beta L_{y_\ell}),$$

$B =$	Supervised learning	Semi-supervised learning
Ridge	$(\lambda_1 I_\ell + K_{X_\ell})^{-1}$	$J(\lambda_1 I_{\ell+n} + K_{X_{\ell+n}}(J^T J + 2\lambda_2 L))^{-1}$
MMR	$\frac{1}{2\lambda_1} \text{diag}(\boldsymbol{\alpha})$	$\frac{1}{2} \text{diag}(\boldsymbol{\alpha}) J(\lambda_1 I_{\ell+n} + 2\lambda_2 K_{X_{\ell+n}} L)^{-1}$

Table 2: Matrix B of the models obtained using the identity decomposable kernel in the case of different settings and loss functions.

where $L_{y_\ell} = D_\ell - A_\ell$ is the graph Laplacian, with D_ℓ the diagonal matrix of degrees. The kernel trick allows to work as if we have chosen the subspace spanned by $\{\mathbf{e}_1, \dots, \mathbf{e}_\ell\}$, the eigenvectors of the matrix K_{Y_ℓ} as a feature space with an associated feature map that verifies:

$$\forall i \in \{1, \dots, \ell\}, \varphi_y(u_i) = [\sqrt{\gamma_1} e_1^i, \dots, \sqrt{\gamma_\ell} e_\ell^i]^T.$$

The kernel $\kappa_y : \mathcal{U} \times \mathcal{U} \rightarrow \mathbb{R}$, also verifies:

$$\forall i, j \in \{1, \dots, \ell\}, \kappa_y(u_i, u_j) = (K_{Y_\ell})_{i,j}.$$

In practise, we only need to know K_{Y_ℓ} . Regarding the operator-valued kernel, we consider here the identity decomposable kernel:

$$\forall (u, u') \in \mathcal{U} \times \mathcal{U}, \mathcal{K}_x(u, u') = \kappa_x(u, u') I.$$

We underline that even if this kernel may seem simple, we must be aware that in this task, we do not have the explicit expressions of outputs $\varphi_y(u)$ and prediction in \mathcal{F}_y is not the final target. Therefore this operator-valued kernel allows us to work properly with output Gram matrix values.

Of particular interest for us is the expression of the scalar product which is the only one we need for link prediction. When using the identity decomposable kernel, the approximation of the output kernel can be written as follows:

$$\widehat{\kappa}_y(u, u') = \langle \hat{h}(u), \hat{h}(u') \rangle_{\mathcal{F}_y} = (\boldsymbol{\kappa}_{x, U_\ell}^u)^T B^T K_{Y_\ell} B \boldsymbol{\kappa}_{x, U_\ell}^{u'}, \quad (13)$$

where B is a matrix of size $\ell \times \ell$ that depends of the loss function used (see Table 2). In the semi-supervised setting, the approximated output kernel has a similar expression, where $\boldsymbol{\kappa}_{x, U_\ell}^u, \boldsymbol{\kappa}_{x, U_\ell}^{u'}$ are replaced by $\boldsymbol{\kappa}_{x, U_{\ell+n}}^u, \boldsymbol{\kappa}_{x, U_{\ell+n}}^{u'}$ and B is a matrix of size $(\ell + n) \times \ell$. We can notice that we do not need to know the explicit expressions of outputs $\varphi_y(u)$ to compute this scalar product. Besides, the approximation of the scalar product $\langle \varphi_y(u), \varphi_y(u') \rangle_{\mathcal{F}_y}$ can be interpreted as a modified scalar product between the inputs $\varphi_x(u)$ and $\varphi_x(u')$.

5.2 Multi-Task Learning

Multi-task learning has been developed based on the observation that it may happen that several learning tasks are not disjoint and are characterized by a relationship such as inclusion or similarity. Learning simultaneously such related tasks has been shown to improve the performance comparing to learning the different tasks independently from each other

(Caruana, 1997; Evgeniou et al., 2005). Examples of multi-task learning problems can be found in document categorization as well as in protein functional annotation prediction. Dependencies among target variables can also be encountered in the case of multiple regression.

We consider here the case of learning d tasks having the same input and output domains. Evgeniou et al. (2005) have shown that this problem is equivalent to learning a vector-valued function $h : \mathcal{X} \rightarrow \mathcal{Y}$ with d components $h^i : \mathcal{X} \rightarrow \mathcal{Y}_i$ using the vector-valued RKHS theory. A natural way to integrate the task relatedness with operator-valued kernels is to use the decomposable kernels introduced in Subsection 3.4: $\mathcal{K}_x(x, x') = \kappa_x(x, x')A$. Several values for the matrix A have been proposed (Evgeniou et al., 2005; Sheldon, 2008; Baldassarre et al., 2012) based on the fact that the regularization term in the RKHS associated to a decomposable OVK can be expressed in function of A :

$$\|h\|_{\mathcal{H}}^2 = \sum_{i,j=1}^d A_{i,j}^\dagger \langle h^i, h^j \rangle_{\mathcal{H}_{\kappa_x}},$$

where \dagger denotes the pseudoinverse and \mathcal{H}_{κ_x} the RKHS associated to the scalar kernel κ_x .

In the IOKR framework, the task structure can be encoded in two different ways. We can use a decomposable OVK in input as described previously and define a regularization term that will penalize the d components of the function h according to the task structure. Another way is to modify the output representation by defining an output kernel that will integrate the task structure. We propose to compare the three following models to solve multi-task learning with our framework:

- Model 0: $\kappa_y(\mathbf{y}, \mathbf{y}') = \mathbf{y}^T \mathbf{y}'$, with the identity kernel $\mathcal{K}_x(x, x') = \kappa_x(x, x') I$,
- Model 1: $\kappa_y(\mathbf{y}, \mathbf{y}') = \mathbf{y}^T A_1 \mathbf{y}'$, with the identity kernel $\mathcal{K}_x(x, x') = \kappa_x(x, x') I$,
- Model 2: $\kappa_y(\mathbf{y}, \mathbf{y}') = \mathbf{y}^T \mathbf{y}'$, with the decomposable kernel $\mathcal{K}_x(x, x') = \kappa_x(x, x') A_2$.

In the first case, the different tasks are learned independently :

$$\forall x \in \mathcal{X}, \hat{h}_0(x) = Y_\ell J (\lambda_1 I_{\ell+n} + K_{X_{\ell+n}} (J^T J + 2\lambda_2 L))^{-1} \boldsymbol{\kappa}_{X_{\ell+n}}^x,$$

while in the other cases, the tasks relatedness is taken into account :

$$\begin{aligned} \forall x \in \mathcal{X}, \hat{h}_1(x) &= \sqrt{A_1} Y_\ell J (\lambda_1 I_{\ell+n} + K_{X_{\ell+n}} (J^T J + 2\lambda_2 L))^{-1} \boldsymbol{\kappa}_{X_{\ell+n}}^x, \\ \forall x \in \mathcal{X}, \hat{h}_2(x) &= \sum_{j=1}^d \gamma_j \mathbf{e}_j \mathbf{e}_j^T Y_\ell J (\lambda_1 I_{\ell+n} + \gamma_j K_{X_{\ell+n}} (J^T J + 2\lambda_2 L))^{-1} \boldsymbol{\kappa}_{X_{\ell+n}}^x, \end{aligned}$$

where γ_j and \mathbf{e}_j are the eigenvalues and eigenvectors of A_2 .

We consider a matrix M of size $d \times d$ that encodes the relations existing between the different tasks. This matrix can be considered as the adjacency matrix of a graph between tasks. We note L_M the graph Laplacian associated to this matrix. The matrices A_1 and A_2 are defined as follow:

$$\begin{aligned} A_1 &= \mu M + (1 - \mu) I_d, \\ A_2 &= (\mu L_M + (1 - \mu) I_d)^{-1}, \end{aligned}$$

where μ is a parameter in $[0, 1]$.

The matrix A_2 was proposed by Evgeniou et al. (2005) and Sheldon (2008) for multi-task learning from the following regularizer:

$$\|h_2\|_{\mathcal{H}}^2 = \frac{\mu}{2} \sum_{i,j=1}^d M_{ij} \|h_2^i - h_2^j\|^2 + (1 - \mu) \sum_{i=1}^d \|h_2^i\|^2.$$

This regularization term forces two tasks h_2^i and h_2^j to be close to each other when the similarity value M_{ij} is high and conversely.

6. Numerical Experiments

In this section, we present the performances obtained with the IOKR approach on two different problems: link prediction and multi-task regression. In these experiments, we examine the effect of the smoothness constraint through the variation of its related hyperparameter λ_2 , using supervised method as a baseline. We evaluate the method in the transductive setting, in which the goal is to predict the correct outputs for the unlabeled examples, as well as in the semi-supervised setting.

6.1 Link Prediction

For the link prediction problem, we considered experiments on three datasets: a collection of synthetic networks, a co-authorship network and a protein-protein interaction (PPI) network.

6.1.1 PROTOCOL

For different percentages of labeled nodes, we randomly selected a subsample of nodes as labeled nodes. We split the remaining nodes in two subsets: one containing the unlabeled nodes and another containing the test nodes. Labeled interactions correspond to interactions between two labeled nodes. This means that when 10% of labeled nodes are selected, it corresponds to only 1% of labeled interactions. The performances were evaluated by averaging the areas under the ROC curve and the precision-recall curve (denoted AUC-ROC and AUC-PR) over ten random choices of the labeled set. A Gaussian kernel was used for the scalar input kernel κ_x . Its corresponding bandwidth σ was selected by a leave-one-out cross-validation procedure on the training set to maximize the AUC-ROC, jointly with the hyperparameter λ_1 . In the case of the least-squares loss function, we used the leave-one-out estimates approach introduced in Section 4. The output kernel used is a diffusion kernel of parameter β . Another diffusion kernel of parameter β_2 was also used for the smoothing penalty: $\exp(-\beta_2 L) = \sum_{i=0}^{\infty} \frac{(-\beta_2 L)^i}{i!}$, where L is the Laplacian of W . Preliminary runs have shown that the values of β and β_2 have a limited influence on the performances, we then have set both parameters to 1. Finally we set W to $K_{X_{\ell+n}}$.

6.1.2 SYNTHETIC NETWORKS

We first illustrate our method on synthetic networks where the input kernel was chosen as a very good approximation of the output kernel. In these experiments we wanted to measure

the improvement brought by the semi-supervised method in extreme cases, i.e. when the percentage of labeled nodes is very low.

The output networks were obtained by sampling random graphs containing 700 nodes from a Erdős-Renyi law with different graph densities. The graph density corresponds to the probability of presence of edges in the graph. In this experiment we chose three densities that are representative of real network densities: 0.007, 0.01 and 0.02. For each network, we used the diffusion kernel on the full graph as output kernel and chose the diffusion parameter such that it maximizes an information criterion. To build an input kernel corresponding to a good approximation of the output kernel, we applied kernel PCA on the output kernel and derived input vectors from the truncated basis of the first components. We can control the quality of the input representation by varying the relative inertia captured by the first components. We then build a Gaussian kernel based on these inputs.

Figures 3 and 4 report respectively the averaged values and standard deviations for the AUC-ROC and AUC-PR obtained for different network densities and different percentages of labeled nodes in the transductive setting. IOKR-ridge corresponds to IOKR with a least-square loss and IOKR-margin to the hinge loss used in MMR. For these results, we used the components capturing 95% of the variance for defining the input vectors. We observe that IOKR-ridge outperforms IOKR-margin in the supervised and in the semi-supervised cases. This improvement is particularly significant for AUC-PR, especially when the network density is strong and the percentage of labeled data is high. It is thus very significant for 10% and 20% of labeled data. In the supervised case, this observation can be explained by the difference between the complexities of the models. As shown in Equation (13), the solution obtained in the supervised case writes as: $\widehat{\kappa}_y(u, u') = (\kappa_{x, U_\ell}^u)^T B^T K_{Y_\ell} B \kappa_{x, U_\ell}^{u'}$. In Table 2, we can see that the matrix B is only a diagonal matrix in the case of IOKR-margin while B is a full matrix for IOKR-ridge. This can also be seen in the dual optimization problem for a general loss function (see Appendix B), where we observe that the dual variables α_i are simply collinear to the vector $\tilde{\mathbf{y}}_i$ for IOKR-margin. The synthetic networks may therefore require a more complex predictor.

We observe an improvement of the performances in terms of AUC-ROC and AUC-PR for both approaches in the semi-supervised setting compared to the supervised setting. This improvement is more significant for IOKR-margin. This can be explained by the fact that the IOKR-margin models obtained in the supervised and in the semi-supervised cases do not have the same complexity. As shown in Table 2, the matrix B of the IOKR-margin model is a much richer matrix in the semi-supervised setting than in the supervised setting where it corresponds to a diagonal matrix. For IOKR-ridge, the improvement of the performance is only observed for low percentages of labeled data. We can therefore make the assumption that for this model, using unlabeled data increases the AUCs for low percentages of labeled data. But when enough information can be found in the labeled data, semi-supervised learning does not improve the performance. Based on these results, we can also formulate the assumption that link prediction is harder in the case of dense networks.

In Appendix C we experimented how the method behaves with perfect to noisy input features. We chose different levels of inertia (75%, 85%, 95% and 100%) for defining the input features. The results obtained with IOKR-ridge and IOKR-margin are shown in Table 8. We also include results on synthetic networks generated using mixtures of Erdős-Renyi random graphs in Table 9.

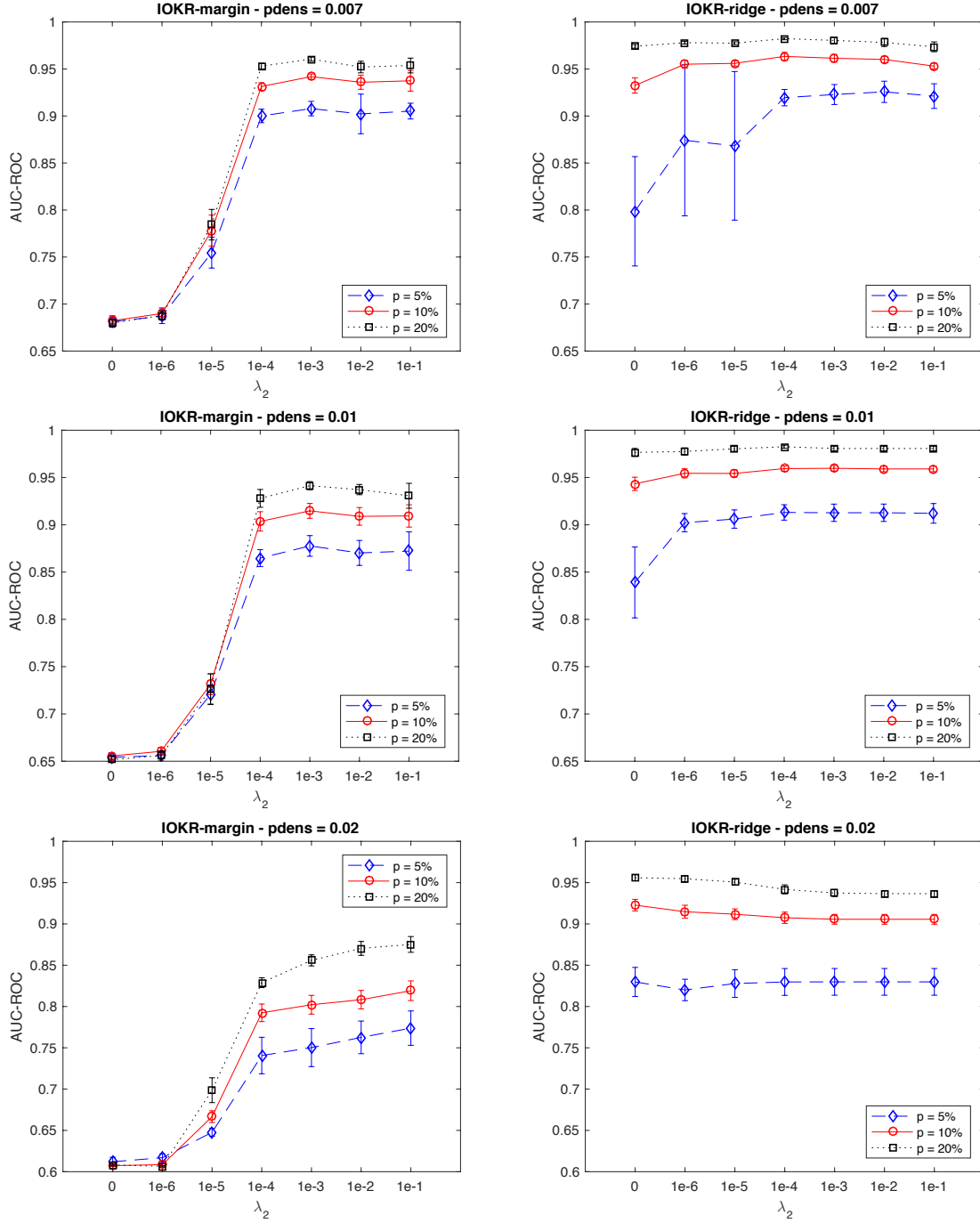


Figure 3: Averaged AUC-ROC for the reconstruction of three synthetic networks with IOKR-margin (left) and IOKR-ridge (right) in the transductive setting. The rows correspond to different graph densities (denoted pdens), which are 0.007, 0.01 and 0.02 respectively.

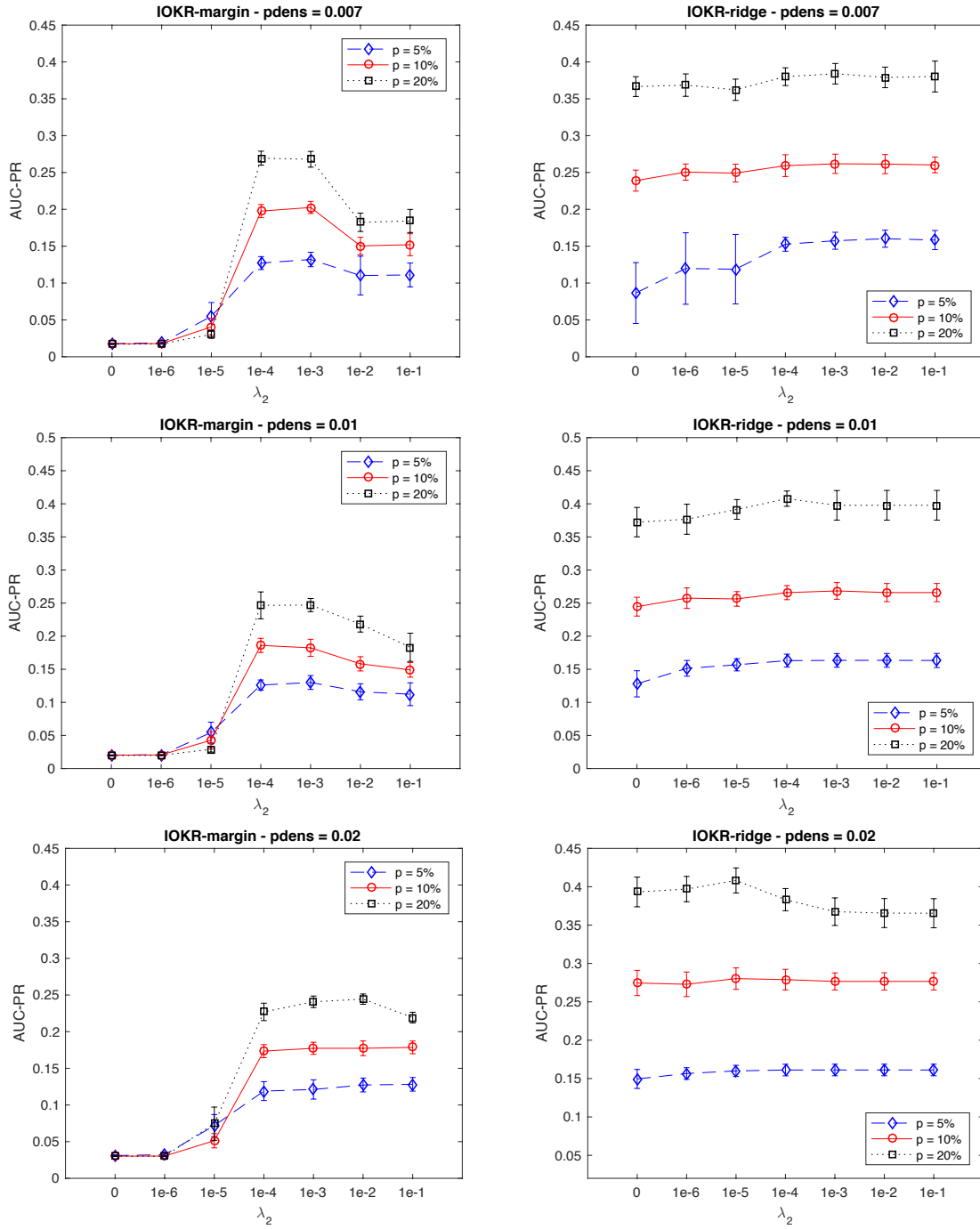


Figure 4: Averaged AUC-PR for the reconstruction of three synthetic networks with IOKR-margin (left) and IOKR-ridge (right) in the transductive setting. The rows correspond to different graph densities (denoted pdens), which are 0.007, 0.01 and 0.02 respectively.

6.1.3 NIPS CO-AUTHORSHIP NETWORK

We applied our method on a co-authorship network containing information on publications of the NIPS conferences between 1988 to 2003 (Globerson et al., 2007). In this network, vertices represent authors and an edge connects two authors if they have at least one NIPS publication in common. Among the 2865 authors, we considered the ones with at least two links in the co-authorship network in order to have a significant density and try to keep close to the original data. We therefore focused on a network containing 2026 authors with an empirical link density of 0.002. Each author was described by a vector of 14036 values, corresponding to the frequency with which he uses each given word in his papers.

Figure 5 reports the averaged AUC-ROC and AUC-PR obtained on the NIPS co-authorship network in the transductive setting for different values of λ_2 and different percentages of labeled nodes. As previously, we observe that the semi-supervised approach

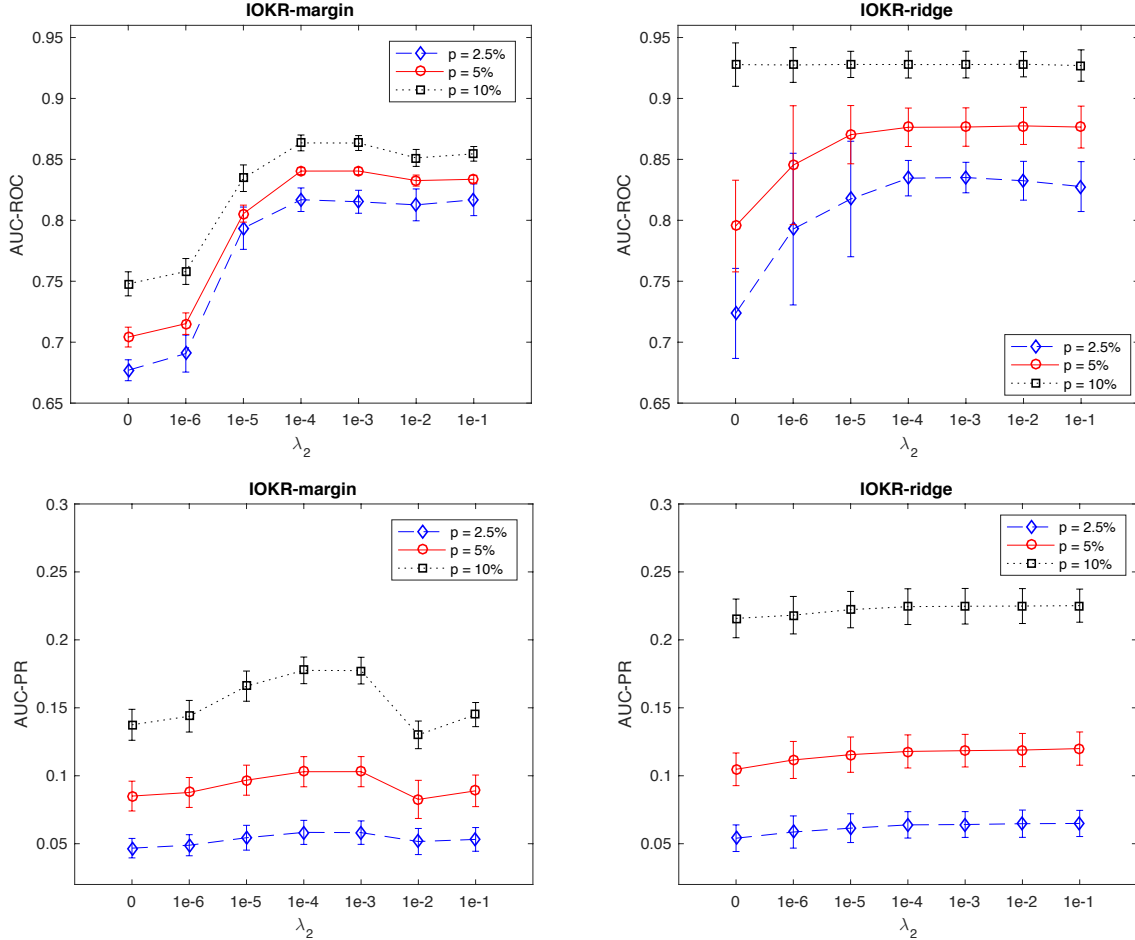


Figure 5: AUC-ROC and AUC-PR obtained for the NIPS co-authorship network inference with IOKR-margin (left) and IOKR-ridge (right) in the transductive setting.

p	AUC-ROC			AUC-PR		
	5%	10%	20%	5%	10%	20%
Transductive setting						
EM	87.3 ± 2.4	92.9 ± 1.7	96.4 ± 0.8	13.8 ± 4.5	22.5 ± 6.6	41.1 ± 2.5
PKMR	85.7 ± 4.1	92.4 ± 1.6	96.4 ± 0.4	9.7 ± 2.8	20.0 ± 4.8	38.8 ± 2.0
IOKR	83.6 ± 5.9	93.6 ± 1.0	96.5 ± 0.4	12.0 ± 3.0	24.5 ± 2.9	43.7 ± 1.9
Semi-supervised setting						
IOKR	86.0 ± 2.7	93.3 ± 0.7	95.7 ± 1.4	7.6 ± 2.3	13.8 ± 1.7	25.3 ± 3.0

Table 3: AUC-ROC and AUC-PR obtained for the NIPS co-authorship network inference with EM, PKMR, IOKR in the transductive setting, and with IOKR in the semi-supervised setting. p indicates the percentage of labeled examples.

improves the performances compared to the supervised one for both models. For AUC-ROC values, this improvement is especially important when the percentage of labeled nodes is low. Indeed, with 2.5% of labeled nodes, the improvement can reach in average up to 0.14 points of AUC-ROC for IOKR-margin and up to 0.11 points for IOKR-ridge. As for the synthetic networks, the IOKR-ridge model outperforms IOKR-margin model in terms of AUC-ROC and AUC-PR, especially when the proportion of labeled examples is large. The explanation provided for the synthetic networks regarding the complexity of the solutions for IOKR-margin and IOKR-ridge holds here also. In the following, we will focus on IOKR-ridge only.

We compared IOKR-ridge with two transductive approaches: the EM-based approach (Tsuda et al., 2003; Kato et al., 2005) and Penalized Kernel Matrix Regression (PKMR) (Yamanishi and Vert, 2007). These two methods regard the link prediction problem as a kernel matrix completion problem. The *EM* method fills the missing entries of the output Gram matrix K_Y by minimizing the information geometry, as measured by the Kullback-Leibler divergence, with the input Gram matrix K_X . The *PKMR* approach considers the kernel matrix completion problem as a regression problem between the labeled input Gram matrix K_{X_ℓ} and the labeled output Gram matrix K_{Y_ℓ} . We did not compare our method with the *Link Propagation* framework (Kashima et al., 2009) because this framework assumes that arbitrary interactions may be considered as labeled while IOKR requires a known subgraph. 500 examples were used for the test set and the remaining 1526 examples for the training set, which corresponds to the union of the labeled and unlabeled sets. For the labeled set we used 5%, 10% and 20% of the training examples and the left examples for the unlabeled set. We averaged the AUC over ten random partitions of the examples in labeled/unlabeled/test sets. The hyperparameters were selected by a 5-CV experiment on the labeled set for the three methods. The hyperparameters were selected separately for the AUC-ROC and the AUC-PR. For IOKR, we selected also the λ_2 parameter in this experiment, and we sparsified the matrix W in the semi-supervised constraint using 10% of the k -nearest-neighbors.

The results obtained for the comparison in the transductive and semi-supervised setting are reported in Table 3. Only the results for IOKR-ridge are reported in the semi-supervised

setting as the other methods are transductive. We observe that IOKR obtains better AUC-ROC and AUC-PR than EM and PKMR when the percentage of labeled data is greater or equal than 10%. For 5% the best performing method is the EM approach. Regarding the results of IOKR in the semi-supervised setting, we observe that the AUC-ROC results stay relatively similar compared to the transductive setting. However the AUC-PR values decrease significantly between the transductive and the semi-supervised settings. Considering the proteins for which we want to predict the interactions in the continuity constraint seems to help a lot the performances in term of AUC-PR.

6.1.4 PROTEIN-PROTEIN INTERACTION NETWORK

We also performed experiments on a protein-protein interaction (PPI) network of the yeast *Saccharomyces Cerevisiae*. This network was built using the DIP database (Salwinski et al., 2004), which contains protein-protein interactions that have been experimentally determined and manually curated. We used more specifically the high confidence DIP core subset of interactions (Deane et al., 2002). For the input kernels, we used the annotations provided by Gene Ontology (GO) (Ashburner et al., 2000) in terms of biological processes, cellular components and molecular functions. These annotations are organized in three different ontologies. Each ontology is represented by a directed acyclic graph, where each node is a GO annotation and edges correspond to relationships between the annotations, like sub-class relationships for example. A protein can be annotated to several terms in an ontology. We chose to represent each protein u_i by a vector \mathbf{s}_i , whose dimension is equal to the total number of terms in the considered ontology. If a protein u_i is annotated by the term t , then :

$$\mathbf{s}_i^{(t)} = -\ln \left(\frac{\text{number of proteins annotated by } t}{\text{total number of proteins}} \right).$$

This encoding allows to take into account the specificity of a term in the ontology. We then used these representations to build a Gaussian kernel for each GO ontology. By considering the set of proteins being annotated for each input kernel and being involved in at least one physical interaction, we obtained a PPI network containing 1242 proteins.

Based on the previous numerical results, we chose to consider only IOKR-ridge in the following experiments. We compared our approach to several supervised methods proposed for biological network inference:

- *Naive* (Yamanishi et al., 2004): this approach predicts an interaction between two proteins u and u' if $\kappa_x(u, u')$ is greater than a threshold θ .
- *kCCA* (Yamanishi et al., 2004): kernel CCA is used to detect correlations existing between the input kernel and a diffusion kernel derived from the adjacency matrix of the labeled PPI network.
- *kML* (Vert and Yamanishi, 2005): kernel Metric Learning consists in learning a new metric such that interacting proteins are close to each other, and conversely for non interacting proteins.
- *Local* (Bleakley et al., 2007): a local model is built for each protein in order to learn the subnetwork associated to each protein and these models are then combined together.

- *OK3+ET* (Geurts et al., 2006, 2007a): Output Kernel Tree with extra-trees is a tree-based method where the output is kernelized and is combined with ensemble methods.

The pairwise kernel method (Ben-Hur and Noble, 2005) was not considered here because this method requires to define a Gram matrix between pairs of nodes, which raises some practical issues in terms of computation time and storage. However we could have used an online implementation of the pairwise kernel method like the one used in Kashima et al. (2009) and thus avoid to store the large Gram matrix.

Each method was evaluated through a 5-fold cross-validation (5-CV) experiment and the hyperparameters were tuned on the training fold using a 4-CV experiment. As the local method can not be used for predicting interactions between two proteins of the test set, AUC-ROC and AUC-PR were only computed for the prediction of interactions between proteins in the test set and proteins in the training set. Input kernel matrices were defined for GO ontology and an integrated kernel, which was obtained by averaging the three input kernels, was also considered. Table 4 reports the results obtained for the comparison of the different methods in the supervised setting. We can see that output kernel regression based methods work better on this dataset than the other methods. In terms of AUC-ROC, the IOKR-ridge method obtains the best results for the four different input kernels, while for AUC-PR, OK3 with extra-trees presents better performances. We also compared the aver-

a) **AUC-ROC:**

Method	GO-BP	GO-CC	GO-MF	int
Naive	60.8 \pm 0.8	64.4 \pm 2.5	64.2 \pm 0.8	67.7 \pm 1.5
kCCA	82.4 \pm 3.6	77.0 \pm 1.7	75.0 \pm 0.6	85.7 \pm 1.6
kML	83.2 \pm 2.4	77.8 \pm 1.1	76.6 \pm 1.9	84.5 \pm 1.5
Local	79.5 \pm 1.6	73.1 \pm 1.3	66.8 \pm 1.2	83.0 \pm 0.5
OK3+ET	84.3 \pm 2.4	81.5 \pm 1.6	79.3 \pm 1.8	86.9 \pm 1.6
IOKR-ridge	88.8 \pm 1.9	87.1 \pm 1.3	84.0 \pm 0.6	91.2 \pm 1.2

b) **AUC-PR:**

Method	GO-BP	GO-CC	GO-MF	int
Naive	4.8 \pm 1.0	2.1 \pm 0.6	2.4 \pm 0.4	8.0 \pm 1.7
kCCA	7.1 \pm 1.5	7.7 \pm 1.4	4.2 \pm 0.5	9.9 \pm 0.4
kML	7.1 \pm 1.3	3.1 \pm 0.6	3.5 \pm 0.4	7.8 \pm 1.6
Local	6.0 \pm 1.1	1.1 \pm 0.3	0.7 \pm 0.0	22.6 \pm 6.6
OK3+ET	19.0 \pm 1.8	21.8 \pm 2.5	10.5 \pm 2.0	26.8 \pm 2.4
IOKR-ridge	15.3 \pm 1.2	20.9 \pm 2.1	8.6 \pm 0.3	22.2 \pm 1.6

Table 4: AUC-ROC and AUC-PR estimated by 5-CV for the yeast PPI network reconstruction in the supervised setting with different input kernels (*GO-BP*: GO biological processes; *GO-CC*: GO cellular components; *GO-MF*: GO molecular functions; *int* : average of the different kernels).

Method	Running time (s)
Naive	0.05 ± 0.01
kCCA	144.60 ± 70.70
kML	18.28 ± 0.78
Local	141.64 ± 14.91
OK3+ET	638.53 ± 69.09
IOKR-ridge	0.49 ± 0.02

Table 5: Averaged running time in seconds for one fold of the 5-CV for the yeast PPI network reconstruction in the supervised setting.

aged running time for one fold of the 5-CV for the different methods. These running times are shown in Table 5 and correspond to the times needed to perform both the training and the prediction steps. All the algorithms were implemented in Matlab and run on a MacBook Pro 2.4 GHz dual-core. For this computation, we fixed the values of the parameters and we did not take into account the computation of the input kernel. In Table 5 we observe that the running time of IOKR-ridge is relatively small compared to the other methods. The fastest method is the naive method. It can be explained by the fact that this method does not have a training step like the other methods. Interactions between two proteins are simply predicted if the proteins are similar according to the input kernel function.

As for the NIPS co-authorship network, we compared IOKR-ridge with the EM and PKMR approaches in the transductive setting. For this network, we used 300 examples for the test set and the remaining 942 examples for the training set. We used as input kernel the integrated kernel introduced in the supervised experiments. The results obtained for this comparison as well as the results for IOKR-ridge in the semi-supervised setting are reported in Table 6. Regarding the AUC-ROC, the EM approach obtains better results when the percentage of labeled data is equal to 5%. For 10% and 20% of labeled data, the difference between EM and IOKR-ridge is not significant. In terms of AUC-PR, EM achieves rather good performances compared to the others, especially for 5% and 10% of labeled data.

p	AUC-ROC			AUC-PR		
	5%	10%	20%	5%	10%	20%
Transductive setting						
EM	82.2 ± 0.6	82.9 ± 0.6	84.6 ± 0.6	15.7 ± 1.4	16.5 ± 2.7	19.7 ± 0.7
PKMR	77.5 ± 2.3	80.8 ± 1.1	83.9 ± 1.2	6.1 ± 1.5	9.8 ± 1.8	13.8 ± 1.2
IOKR	80.6 ± 0.7	83.1 ± 0.5	83.9 ± 0.5	7.1 ± 1.1	11.7 ± 1.1	17.8 ± 1.5
Semi-supervised setting						
IOKR	81.0 ± 1.1	82.9 ± 1.2	83.8 ± 1.0	6.6 ± 1.6	10.5 ± 1.3	16.0 ± 2.3

Table 6: AUC-ROC and AUC-PR obtained for the PPI network inference with EM, PKMR, IOKR in the transductive setting, and with IOKR in the semi-supervised setting.

p	5%	10%	20%
EM	0.19 ± 0.01	0.19 ± 0.00	0.22 ± 0.04
PKMR	0.16 ± 0.01	0.18 ± 0.00	0.19 ± 0.01
IOKR	1.61 ± 0.01	1.63 ± 0.01	1.76 ± 0.22

Table 7: Averaged running time in seconds of one repetition for the yeast PPI network reconstruction in the transductive setting.

However we can notice that the EM-based approach is purely transductive while IOKR-ridge learns a function and can therefore be used in the semi-supervised learning, which is more general. Regarding the IOKR-ridge results in the semi-supervised setting, we observe that the performances are very similar to the ones obtained in the transductive setting. We also compared in Table 7 the averaged running time for different percentages of labeled data. We can first observe that the three methods have a small running time (less than 2 seconds). EM and PKMR are a bit faster than IOKR-ridge as these methods require to inverse a matrix of size $\ell \times \ell$ while IOKR-ridge needs to inverse a matrix of size $(\ell+n) \times (\ell+n)$.

6.2 Application to Multi-Task Regression

In the following, we compare the behavior of the three models proposed for multi-task learning with IOKR in Section 5 on a drug activity prediction problem. The goal of this problem is to predict the activities of molecules in different cancer cell lines (cancer types). This problem has potential applications in cancer drug discovery. In this application, \mathcal{X} corresponds to the set of molecules and $\mathcal{Y} = \mathcal{F}_y = \mathbb{R}^d$, where d is the number of cell lines.

6.2.1 DATASET

We used the dataset of Su et al. (2010) that contains the biological activities of molecules against a set of 59 human cancer cell lines. These data have been extracted from the NCI-Cancer dataset. We used the "No-Zero-Active" version of the dataset which contains the 2303 molecules that are all active against at least one cell line. Each molecule is represented by a graph, where nodes correspond to atoms and edges to bonds between atoms. The Tanimoto kernel (Ralaivola et al., 2005) is used for the scalar input kernel:

$$\kappa_x(x, x') = \frac{k_m(x, x')}{k_m(x, x) + k_m(x', x') - k_m(x, x')}.$$

In this application, k_m is chosen as a linear path kernel. The corresponding input feature vectors $\varphi_{x_m}(x)$ are binary vectors that indicate the presences and absences in the molecules of all existing paths containing a maximum of m bonds. In this experiment, the value of m was set to 6.

6.2.2 PROTOCOL

We evaluated the behavior of the IOKR-ridge model in the transductive setting. The performances were measured by computing the mean squared error (MSE) on the unlabeled

set:

$$MSE = \frac{1}{n} \sum_{i=\ell+1}^{\ell+n} \|h(x_i) - \varphi_y(\mathbf{y}_i)\|_{\mathcal{F}_y}^2.$$

We estimated the task structure between the cancer types by comparing the molecular activities associated to each cancer type on the training set:

$$M_{ij} = \exp\left(-\gamma \|Y_\ell^i - Y_\ell^j\|^2\right), \quad i, j = 1, \dots, d,$$

where $Y_\ell^i = (\mathbf{y}_1^i, \mathbf{y}_2^i, \dots, \mathbf{y}_\ell^i)$.

The parameter γ of the matrix M was chosen to maximize an information criterion and the regularization parameter λ_1 was set to 1. Regarding the matrix W used in the semi-supervised term, we sparsified the Gram matrix $K_{x_{\ell+n}}$ of the scalar input kernel κ_x using a k -nearest neighbors procedure with $k = 50$. We then computed the graph Laplacian of the obtained graph and considered the Laplacian iterated to degree 5.

6.2.3 RESULTS

The results presented in Figure 6 were obtained from ten random choices of the training set. The performances obtained with model 1 and model 2 for different percentages of labeled data are represented as a function of the parameters μ and λ_2 .

We observe on this figure that for both models, using unlabeled data helps to improve the performances. We also observe that when μ is increased from 0 to 0.8 or 1, the mean squared errors are decreased. The obtained results therefore show the benefit of taking into account the relationships existing between the outputs for both models and both settings (supervised and semi-supervised).

We reported on Figure 7 the MSE obtained with models 1 and 2 for the best parameter μ and added the results obtained with the model 0, which corresponds to the case where $A = I$. We observe on this figure that the model 2 obtains better results than the model 1 when the percentage of labeled data is small ($p = 5\%$). For $p = 10\%$, the two models behave similarly, while for 20% of labeled data, the model 1 improves significantly the performances, compared to model 2. Therefore, we observe that using the output structure information either in the input operator-valued kernel or in the output kernel leads to different results. And depending on the amount of labeled data, one of the two models can be more interesting to use.

7. Conclusion and Perspectives

Operator-valued kernels and the associated RKHS theory provide a general framework to address approximation of functions with values in some Hilbert space. When characterizing the output Hilbert space as a feature space related to some real-valued scalar kernel, we get an original framework to deal with structured outputs. Extending our previous work (Brouard et al., 2011) which introduced a new representer theorem for semi-supervised learning with vector-valued functions, we presented solutions of semi-supervised penalized regression developed for two empirical loss functions, the square loss and the hinge loss in the general case and in the special case of decomposable kernels using tensors. We also showed

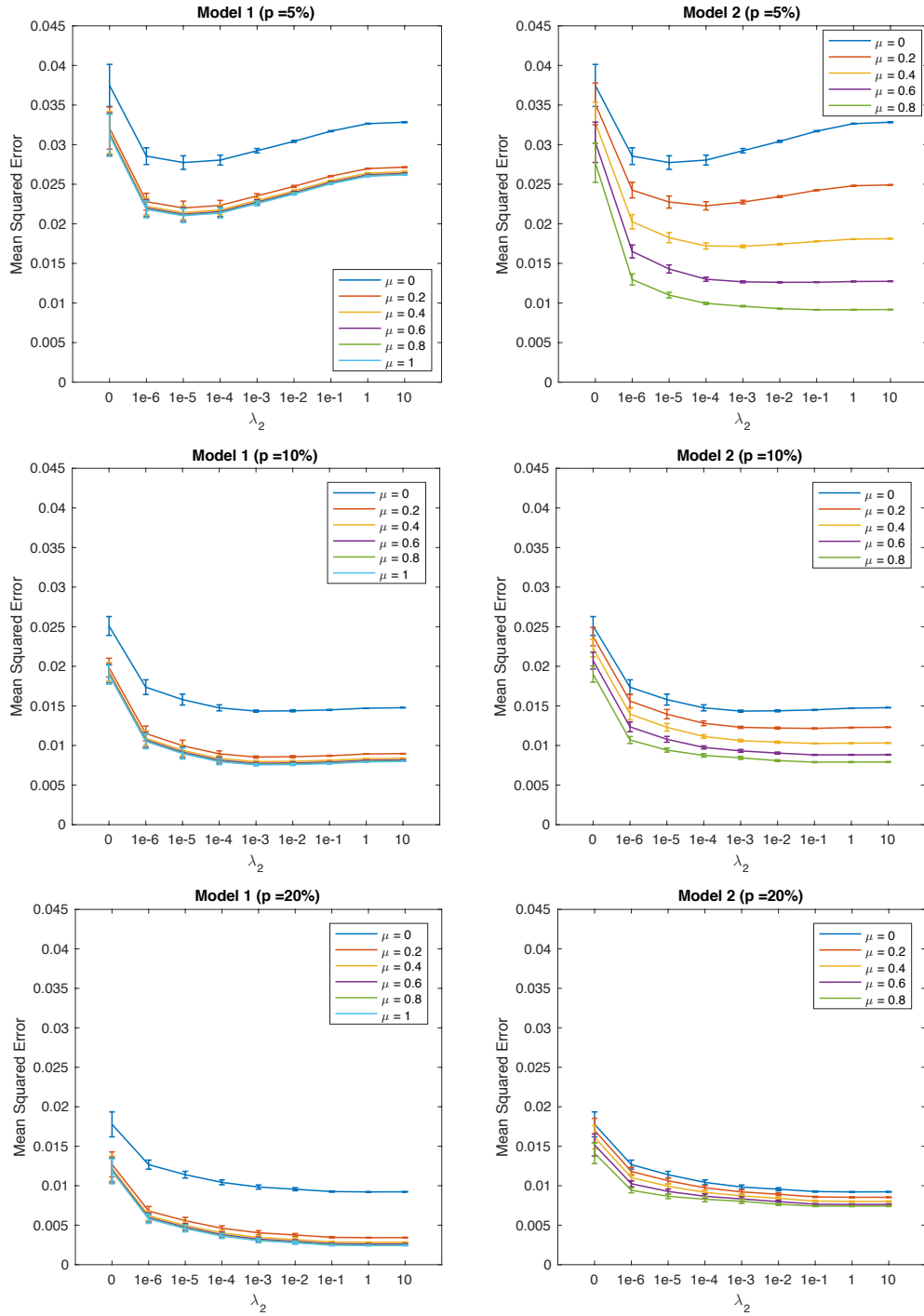


Figure 6: Mean squared errors obtained with the two models for the prediction of molecular activities. The results are averaged over ten random choices of the training set and are given for different percentages of labeled data (5%, 10% and 20%).

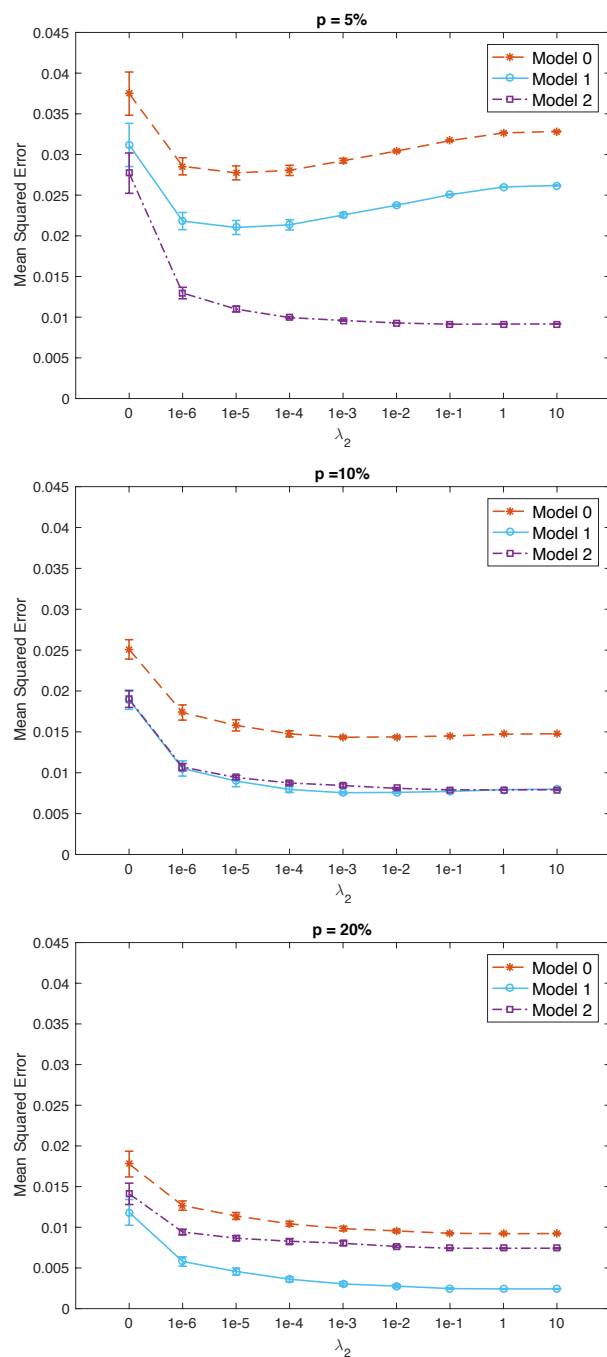


Figure 7: Mean squared errors obtained for the prediction of molecular activities for the model 0 (corresponding to $A = I$), model 1 ($\mu = 1$) and model 2 ($\mu = 0.8$). The results are averaged over ten random training sets and are given for different percentages of labeled data (5%, 10% and 20%).

that Generalized Cross-Validation extends in the case of the closed-form solution of IOKR-ridge, providing an efficient tool for model selection. Perspectives to this work concern the construction of new models by minimizing loss functions with different penalties, for instance, penalties that enforce the parsimony of the model. For these non-smooth penalties, proximal gradient descent methods can be applied such as in Lim et al. (2013). A more general research direction is related to the design of new kernels and appropriate kernel learning algorithms. Finally, although the pre-image problem has received a lot of attention in the literature, there is still room for improvement in order to apply IOKR in other tasks than link prediction or multiple output structured regression.

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Appendix A. Technical Proofs

In this appendix section, we provide the proofs for some theorems and propositions presented in the paper.

A.1 Proof of Theorem 7

We derive here the solution obtained for the Maximum Margin Regression optimization problem in the semi-supervised setting (Equation 8). We begin by writing the primal formulation of this optimization problem:

$$\begin{aligned} \min_{h \in \mathcal{H}, \xi \in \mathbb{R}^\ell} \quad & \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h(x_i), h(x_j) \rangle_{\mathcal{F}_y} + \sum_{i=1}^{\ell} \xi_i \\ \text{s.t.} \quad & \langle \tilde{\mathbf{y}}_i, h(x_i) \rangle_{\mathcal{F}_y} \geq 1 - \xi_i, i = 1, \dots, \ell \\ & \xi_i \geq 0, i = 1, \dots, \ell. \end{aligned}$$

We write the corresponding Lagrangian:

$$\begin{aligned} \mathcal{L}_a(h, \xi, \alpha, \eta) = & \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h(x_i), h(x_j) \rangle_{\mathcal{F}_y} + \sum_{i=1}^{\ell} \xi_i \\ & - \sum_{i=1}^{\ell} \alpha_i (\langle \tilde{\mathbf{y}}_i, h(x_i) \rangle_{\mathcal{F}_y} - 1 + \xi_i) - \sum_{i=1}^{\ell} \eta_i \xi_i. \end{aligned}$$

In the following we note $K_x = \mathcal{K}_x(\cdot, x)$ and $K_x^* = \mathcal{K}_x(x, \cdot)$. By using the reproducing property the expression of the Lagrangian becomes:

$$\begin{aligned}
 \mathcal{L}_a &= \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle K_{x_i}^* h, K_{x_j}^* h \rangle_{\mathcal{H}} - \sum_{i=1}^{\ell} \alpha_i (\langle \tilde{\mathbf{y}}_i, K_{x_i}^* h \rangle_{\mathcal{H}} - 1) + \sum_{i=1}^{\ell} (1 - \alpha_i - \eta_i) \xi_i \\
 &= \langle (\lambda_1 I + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} K_{x_j} K_{x_i}^*) h, h \rangle_{\mathcal{H}} - \sum_{i=1}^{\ell} \alpha_i \langle K_{x_i} \tilde{\mathbf{y}}_i, h \rangle_{\mathcal{H}} + \sum_{i=1}^{\ell} \alpha_i + \sum_{i=1}^{\ell} (1 - \alpha_i - \eta_i) \xi_i \\
 &= \langle Bh, h \rangle_{\mathcal{H}} - \sum_{i=1}^{\ell} \alpha_i \langle K_{x_i} \tilde{\mathbf{y}}_i, h \rangle_{\mathcal{H}} + \sum_{i=1}^{\ell} \alpha_i + \sum_{i=1}^{\ell} (1 - \alpha_i - \eta_i) \xi_i,
 \end{aligned}$$

where $B \in \mathcal{B}(h)$ is the operator defined as: $B = \lambda_1 I + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} K_{x_i} K_{x_j}^*$. Due to the symmetry of the Laplacian L , this operator is self-adjoint:

$$B^* = \lambda_1 I + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} K_{x_j} K_{x_i}^* = \lambda_1 I + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ji} K_{x_i} K_{x_j}^* = \lambda_1 I + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} K_{x_i} K_{x_j}^* = B.$$

Differentiating the Lagrangian with respect to ξ_i and h gives:

$$\begin{aligned}
 \frac{\partial \mathcal{L}_a}{\partial \xi_i} &= 0 \Rightarrow 1 - \alpha_i - \eta_i = 0 \\
 \frac{\partial \mathcal{L}_a}{\partial h} &= 0 \Rightarrow 2Bh - \sum_{i=1}^{\ell} \alpha_i K_{x_i} \tilde{\mathbf{y}}_i = 0 \Rightarrow h = \frac{1}{2} B^{-1} \left(\sum_{i=1}^{\ell} \alpha_i K_{x_i} \tilde{\mathbf{y}}_i \right).
 \end{aligned}$$

B is invertible as it is a positive definite operator:

$$\begin{aligned}
 \forall h \in \mathcal{H}, \langle h, Bh \rangle_{\mathcal{H}} &= \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h, K_{x_j} K_{x_i}^* h \rangle_{\mathcal{H}} \\
 &= \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h(x_j), h(x_i) \rangle_{\mathcal{F}_y} \\
 &= \lambda_1 \|h\|_{\mathcal{H}}^2 + \lambda_2 \sum_{i,j=1}^{\ell+n} W_{ij} \|h(x_j) - h(x_i)\|_{\mathcal{F}_y}^2 \\
 &> 0 \text{ for all non-zero function } h.
 \end{aligned}$$

The last inequality is deduced from the assumption that the values of W are non-negative. We formulate a reduced Lagrangian :

$$\begin{aligned}
 \mathcal{L}_r(\alpha) &= \frac{1}{4} \sum_{i,j=1}^{\ell} \alpha_i \alpha_j \langle BB^{-1} K_{x_i} \tilde{\mathbf{y}}_i, B^{-1} K_{x_j} \tilde{\mathbf{y}}_j \rangle_{\mathcal{H}} - \frac{1}{2} \sum_{i,j=1}^{\ell} \alpha_i \alpha_j \langle K_{x_i} \tilde{\mathbf{y}}_i, B^{-1} K_{x_j} \tilde{\mathbf{y}}_j \rangle_{\mathcal{H}} + \sum_{i=1}^{\ell} \alpha_i \\
 &= -\frac{1}{4} \sum_{i,j=1}^{\ell} \alpha_i \alpha_j \langle K_{x_i} \tilde{\mathbf{y}}_i, B^{-1} K_{x_j} \tilde{\mathbf{y}}_j \rangle_{\mathcal{H}} + \sum_{i=1}^{\ell} \alpha_i.
 \end{aligned}$$

The dual formulation of the optimization problem (8) can thus be expressed as:

$$\begin{aligned} \min_{\alpha \in \mathbb{R}^\ell} \quad & \frac{1}{4} \sum_{i,j=1}^{\ell} \alpha_i \alpha_j \langle K_{x_i} \tilde{y}_i, B^{-1} K_{x_j} \tilde{y}_j \rangle_{\mathcal{H}} - \sum_{i=1}^{\ell} \alpha_i \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq 1, i = 1, \dots, \ell. \end{aligned}$$

This concludes the proof.

A.2 Proof of Proposition 9

We start from the expression of $\text{vec}(C_{\ell+n})$ given in Section 3.3 for the least-squares loss and replace A by its eigendecomposition:

$$\text{vec}(C_{\ell+n}) = (\lambda_1 I_{(\ell+n)d} + M \otimes A)^{-1} \text{vec}(\tilde{Y}_\ell J),$$

where $M = (J^T J + 2\lambda_2 L) K_{X_{\ell+n}}$.

We introduce the vec-permutation matrices P_{mn} and P_{nm} defined as:

$$\forall A \in \mathbb{R}^{m \times n}, \text{vec}(A^T) = P_{mn} \text{vec}(A) \text{ and } \text{vec}(A) = P_{nm} \text{vec}(A^T).$$

For any $m \times n$ matrix A and $p \times q$ matrix B ,

$$B \otimes A = P_{pm}(A \otimes B)P_{nq}.$$

Using these properties, we can write:

$$\begin{aligned} \text{vec}(C_{\ell+n}^T) &= P_{d(\ell+n)} \text{vec}(C_{\ell+n}) \\ &= P_{d(\ell+n)} (\lambda_1 I_{(\ell+n)d} + P_{(\ell+n)d}(A \otimes M)P_{d(\ell+n)})^{-1} \text{vec}(\tilde{Y}_\ell J) \\ &= (\lambda_1 I_{(\ell+n)d} + P_{d(\ell+n)} P_{(\ell+n)d}(A \otimes M))^{-1} P_{d(\ell+n)} \text{vec}(\tilde{Y}_\ell J) \\ &= (\lambda_1 I_{(\ell+n)d} + A \otimes M)^{-1} \text{vec}(J^T \tilde{Y}_\ell^T) \\ &= (\lambda_1 I_{(\ell+n)d} + E \Gamma E^T \otimes M)^{-1} \text{vec}(J^T \tilde{Y}_\ell^T). \end{aligned}$$

We multiply each side by $(E^T \otimes I_{\ell+n})$

$$\begin{aligned} (E^T \otimes I_{\ell+n}) \text{vec}(C_{\ell+n}^T) &= \\ (E^T \otimes I_{\ell+n}) (\lambda_1 I_{(\ell+n)d} + (E \otimes I_{\ell+n})(\Gamma \otimes M)(E^T \otimes I_{\ell+n}))^{-1} \text{vec}(J^T \tilde{Y}_\ell^T). \end{aligned}$$

We use the facts that $\text{vec}(AXB) = (B^T \otimes A) \text{vec}(X)$ and that $E^T E = I_d$ to obtain the following equation:

$$\text{vec}(C_{\ell+n}^T E) = (\lambda_1 I_{(\ell+n)d} + \Gamma \otimes M)^{-1} \text{vec}(J^T \tilde{Y}_\ell^T E).$$

The matrix $(\lambda_1 I_{(\ell+n)d} + \Gamma \otimes M)$ being block-diagonal, we have

$$C_{\ell+n}^T \mathbf{e}_i = (\lambda_1 I_{\ell+n} + \gamma_i M)^{-1} J^T \tilde{Y}_\ell^T \mathbf{e}_i, \text{ for } i = 1, \dots, \ell + n.$$

Then, we can express the model h as:

$$\begin{aligned} \forall x \in \mathcal{X}, h(x) &= AC_{\ell+n}\boldsymbol{\kappa}_{x_{\ell+n}}^x = \sum_{j=1}^d \gamma_j \mathbf{e}_j \mathbf{e}_j^T C_{\ell+n} \boldsymbol{\kappa}_{x_{\ell+n}}^x \\ &= \sum_{j=1}^d \gamma_j \mathbf{e}_j \mathbf{e}_j^T \tilde{Y}_\ell J (\lambda_1 I_{\ell+n} + \gamma_j K_{X_{\ell+n}} (J^T J + 2\lambda_2 L))^{-1} \boldsymbol{\kappa}_{X_{\ell+n}}^x. \end{aligned}$$

In the supervised setting ($\lambda_2 = 0$), the model h writes as:

$$\forall x \in \mathcal{X}, h(x) = \sum_{j=1}^d \gamma_j \mathbf{e}_j \mathbf{e}_j^T \tilde{Y}_\ell (\lambda_1 I_\ell + \gamma_j K_{X_\ell})^{-1} \boldsymbol{\kappa}_{X_\ell}^x.$$

This completes the proof.

A.3 Proof of Proposition 10

Let $Z_\ell = \tilde{Y}_\ell \text{diag}(\boldsymbol{\alpha})J$. We start from the expression of the Lagrangian in the case of a general operator-valued kernel (Equation 10) and replace A by its eigendecomposition:

$$\begin{aligned} \mathcal{L}_a(\boldsymbol{\alpha}) &= -\frac{1}{4} \text{vec}(Z_\ell)^T (\lambda_1 I_{(\ell+n)d} + 2\lambda_2 K_{X_{\ell+n}} L \otimes A)^{-1} (K_{X_{\ell+n}} \otimes A) \text{vec}(Z_\ell) + \boldsymbol{\alpha}^T \mathbf{1} \\ &= -\frac{1}{4} \text{vec}(Z_\ell)^T (\lambda_1 I_{(\ell+n)d} + 2\lambda_2 (I_{\ell+n} \otimes E)(K_{X_{\ell+n}} L \otimes \Gamma)(I_{\ell+n} \otimes E^T))^{-1} \\ &\quad (I_{\ell+n} \otimes E)(K_{X_{\ell+n}} \otimes \Gamma)(I_{\ell+n} \otimes E^T) \text{vec}(Z_\ell) + \boldsymbol{\alpha}^T \mathbf{1}. \\ &= -\frac{1}{4} \text{vec}(E^T Z_\ell)^T (\lambda_1 I_{(\ell+n)d} + 2\lambda_2 K_{X_{\ell+n}} L \otimes \Gamma)^{-1} (K_{X_{\ell+n}} \otimes \Gamma) \text{vec}(E^T Z_\ell) + \boldsymbol{\alpha}^T \mathbf{1}. \end{aligned}$$

Using the vec-permutation matrices, we can show that:

$$\mathcal{L}_a(\boldsymbol{\alpha}) = -\frac{1}{4} \text{vec}(Z_\ell^T E)^T (\lambda_1 I_{(\ell+n)d} + 2\lambda_2 \Gamma \otimes K_{X_{\ell+n}} L)^{-1} (\Gamma \otimes K_{X_{\ell+n}}) \text{vec}(Z_\ell^T E) + \boldsymbol{\alpha}^T \mathbf{1}.$$

As $(\lambda_1 I_{(\ell+n)d} + 2\lambda_2 \Gamma \otimes K_{X_{\ell+n}} L)$ is a block diagonal matrix, we can write:

$$\begin{aligned} \mathcal{L}_a(\boldsymbol{\alpha}) &= -\frac{1}{4} \sum_{i=1}^d \mathbf{e}_i^T Z_\ell (\lambda_1 I_{\ell+n} + 2\lambda_2 \gamma_i K_{X_{\ell+n}} L)^{-1} \gamma_i K_{X_{\ell+n}} Z_\ell^T \mathbf{e}_i + \boldsymbol{\alpha}^T \mathbf{1} \\ &= -\frac{1}{4} \sum_{i=1}^d \gamma_i \text{trace} \left(\tilde{Y}_\ell^T \mathbf{e}_i \mathbf{e}_i^T \tilde{Y}_\ell \text{diag}(\boldsymbol{\alpha}) J (\lambda_1 I_{\ell+n} + 2\lambda_2 \gamma_i K_{X_{\ell+n}} L)^{-1} K_{X_{\ell+n}} J^T \text{diag}(\boldsymbol{\alpha}) \right) \\ &\quad + \boldsymbol{\alpha}^T \mathbf{1}. \end{aligned}$$

Using the fact that $\mathbf{y}^T (A \circ B) \mathbf{x} = \text{trace}(\text{diag}(\mathbf{y})^T A \text{diag}(\mathbf{x}) B^T)$, the Lagrangian can be written as:

$$\mathcal{L}_a(\boldsymbol{\alpha}) = -\frac{1}{4} \sum_{i=1}^d \gamma_i \boldsymbol{\alpha}^T (\tilde{Y}_\ell^T \mathbf{e}_i \mathbf{e}_i^T \tilde{Y}_\ell \circ J (\lambda_1 I_{\ell+n} + 2\lambda_2 \gamma_i K_{X_{\ell+n}} L)^{-1} K_{X_{\ell+n}} J^T) \boldsymbol{\alpha} + \boldsymbol{\alpha}^T \mathbf{1}.$$

In the supervised setting ($\lambda_2 = 0$), the Lagrangian becomes:

$$\begin{aligned}\mathcal{L}_a(\boldsymbol{\alpha}) &= -\frac{1}{4\lambda_1} \sum_{i=1}^d \gamma_i \boldsymbol{\alpha}^T (\tilde{Y}_\ell^T \mathbf{e}_i \mathbf{e}_i^T \tilde{Y}_\ell \circ K_{X_\ell}) \boldsymbol{\alpha} + \boldsymbol{\alpha}^T \mathbf{1} \\ &= -\frac{1}{4\lambda_1} \boldsymbol{\alpha}^T (\tilde{Y}_\ell^T A \tilde{Y}_\ell \circ K_{X_\ell}) \boldsymbol{\alpha} + \boldsymbol{\alpha}^T \mathbf{1},\end{aligned}$$

which concludes the proof.

Appendix B. Dual Optimization Problem for a General Convex Loss Function

In this appendix we derive the dual optimization problem for a general convex loss function in the supervised and semi-supervised settings using the Fenchel duality.

B.1 Supervised Setting

We consider the following optimization problem where the cost function $\mathcal{L} : \mathcal{F}_y \times \mathcal{F}_y \rightarrow \mathbb{R}$ is convex in its first variable:

$$\min_{h \in \mathcal{H}} \sum_{i=1}^{\ell} \mathcal{L}(h(x_i), \tilde{\mathbf{y}}_i) + \lambda \|h\|_{\mathcal{H}}^2.$$

It can be rewritten by introducing the constraint $\mathbf{u}_i = h(x_i)$ and the function $\mathcal{L}_i : \mathcal{F}_y \rightarrow \mathbb{R}$ defined as $\mathcal{L}_i(\mathbf{u}_i) = \mathcal{L}(\mathbf{u}_i, \tilde{\mathbf{y}}_i)$ for $i \in [1, \ell]$:

$$\begin{aligned}\min_{h \in \mathcal{H}, \{\mathbf{u}_i \in \mathcal{F}_y\}_{i=1}^{\ell}} \quad & \sum_{i=1}^{\ell} \mathcal{L}_i(\mathbf{u}_i) + \lambda \|h\|_{\mathcal{H}}^2 \\ \text{s.t.} \quad & \mathbf{u}_i = h(x_i), \quad i = 1, \dots, \ell.\end{aligned}$$

We write the expression of the Lagrangian:

$$\begin{aligned}\mathcal{L}_a(h, \mathbf{u}_i, \boldsymbol{\alpha}_i) &= \sum_{i=1}^{\ell} \mathcal{L}_i(\mathbf{u}_i) + \lambda \|h\|_{\mathcal{H}}^2 + \sum_{i=1}^{\ell} \langle \boldsymbol{\alpha}_i, \mathbf{u}_i - h(x_i) \rangle_{\mathcal{F}_y} \\ &= \sum_{i=1}^{\ell} \mathcal{L}_i(\mathbf{u}_i) + \lambda \|h\|_{\mathcal{H}}^2 + \sum_{i=1}^{\ell} \langle \boldsymbol{\alpha}_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} - \sum_{i=1}^{\ell} \langle \mathcal{K}_x(\cdot, x_i) \boldsymbol{\alpha}_i, h \rangle_{\mathcal{H}}.\end{aligned}$$

The dual function can be written:

$$\begin{aligned}
 g(\alpha) &= \inf_{h \in \mathcal{H}, \{\mathbf{u}_i \in \mathcal{F}_y\}_{i=1}^\ell} \left(\sum_{i=1}^\ell \mathcal{L}_i(\mathbf{u}_i) + \lambda \|h\|_{\mathcal{H}}^2 + \sum_{i=1}^\ell \langle \alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} - \sum_{i=1}^\ell \langle \mathcal{K}_x(\cdot, x_i) \alpha_i, h \rangle_{\mathcal{H}} \right) \\
 &= \sum_{i=1}^\ell \inf_{\mathbf{u}_i \in \mathcal{F}_y} (\mathcal{L}_i(\mathbf{u}_i) + \langle \alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y}) + \inf_h \left(\lambda \|h\|_{\mathcal{H}}^2 - \sum_{i=1}^\ell \langle \mathcal{K}_x(\cdot, x_i) \alpha_i, h \rangle_{\mathcal{H}} \right) \\
 &= - \sum_{i=1}^\ell \sup_{\mathbf{u}_i \in \mathcal{F}_y} (-\mathcal{L}_i(\mathbf{u}_i) + \langle -\alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y}) + \inf_h \left(\lambda \|h\|_{\mathcal{H}}^2 - \sum_{i=1}^\ell \langle \mathcal{K}_x(\cdot, x_i) \alpha_i, h \rangle_{\mathcal{H}} \right) \\
 g(\alpha) &= - \sum_{i=1}^\ell \mathcal{L}_i^*(-\alpha_i) - \frac{1}{4\lambda} \sum_{i,j=1}^\ell \langle \alpha_i, \mathcal{K}_x(x_i, x_j) \alpha_j \rangle_{\mathcal{F}_y},
 \end{aligned}$$

where \mathcal{L}_i^* denotes the convex conjugate, also called Fenchel conjugate, of the function \mathcal{L}_i :

$$\mathcal{L}_i^*(\alpha_i) = \sup_{\mathbf{u}_i \in \mathcal{F}_y} \langle \alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} - \mathcal{L}_i(\mathbf{u}_i)$$

and $h = \frac{1}{2\lambda} \sum_{i=1}^\ell \mathcal{K}_x(\cdot, x_i) \alpha_i$.

The dual optimization problem for a general convex loss function writes as follows:

$$\max_{\{\alpha_i \in \mathcal{F}_y\}_{i=1}^\ell} - \sum_{i=1}^\ell \mathcal{L}_i^*(-\alpha_i) - \frac{1}{4\lambda} \sum_{i,j=1}^\ell \langle \alpha_i, \mathcal{K}_x(x_i, x_j) \alpha_j \rangle_{\mathcal{F}_y}. \quad (14)$$

In the following, we derive it for the least-squares and the MMR loss functions.

B.1.1 LEAST-SQUARES LOSS

We compute the convex conjugate of the least-squares loss:

$$\mathcal{L}_i^*(-\alpha_i) = \sup_{\mathbf{u}_i \in \mathcal{F}_y} -\langle \alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} - \|\mathbf{u}_i - \tilde{\mathbf{y}}_i\|_{\mathcal{F}_y}^2.$$

By setting the derivative $\frac{\partial \mathcal{L}_i^*}{\partial \mathbf{u}_i}$ to 0 we find that $\mathbf{u}_i = \tilde{\mathbf{y}}_i - \frac{1}{2} \alpha_i$. By substituting we see that:

$$\mathcal{L}_i^*(-\alpha_i) = \frac{1}{4} \|\alpha_i\|_{\mathcal{F}_y}^2 - \langle \alpha_i, \tilde{\mathbf{y}}_i \rangle_{\mathcal{F}_y}.$$

We replace the expression of $\mathcal{L}_i^*(-\alpha_i)$ in the dual problem:

$$\max_{\{\alpha_i \in \mathcal{F}_y\}_{i=1}^\ell} - \frac{1}{4} \sum_{i=1}^\ell \|\alpha_i\|_{\mathcal{F}_y}^2 + \sum_{i=1}^\ell \langle \alpha_i, \tilde{\mathbf{y}}_i \rangle_{\mathcal{F}_y} - \frac{1}{4\lambda} \sum_{i,j=1}^\ell \langle \alpha_i, \mathcal{K}_x(x_i, x_j) \alpha_j \rangle_{\mathcal{F}_y}.$$

We derive with respect to α_i , $i = 1, \dots, \ell$ and find that the solution of the dual optimization problem satisfy the following equations:

$$\sum_{j=1}^\ell (\mathcal{K}_x(x_i, x_j) + \lambda \delta_{ij}) \alpha_j = 2\lambda \tilde{\mathbf{y}}_i, \quad i = 1, \dots, \ell.$$

B.1.2 MAXIMUM MARGIN REGRESSION

We compute the convex conjugate function of the MMR loss using the Lagrange technique:

$$\begin{aligned}
 -\mathcal{L}_i^*(-\alpha_i) &= - \sup_{\mathbf{u}_i \in \mathcal{F}_y} \{ -\langle \alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} - \max(0, 1 - \langle \tilde{\mathbf{y}}_i, \mathbf{u}_i \rangle_{\mathcal{F}_y}) \} \\
 &= \inf_{\substack{\mathbf{u}_i \in \mathcal{F}_y, \xi_i \in \mathbb{R} \\ \xi_i \geq 0, \xi_i \geq 1 - \langle \tilde{\mathbf{y}}_i, \mathbf{u}_i \rangle_{\mathcal{F}_y}}} \{ \langle \alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} + \xi_i \} \\
 &= \sup_{\beta_i, \eta_i \geq 0} \left\{ \inf_{\mathbf{u}_i \in \mathcal{F}_y, \xi_i \in \mathbb{R}} \{ \langle \alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} + \xi_i + \beta_i(1 - \langle \tilde{\mathbf{y}}_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} - \xi_i) - \eta_i \xi_i \} \right\} \\
 &= \sup_{\beta_i, \eta_i \geq 0} \left\{ \inf_{\mathbf{u}_i \in \mathcal{F}_y} \{ \langle \alpha_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} - \beta_i \langle \tilde{\mathbf{y}}_i, \mathbf{u}_i \rangle_{\mathcal{F}_y} \} + \inf_{\xi_i \in \mathbb{R}} \{ \xi_i - \beta_i \xi_i - \eta_i \xi_i \} + \beta_i \right\} \\
 &= \sup_{\substack{0 \leq \beta_i \leq 1 \\ \alpha_i = \beta_i \tilde{\mathbf{y}}_i}} \beta_i.
 \end{aligned}$$

This means that $-\mathcal{L}_i^*(-\alpha_i) = \beta_i$ at the condition that $\alpha_i = \beta_i \tilde{\mathbf{y}}_i$ and $0 \leq \beta_i \leq 1$. Otherwise it is unbounded. We replace in the dual problem in Equation (14):

$$\begin{aligned}
 \max_{\beta \in \mathbb{R}^\ell} \quad & \sum_{i=1}^{\ell} \beta_i - \frac{1}{4\lambda} \sum_{i,j=1}^{\ell} \beta_i \beta_j \langle \tilde{\mathbf{y}}_i, \mathcal{K}_x(x_i, x_j) \tilde{\mathbf{y}}_j \rangle_{\mathcal{F}_y} \\
 \text{s.t.} \quad & 0 \leq \beta_i \leq 1, \quad i = 1, \dots, \ell.
 \end{aligned}$$

B.2 Semi-supervised Setting

In the semi-supervised setting, the optimization problem can be written as:

$$\begin{aligned}
 \min_{h \in \mathcal{H}, \{\mathbf{u}_i \in \mathcal{F}_y\}_{i=1}^{\ell}} \quad & \sum_{i=1}^{\ell} \mathcal{L}(\mathbf{u}_i, \tilde{\mathbf{y}}_i) + \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h(x_i), h(x_j) \rangle_{\mathcal{F}_y} \\
 \text{s.t.} \quad & \mathbf{u}_i = h(x_i), \quad i = 1, \dots, \ell.
 \end{aligned}$$

We write the expression of the dual function:

$$\begin{aligned}
 g(\alpha) &= \inf_{\substack{h \in \mathcal{H} \\ \mathbf{u}_i \in \mathcal{F}_y}} \sum_{i=1}^{\ell} \mathcal{L}(\mathbf{u}_i, \tilde{\mathbf{y}}_i) + \lambda_1 \|h\|_{\mathcal{H}}^2 + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \langle h(x_i), h(x_j) \rangle_{\mathcal{F}_y} + \sum_{i=1}^{\ell} \langle \alpha_i, \mathbf{u}_i - h(x_i) \rangle_{\mathcal{F}_y} \\
 &= - \sum_{i=1}^{\ell} \mathcal{L}_i^*(-\alpha_i) + \inf_{h \in \mathcal{H}} \left(\langle Bh, h \rangle_{\mathcal{H}} - \sum_{i=1}^{\ell} \langle K_{x_i} \alpha_i, h \rangle_{\mathcal{H}} \right),
 \end{aligned}$$

where $B \in \mathcal{B}(h)$ is the operator defined as: $B = \lambda_1 I + 2\lambda_2 \sum_{i,j=1}^{\ell+n} L_{ij} \mathcal{K}_x(\cdot, x_j) \mathcal{K}_x(x_i, \cdot)$.

By setting the derivative of the second term with respect to h to zero we find that: $h = \frac{1}{2} B^{-1} \left(\sum_{i=1}^{\ell} \mathcal{K}_x(\cdot, x_i) \alpha_i \right)$. The proof that B can be inverted was already given in Appendix A.1.

We replace in the dual function and obtain the following dual optimization problem:

$$\max_{\{\alpha_i \in \mathcal{F}_y\}_{i=1}^\ell} - \sum_{i=1}^\ell \mathcal{L}_i^*(-\alpha_i) - \frac{1}{4} \sum_{i,j=1}^\ell \langle K_{x_i} \alpha_i, B^{-1} K_{x_j} \alpha_j \rangle_{\mathcal{H}}.$$

Appendix C. Additional Results on Synthetic Networks

This appendix contains additional results on synthetic networks.

C.1 Influence of the Level of Inertia

We experimented how IOKR behaves with perfect to noisy input features on the synthetic networks. We modified the quality of the input representation by varying the relative inertia captured by the first components. We chose four different levels of inertia: 75%, 85%, 95% and 100%. The results obtained with IOKR-ridge and IOKR-margin are shown in Table 8.

For both methods we observe small differences in term of AUC-ROC when the inertia varies between 75% and 100%. On the other hand, there is more variation in the AUC-PR results, especially for a low graph density. The difference between the AUC-PRs for 75% and 100% of inertia increases when the percentage of labeled nodes is increased. Overall IOKR is robust to the noise level of the input data in all the cases for the AUC-ROC, and in the networks of density 0.01 and 0.02 for the AUC-PR.

C.2 Mixture of Erdős-Renyi Random Graphs

We generated synthetic networks using mixtures of Erdős-Renyi random graphs. The 700 nodes of the graphs were divided equally in three classes. We considered that the connection probability between a node belonging to the class i and a node in the class j can take two values:

$$\forall i, j \in \{1, \dots, 3\}, p_{i,j} = \begin{cases} p_{intra} & \text{if } i = j, \\ p_{inter} & \text{if } i \neq j. \end{cases}$$

We evaluated the performances of IOKR-ridge and IOKR-margin on these random networks for $p_{intra} \in \{0.02, 0.03\}$ and $p_{inter} \in \{5 * 10^{-4}, 10^{-3}\}$. The input vectors were derived from the diffusion kernel applied on the network as described in Section 6.1.2. These results are reported in Table 9. For IOKR-margin, we observe that the AUC values stay relatively similar for the different networks and also for the different percentage of labeled data. On the opposite, IOKR-ridge presents better performances when the inter-class connection probability is higher. As in Section 6.1.2, in which we noted that denser networks are more difficult to predict, we observe here that the AUC values decrease when the intra-class connection probability increases.

In Figure 8, we illustrate the fact that IOKR is able to recover the clusters present in a synthetic network ($p_{intra} = 0.02$, $p_{inter}=5e-4$). The true network is shown on the left and the network predicted with IOKR-ridge is shown on the right. The predicted network was obtained by thresholding the values in the predicted output kernel. The value of the threshold was selected with the other parameters on the training set such that it maximizes the F1-score value.

a) IOKR-ridge:

pdens	var %	nc	AUC-ROC			AUC-PR		
			p=5%	p=10%	p=20%	p=5%	p=10%	p=20%
0.007	75	69	92.3 ± 0.4	95.9 ± 0.2	97.7 ± 0.2	12.9 ± 0.9	21.9 ± 0.8	30.0 ± 1.8
	85	100	92.1 ± 0.9	95.6 ± 0.3	97.9 ± 0.2	14.2 ± 0.9	22.7 ± 1.0	35.3 ± 1.5
	95	159	92.2 ± 1.2	95.6 ± 0.3	97.8 ± 0.2	15.4 ± 1.5	24.7 ± 1.7	36.1 ± 1.5
	100	700	92.1 ± 1.2	95.6 ± 0.3	97.7 ± 0.2	15.5 ± 1.5	25.0 ± 1.5	36.2 ± 1.5
0.01	75	104	90.3 ± 1.3	94.8 ± 0.9	97.1 ± 0.9	14.1 ± 1.4	22.8 ± 2.3	32.5 ± 3.6
	85	145	90.5 ± 1.3	94.9 ± 0.5	97.6 ± 0.1	15.0 ± 1.5	23.6 ± 1.1	35.1 ± 0.9
	95	227	90.6 ± 1.0	95.4 ± 0.4	98.0 ± 0.3	15.7 ± 1.0	25.6 ± 1.2	39.2 ± 1.6
	100	700	90.5 ± 1.0	95.6 ± 0.4	98.1 ± 0.1	15.7 ± 1.0	26.0 ± 1.0	39.5 ± 0.8
0.02	75	201	82.6 ± 1.4	91.2 ± 0.8	95.4 ± 0.4	15.3 ± 0.8	26.7 ± 1.9	38.2 ± 2.0
	85	274	83.0 ± 1.7	90.6 ± 0.6	94.6 ± 0.5	16.1 ± 0.8	26.3 ± 1.3	36.3 ± 1.8
	95	411	82.8 ± 1.8	91.2 ± 0.7	95.1 ± 0.4	16.0 ± 0.8	28.0 ± 1.5	40.8 ± 1.7
	100	700	82.8 ± 1.8	91.1 ± 0.7	95.0 ± 0.4	16.0 ± 0.8	27.9 ± 1.5	40.5 ± 1.7

b) IOKR-margin:

pdens	var %	nc	AUC-ROC			AUC-PR		
			p=5%	p=10%	p=20%	p=5%	p=10%	p=20%
0.007	75	69	91.3 ± 0.7	93.4 ± 0.7	94.7 ± 0.6	10.5 ± 1.1	12.5 ± 1.2	14.4 ± 1.5
	85	100	91.0 ± 0.8	93.5 ± 0.8	95.2 ± 0.7	12.0 ± 0.8	15.2 ± 2.6	19.6 ± 4.4
	95	159	90.5 ± 0.9	93.1 ± 0.5	95.3 ± 0.3	12.5 ± 0.9	18.9 ± 2.5	26.5 ± 1.0
	100	700	90.5 ± 0.8	93.1 ± 0.4	95.3 ± 0.3	13.0 ± 0.8	19.8 ± 0.9	26.9 ± 1.0
0.01	75	104	87.9 ± 0.9	91.0 ± 0.8	93.5 ± 0.4	12.1 ± 1.2	16.5 ± 1.0	22.8 ± 1.0
	85	145	87.7 ± 1.0	91.1 ± 1.2	92.9 ± 0.5	12.5 ± 1.0	16.9 ± 0.9	23.3 ± 1.1
	95	227	87.3 ± 1.6	91.3 ± 0.8	94.1 ± 0.5	12.5 ± 1.6	17.9 ± 1.3	24.7 ± 1.0
	100	700	87.2 ± 1.6	91.2 ± 0.8	94.1 ± 0.5	12.4 ± 1.6	17.9 ± 1.3	24.9 ± 1.1
0.02	75	201	78.4 ± 2.1	83.2 ± 1.2	88.4 ± 0.7	12.0 ± 1.0	17.3 ± 0.7	24.0 ± 0.9
	85	274	77.6 ± 2.1	81.9 ± 1.6	87.5 ± 0.8	12.5 ± 1.0	17.3 ± 1.0	24.3 ± 0.8
	95	411	77.3 ± 2.3	81.7 ± 1.6	87.0 ± 0.9	12.8 ± 1.0	17.8 ± 1.2	24.4 ± 0.7
	100	700	77.3 ± 2.3	82.0 ± 1.6	87.1 ± 0.9	12.8 ± 1.0	18.3 ± 1.1	24.5 ± 0.7

Table 8: Averaged AUCs obtained with IOKR for the reconstruction of three synthetic networks. The first column indicates the link probability between two nodes, var corresponds to the percentage of variance, or inertia, used to truncate the principal components and nc indicates the corresponding number of principal components.

a) IOKR-ridge:

p_{intra}	p_{inter}	var %	AUC-ROC			AUC-PR		
			p=5%	p=10%	p=20%	p=5%	p=10%	p=20%
0.02	5e-4	75	85.0 \pm 0.7	86.8 \pm 0.9	93.1 \pm 2.2	2.8 \pm 0.4	3.5 \pm 0.5	10.3 \pm 2.7
		85	85.7 \pm 0.7	90.4 \pm 3.5	95.5 \pm 0.3	3.0 \pm 0.4	7.3 \pm 3.8	15.9 \pm 1.2
		95	86.6 \pm 1.8	93.2 \pm 2.8	96.6 \pm 0.3	3.8 \pm 1.9	12.7 \pm 4.7	21.2 \pm 1.8
		100	87.0 \pm 2.3	93.3 \pm 2.8	96.6 \pm 0.3	4.5 \pm 2.7	13.1 \pm 4.8	22.1 \pm 1.9
	1e-3	75	87.1 \pm 2.2	93.4 \pm 2.7	96.9 \pm 0.2	5.3 \pm 2.5	15.1 \pm 5.2	23.9 \pm 1.3
		85	88.4 \pm 2.1	93.2 \pm 2.6	97.2 \pm 0.2	7.7 \pm 3.7	16.2 \pm 5.7	27.1 \pm 1.4
		95	88.8 \pm 1.7	93.1 \pm 2.6	97.4 \pm 0.5	8.9 \pm 3.7	17.0 \pm 5.8	31.3 \pm 4.0
		100	89.2 \pm 1.6	93.1 \pm 2.5	97.9 \pm 0.4	9.8 \pm 3.6	17.1 \pm 5.8	34.5 \pm 3.1
0.03	5e-4	75	83.5 \pm 0.1	83.6 \pm 0.1	84.5 \pm 1.2	3.2 \pm 0.0	3.2 \pm 0.0	3.7 \pm 0.5
		85	83.7 \pm 0.1	83.8 \pm 0.1	86.4 \pm 1.4	3.3 \pm 0.0	3.3 \pm 0.0	4.6 \pm 0.7
		95	84.2 \pm 1.3	84.5 \pm 1.4	88.8 \pm 1.0	3.6 \pm 0.6	3.8 \pm 0.9	6.1 \pm 1.0
		100	84.2 \pm 1.3	84.7 \pm 1.7	89.7 \pm 1.6	3.6 \pm 0.6	3.9 \pm 1.0	7.2 \pm 1.9
	1e-3	75	86.2 \pm 1.9	91.1 \pm 1.7	93.7 \pm 0.3	5.9 \pm 2.2	12.1 \pm 2.4	16.5 \pm 1.3
		85	86.3 \pm 1.8	91.8 \pm 0.6	94.3 \pm 0.3	6.3 \pm 2.3	14.3 \pm 1.3	19.4 \pm 1.6
		95	86.8 \pm 2.2	91.7 \pm 0.6	94.8 \pm 0.7	6.9 \pm 3.1	14.8 \pm 1.4	22.3 \pm 3.1
		100	86.8 \pm 2.2	92.1 \pm 1.1	95.2 \pm 1.0	7.0 \pm 3.1	15.7 \pm 2.5	23.9 \pm 4.2

b) IOKR-margin:

p_{intra}	p_{inter}	inertia	AUC-ROC			AUC-PR		
			p=5%	p=10%	p=20%	p=5%	p=10%	p=20%
0.02	5e-4	0.75	84.5 \pm 0.6	84.6 \pm 0.4	84.5 \pm 0.3	2.6 \pm 0.1	2.5 \pm 0.1	2.5 \pm 0.1
		0.85	84.8 \pm 0.7	84.9 \pm 0.5	84.9 \pm 0.4	2.7 \pm 0.1	2.6 \pm 0.1	2.6 \pm 0.2
		0.95	85.1 \pm 0.9	85.2 \pm 0.5	85.2 \pm 0.5	2.8 \pm 0.1	2.8 \pm 0.1	2.7 \pm 0.2
		1	85.2 \pm 0.9	85.3 \pm 0.5	85.3 \pm 0.5	2.9 \pm 0.2	2.8 \pm 0.1	2.8 \pm 0.2
	1e-3	0.75	84.8 \pm 0.6	85.0 \pm 0.3	84.7 \pm 0.6	3.4 \pm 0.4	3.3 \pm 0.3	3.0 \pm 0.2
		0.85	85.1 \pm 0.6	85.3 \pm 0.3	85.3 \pm 0.4	3.6 \pm 0.4	3.7 \pm 0.3	3.4 \pm 0.3
		0.95	85.2 \pm 0.7	85.5 \pm 0.4	85.6 \pm 0.2	3.8 \pm 0.4	3.9 \pm 0.3	3.9 \pm 0.1
		1	85.5 \pm 0.4	85.6 \pm 0.4	85.7 \pm 0.2	3.9 \pm 0.4	3.9 \pm 0.3	3.9 \pm 0.1
0.03	5e-4	0.75	83.4 \pm 0.2	83.5 \pm 0.2	83.5 \pm 0.2	3.2 \pm 0.0	3.2 \pm 0.0	3.2 \pm 0.0
		0.85	83.6 \pm 0.2	83.7 \pm 0.2	83.6 \pm 0.2	3.3 \pm 0.0	3.3 \pm 0.0	3.3 \pm 0.0
		0.95	83.6 \pm 0.2	83.7 \pm 0.2	83.7 \pm 0.2	3.3 \pm 0.0	3.4 \pm 0.0	3.3 \pm 0.0
		1	83.6 \pm 0.2	83.8 \pm 0.2	83.7 \pm 0.2	3.3 \pm 0.0	3.4 \pm 0.0	3.3 \pm 0.0
	1e-3	0.75	84.0 \pm 0.6	83.9 \pm 0.4	84.0 \pm 0.1	3.8 \pm 0.2	3.7 \pm 0.2	3.7 \pm 0.1
		0.85	84.2 \pm 0.6	84.1 \pm 0.4	84.1 \pm 0.1	4.0 \pm 0.3	3.9 \pm 0.2	3.9 \pm 0.1
		0.95	84.3 \pm 0.7	84.2 \pm 0.4	84.2 \pm 0.1	4.1 \pm 0.3	4.0 \pm 0.2	4.0 \pm 0.1
		1	84.3 \pm 0.7	84.2 \pm 0.4	84.2 \pm 0.1	4.2 \pm 0.3	4.0 \pm 0.2	4.0 \pm 0.1

Table 9: Averaged AUCs obtained with IOKR on different mixtures of Erdős-Renyi random graphs. p_{intra} and p_{inter} denote respectively the intra- and inter-class connection probabilities. The third column indicates the percentage of variance used to define the input vectors from the principal components.

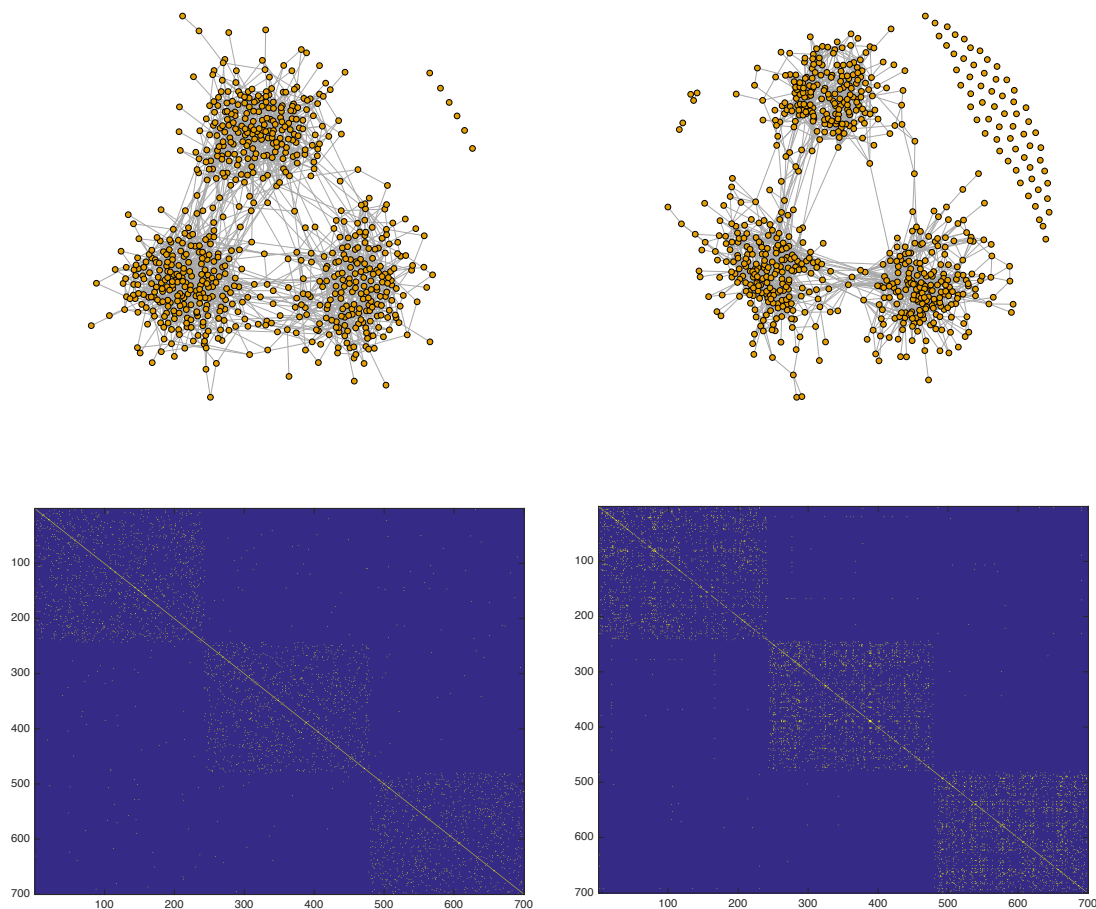


Figure 8: Prediction of a mixture of Erdős-Renyi random graphs with IOKR. The true network is shown on the left and the network predicted with IOKR-ridge on the right. The respective adjacency matrices are displayed under the two networks.

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