Determinantal Point Processes Implicitly Regularize
Semi-parametric Regression Problems

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Abstract

Semi-parametric regression models are used in several applications which require comprehensibility without sacrificing accuracy. Examples are spline interpolation in geophysics, or non-linear time series problems, where the system includes for instance a linear and non-linear component. We discuss here the use of a finite Determinantal Point Process (DPP) sampling for approximating semi-parametric models in two cases. On the one hand, in the case of large training data sets, DPP sampling is used to reduce the number of model parameters. On the other hand, DPPs can determine experimental designs in the case of the optimal interpolation models. Recently, Barthelmé, Tremblay, Usevich, and Amblard introduced a novel representation of finite DPP’s. They formulated extended L-ensembles that can conveniently represent for instance partial-projection DPPs and suggest their use for optimal interpolation. With the help of this formalism, we derive a key identity illustrating the implicit regularization effect of determinantal sampling for semi-parametric regression and interpolation. Also, a novel projected Nyström approximation is defined and used to derive a bound on the expected risk for the corresponding approximation of semi-parametric regression. This work naturally extends similar results obtained for kernel ridge regression.

Keywords — determinantal point processes, semi-parametric regression, Nyström approximation, implicit regularization

1 Introduction

Kernel methods provide a consistent framework for non-parametric regression and have been able to achieve excellent performance [39] in the last years. Also, in the case of massive data sets, smart sampling and sketching methods have allowed to scale up kernel ridge regression [33], while preserving its theoretical guarantees. Besides, sampling methods are interesting to reduce the number of parameters for enhancing prediction speed, for instance, in the context of embedded applications. In this paper, we consider the specific setting of semi-parametric regression which generalizes and improves the interpretability of kernel ridge regression for the applications where a parametric (polynomial) estimator can be conjectured to be a good guess. We combine this semi-parametric approach with a custom sampling scheme based on Determinantal Point Processes.

Discrete Determinantal Point Processes (DPPs) provide elegant ways to sample subsets $C \subseteq \{1, \ldots, n\}$, sometimes called coresets [44], so that the selected items are diverse. In a word, discrete DPPs are represented by a marginal kernel, that is, a $n \times n$ matrix $P$ with eigenvalues within $[0, 1]$, giving the inclusion probabilities: if $C$ be distributed according to a DPP with marginal kernel $P$, then we have

$$\Pr (E \subseteq C) = \det P_{EE},$$

where $P_{EE}$ is the square submatrix indexed by $E$. It is often very convenient to work with L-ensembles, which constitute a class of DPPs satisfying $\Pr (C) \propto \det L_{CC}$ where $L$ is a $n \times n$ positive semi-definite matrix. In the case of L-ensembles, the marginal kernel reads

$$P = L(L + I)^{-1}.$$

In the context of kernel ridge regression, the implicit regularization effect of sampling landmarks from L-ensemble DPPs was investigated in [23]. Given a $n \times n$ positive semi-definite kernel matrix $K$, an L-ensemble DPP can be used

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to sample subsets of \( k \) landmarks \( C \subseteq \{1, \ldots, n\} \). Then, the matrix \( K \) can be approximated thanks to the Nyström method which uses its submatrices, such as the square \( k \times k \) submatrix \( K_{CC} \). This is conveniently done with the use of a \( n \times k \) sampling matrix \( C \) obtained by sampling the columns indexed by \( C \) of the identity matrix. For instance, in the case of the Nyström approximation, one considers the pseudo-inverse of the sparse matrix \( C K_{CC} C^\top \), which is a \( n \times n \) matrix whose entry \( (i, j) \) is \( K_{ij} \) if \( i, j \in C \) and zero otherwise. This subsampling with \( C \)-ensembles has an implicit regularization effect \cite{23}, which is based on the following expectation formula, also independently shown by \cite{37}:

\[
\mathbb{E}_C \left( C K_{CC} C^\top \right)^{-1} = (K + \lambda I)^{-1},
\]

where the subset \( C \) is sampled according to a \( L \)-ensemble DPP with \( L = K/\lambda \) with \( \lambda > 0 \). The role of \( \lambda \) is to vary the expected size of the subset and the amount of regularization. A similar identity has been revisited in the context of fixed-size \( L \)-ensemble DPP in \cite{41}. Implicit regularization is not specific to sampling, since it is also observed with Gaussian and Rademacher sketches of Gram matrices in \cite{13}, although a closed-form formula can derived be advantageously with \( L \)-ensemble sampling.

There are DPPs which are not \( L \)-ensembles, for instance, the projection DPPs. Therefore, the elegant framework of `extended \( L \)-ensembles' has been introduced in \cite{3} to represent any finite DPP, and it is used extensively in this paper to deal with partial-projection DPPs. For a partial-projection DPP, denoted by \( DPP(\tilde{L}, V) \), the marginal kernel is of the following form

\[
P = PV + \tilde{L}(\tilde{L} + \|)^{-1},
\]

where \( V = V(V^\top V)^{-1}V^\top \) is the projection part, with \( V \) a \( n \times p \) matrix with full column rank. The matrix

\[
\tilde{L} = \tilde{K}/\lambda \quad \text{with} \quad \tilde{K} = PV_{\perp} K P V_{\perp},
\]

is defined thanks to the \( n \times n \) projected kernel which is denoted by using a tilde. It is natural to assume \( \tilde{L} \) to be positive semi-definite so that it is analogous to an \( L \)-ensemble. If we perform the QR-decomposition \( V = QR \), the above projection can be easily written as \( \tilde{PV}_{\perp} = I - QQ^\top \), where \( Q \) is a \( n \times p \) matrix with orthonormal columns.

Extended \( L \)-ensembles, that we describe hereafter, represent more conveniently partial-projection DPPs by giving a handy formula for \( \text{Pr}(C) \). The reference \cite{3} also points out a connection between `extended \( L \)-ensembles' and optimal interpolation in Section 2.8.2. This remark has motivated the following case study: the Nyström approximation of semi-parametric regression problem. While the Nyström approximation has been studied in the case of kernel ridge regression \cite{30,29,23,22} where the estimated function is of the form \( f(x) = \sum_{i=1}^n \alpha_i k(x, x_i) \) with a positive semi-definite \( k(x, x') \), we consider here the semi-parametric form

\[
f(x) = \sum_{i=1}^n \alpha_i k(x, x_i) + \sum_{j=1}^p \beta_j p_j(x),
\]

where the first term is the non-parametric component associated to a conditionally positive semi-definite kernel \( k(x, x') \), while the second term is the parametric component that is typically given by polynomials. We consider noisy queried values of the unknown function

\[
y_i = z_i + \epsilon_i \quad \text{with} \quad z_i = f(x_i), \quad \text{and} \quad 1 \leq i \leq n,
\]

where \( \epsilon_i \) denotes i.i.d. \( N(0, \sigma^2) \) noise. Then, the marginal kernel \cite{3} appears interestingly in the known formula for the in-sample estimate of a semi-parametric \( \gamma \)-regularized least squares problem (see Section 3.3).

\[
\hat{z} = P y \quad \text{with} \quad P = PV + \tilde{L}(\tilde{L} + \|)^{-1},
\]

with \( \tilde{L} = \tilde{K}/(n\gamma) \). In this setting, the \( V \) and \( K \) matrices used in \cite{3} are identified with the following matrices obtained from the parametric and non-parametric components: \( V_{\gamma} = [y_i(x_i)] \) for \( 1 \leq i \leq n \) and \( 1 \leq j \leq p \) whereas \( K_{ij} = [k(x_i, x_j)] \) for \( 1 \leq i, j \leq n \). We outline now the contributions of this paper.

### 1.1 Contributions

A key contribution of this paper is a formula analogous to \cite{1} involving a sampling with a custom partial-projection DPP. Namely, Theorem 1 given hereafter implies the following identity for the expectation of the pseudo-inverse \cite{47}:

\[
\mathbb{E}_C \left( C P V_{\perp} K_{CC} P V_{\perp} C^\top \right)^{-1} = P_{V_{\perp}} (K + \lambda I)^{-1} P_{V_{\perp}} \quad \text{with} \quad \tilde{K} = P_{V_{\perp}} K P_{V_{\perp}}.
\]

\(^{1}\)Technically, we require here that \( K \) is conditionally positive semi-definite definite with respect to \( V \), i.e., \( P_{V_{\perp}} K P_{V_{\perp}} \) is positive semi-definite. The existence of the LHS of \cite{47} is also shown in the sequel.
where $C$ is sampled according to the partial-projection $DPP(K/\lambda, V)$ where $\mathbb{P}_{V'}$ (resp. $\mathbb{P}_{V'_\perp}$) is the projector onto the orthogonal of $V$ (resp. $C^\top V$). We emphasize that the implicit regularization is ‘conditional’ since it occurs only within the subspace orthogonal to $V$. The identity [3] is novel to the best of our knowledge and is also instrumental to derive two key contributions of this paper:

- in Section 5.1 we define a projected Nyström approximation $\widehat{L}(C)$ of the projected kernel matrix $\widehat{K}$ under the assumption that $\widehat{K}$ is positive semi-definite:

$$
\widehat{L}(C) = \widehat{K}S(C) \left( S(C)^\top \widehat{K}S(C) \right)^{-1} S(C)\widehat{K}
$$

where the sketching matrix is $S(C) = CB(C) \in \mathbb{R}^{n \times (k-p)}$, with $B(C) \in \mathbb{R}^{k \times (k-p)}$ a matrix whose columns are an orthonormal basis of $(C^\top V)^\perp$. This low rank approximation of the projected kernel matrix can be constructed conveniently with submatrices of the original kernel $K$. Indeed, it is not necessary to construct explicitly the sketching matrix $S(C)$. Importantly, we give an expected error formula in Corollary 2:

$$
\mathbb{E}_{C}[\widehat{K} - \widehat{L}(C)] = \lambda \widehat{K}(\widehat{K} + \lambda I)^{-1}, \text{ where } C \sim DPP(K/\lambda, V).
$$

Notice that the expected subset size of $C \sim DPP(K/\lambda, V)$ is given by

$$
\mathbb{E}_C[|C|] = p + d_{\text{eff}}(\widehat{K}/\lambda), \text{ with } d_{\text{eff}}(\widehat{K}/\lambda) = \text{Tr} \left( \widehat{K}(\widehat{K} + \lambda I_n)^{-1} \right),
$$

where $p$ is the number of columns of $V$ and with $\widehat{K} = \mathbb{P}_{V'} K \mathbb{P}_{V'_\perp}$. The interpretation of this identity is that a small $\lambda > 0$ yields a large number of samples and a small error on expectation. We emphasize that the projected Nyström approximation exists almost surely if $C \sim DPP(K/\lambda, V)$. This extends similar results obtained independently in [29 Corollary 2] and [12].

- in Section 5.3 we give an expected risk bound for the estimator $\hat{z}_N$ of the $\gamma$-regularized semi-parametric regression obtained with the projected Nyström approximation, that is,

$$
\mathbb{E}_C \left[ \frac{R(\hat{z}_N)}{R(\hat{z})} \right] \leq 1 + \frac{\lambda}{\gamma^2} d_{\text{eff}}(\widehat{K}/\lambda), \text{ with } C \sim DPP(K/\lambda, V).
$$

where the expected risk of the estimator $\hat{z}$ is $R(\hat{z}) = \mathbb{E}_z \| \hat{z} - z \|^2$, as it is detailed in Theorem 2 hereafter. This result indicates that the estimation thanks to the Nyström approximation cannot be arbitrarily worse than the estimation obtained without approximation.

Two different applications are considered within the penalized kernel regression framework. 1) The case where $y$, values are initially unknown to the user and costly to retrieve. This is for example the case in an active learning approach where datapoints have to be manually labelled or when measurements are expensive. This application is known as experimental design and was previously studied, e.g., for linear regression in [17, 15, 11]. In this setting, one interpolates on a small selected number of landmark points to minimize the number of necessary labeled points. The question now poses itself: what is a good way of selecting points such that the performance is maintained together with a good conditioning of the linear system? In this paper, we propose a determinantal design approach. 2) The user has knowledge of the full $y$ response vector, but the (embedded) application requires a number of parameters smaller than $n + p$, or the number of datapoints $n$ is too large to solve the corresponding linear system.

### 1.2 Related work

While it is currently an active topic of research in the context of deep neural networks, implicit regularization has been studied already previously in [20, 31]. Recently, DPPs and implicit regularization also appeared in the context of double descent phenomena [14], while we refer to [16] for a review. DPPs are useful methods to sample diverse subsets that have been applied in machine learning in variety of tasks, such as diverse recommendations, summarizing text or search tasks [29].

Semi-parametric models are useful tools when some domain knowledge exists about the function to be estimated (e.g. the user want to correct the data for a linear trend) or more understandability is required of the model [20, 28]. These models combine a parametric part which is easy to understand and non-parametric term to improve performance. Semi-parametric models are often used in critical applications where the user wants to have an understandable model, without sacrificing accuracy [20, 21, 22].

A natural application of conditionally positive semi-definite matrices is radial basis function interpolation [35]. Radial basis function interpolation is an attractive method for interpolating and smoothing function values on scattered points in the plane. However, a potential problem is that their computation involves the solution of a linear
system that is ill-conditioned for large data sets. Thin-plate spline basis functions have been shown to be very accurate in medical imaging [9], surface reconstruction [8], as well as other engineering applications [6]. Importantly, the paper [1] studies a slightly different question, which mainly concerns the case of thin-plate splines. Given a fixed set of landmark points, it proposes an elegant method for choosing a suitable basis of the function space so that the linear system under study has an improved condition number. This strategy is also described in [15].

1.3 Organization of the paper

In Section 2 we introduce basic definitions. Then, the penalized semi-parametric regression and interpolation problems that we study in this paper are discussed in Section 3. There, we consider two case studies: thin-plate splines regression and Gaussian kernel semi-parametric regression. Next, in Section 4 we explain the implicit regularization effect of a determinantal design for optimal interpolation. In Section 5 we discuss the large scale semi-parametric regression problem that can be simplified thanks to a determinantal sampling together with a custom Nyström approximation. We also provide a stability result for the expected risk of the approximation. Technical proofs and results are deferred to the appendix.

1.4 Notations

Matrices $(A,B,K,\ldots)$ are denoted by upper-case letters, whereas column vectors are denoted by bold lower-case letters, e.g., $x = [x_1, \ldots, x_d]^\top \in \mathbb{R}^d$. The constant $n \times 1$ vector of ones is $1_n$. We write $A \succeq 0$ (resp. $A \preceq 0$) if $A$ (resp. $-A$) is positive semi-definite (psd), while $A \succeq B$ indicates that $A-B$ is psd. The Moore-Penrose pseudo-inverse of a matrix $A$ is denoted here by $A^\dagger$. We use calligraphic letters to denote sets. In this paper, we consider the problem of sampling subsets $C \subseteq [n]$, where $[n] = \{1, \ldots, n\}$. Then, it is convenient to use a sampling matrix $\tilde{C} = \mathbb{I}^d_n \in \mathbb{R}^{n \times k}$ obtained by selecting the columns of the identity matrix corresponding to $C$. The sampled sub-matrices are then denoted as follows: $V_C = \tilde{C}^\top V$ where $V \in \mathbb{R}^{n \times p}$ and $A_C = \tilde{C}^\top A \tilde{C}$ with $A \in \mathbb{R}^{n \times n}$.

2 Extended L-ensembles and definitions

To begin with, we recall some definitions that were introduced in [3]. Typically, a finite DPP can be described thanks to its marginal kernel, which incorporates the inclusion probabilities. The subclass of DPPs called L-ensembles admits a more convenient representation that allows to express directly the probability to sample of subset $C$ with respect to $\tilde{C}$

\[ C \subseteq \{1, \ldots, n\} \]

\[ \text{Pr}(C) = \det(A_C)/\det(A) \]

Moreover, the orthogonal of the space spanned by the columns of $A$ is denoted as follows:

\[ A_C = \tilde{C}^\top A \tilde{C} \]

\[ A_C = \tilde{C}^\top A \tilde{C} \]

Example 1. The kernel $k(x,x') = -\|x-x'\|^2_2$ is a conditionally positive semi-definite kernel with respect to the constant function. Indeed, let $x_i \in \mathbb{R}^d$ with $1 \leq i \leq n$. Then, the Gram matrix $K = [k(x_i,x_j)]_{i,j}$ satisfies $v^\top K v \geq 0$ for all $v \in \mathbb{R}^d$ such that $1^\top v = 0$. Then, $(K,1)$ is a NNP. Other examples are given by generalized multiquadrics mentioned in [20].

Equipped with these definitions, a DPP associated to a NNP can be defined thanks to the representation called extended L-ensemble and introduced in [3].
Definition 3 (Extended L-ensembles [3]). Let $(L,V)$ a NNP and $\tilde{L} = \mathbb{P}_{V^\perp}L\mathbb{P}_{V^\perp}$. Then, an extended L-ensemble $\mathcal{Y} \sim DPP(L,V)$ satisfies

$$\Pr(\mathcal{Y} = \mathcal{C}) = N^{-1} \times \det \left( \frac{Lc}{Vc} \begin{bmatrix} Vc & Vc \\ 0 & 0 \end{bmatrix} \right)$$

where $N = (-1)^p \det(\tilde{L} + \mathbb{I}) \det(V^\top V)$.

The size of an extended L-ensemble is itself a random variable, and its expected sample size can be calculated. Indeed, let $\lambda > 0$ be a scale parameter. The expected size of $\mathcal{C} \sim DPP(K/\lambda, V)$ is

$$\mathbb{E}[|\mathcal{C}|] = \text{Tr} \left( \tilde{K}(\tilde{K} + \lambda \mathbb{I})^{-1} \right) + p,$$

where $\lambda > 0$ allows to vary the sample size, i.e., a small $\lambda$ value yields a large sample size on expectation and conversely. This can be shown thanks to the marginal kernel of an extended L-ensemble, which was given in [2] in the introduction. In the next section, we introduce semi-parametric penalized least-squares regression problems that can be combined conveniently with extended L-ensembles.

Remark 1 (Sampling). The sampling algorithm used in this paper relies on Algorithm 3 in [44] (see also [29]). In all numerical simulation, we use a fixed size DPP sampling and rely on the asymptotic equivalence between DPPs and fixed size DPPs [3].

3 Basics of penalized semi-parametric regression

We start by introducing the framework of semi-parametric regression with a psd kernel while an example with a conditionally positive semi-definite kernel is given in the sequel.

3.1 Semi-parametric regression with semi-positive definite kernels

Let $(\mathcal{H}_1, \langle \cdot, \cdot \rangle_1)$ be a Reproducing Kernel Hilbert Space (RKHS) with kernel $k(x,x')$. Also, let $\mathcal{H}_0$ be a Hilbert space of dimension $p < \infty$ with a basis given by $p_i(x)$ for $1 \leq j \leq p$ and such that that $\mathcal{H}_0 \cap \mathcal{H}_1 = \{0\}$.

The function space that we consider is the direct sum $\mathcal{H}_0 \oplus \mathcal{H}_1$. By construction, every $f \in \mathcal{H}_0 \oplus \mathcal{H}_1$ can be decomposed uniquely as $f = f_0 + f_1$ with $f_0 \in \mathcal{H}_0$ and $f_1 \in \mathcal{H}_1$. Hence, we define the penalty functional

$$J(f) = \langle f_1, f_1 \rangle_1,$$

so that its null space is naturally $\mathcal{N}_J = \{f \in \mathcal{H}_0 \oplus \mathcal{H}_1 : J(f) = 0\} = \mathcal{H}_0$. The penalized least-squares (PLS) problem reads

$$\min_{f \in \mathcal{N}_J \oplus \mathcal{H}_1} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \gamma J(f). \quad (\text{PLS})$$

When $\mathcal{N}_J = \{0\}$, (PLS) reduces to Kernel Ridge Regression (KRR). By a classical argument (‘representer theorem’, see, e.g., Section 2.3.2 of [27] or [38]), the solutions of (PLS) are in the semi-parametric form $f(x) = \sum_{i=1}^{n} \alpha_i k(x,x_i) + \sum_{j=1}^{p} \beta_j p_j(x)$, where the first term includes only a finite number of terms. By plugging the above expression into the minimization problem (PLS), we find the discrete minimization problem

$$\min_{\alpha,\beta} \frac{1}{n} \|y - V\beta - K\alpha\|^2 + \gamma \alpha^\top K\alpha, \quad (4)$$

with $V_{ij} = [p_j(x_i)]$ for $1 \leq i \leq n$ and $1 \leq j \leq p$. Notice that $\frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$ is strictly convex on $\mathcal{N}_J$ whenever $V$ is full column rank. Furthermore, (PLS) is strictly convex on $\mathcal{H}_0 \oplus \mathcal{H}_1$ if $V$ is full column rank. Therefore, we assume in the sequel that the data set is "unisolvent" with respect to $(p_j)_j$, i.e., such that $V$ is full column rank. In this case, the solution of (PLS) is unique in view of Theorem 3 in Appendix [27]. The first order optimality condition of the optimization problem (4) reads

$$K (K + n\gamma I) \alpha + V\beta - y = 0,$$

$$V^\top (K\alpha + V\beta - y) = 0.$$

Any finite dimensional Hilbert space can be endowed with a suitable scalar product so that is also a RKHS. Let $(\mathcal{H}_0, \langle \cdot, \cdot \rangle_0)$ be a RKHS. Then, $\mathcal{H}_0$ is the orthogonal complement of $\mathcal{H}_1$ with respect to the following inner product: $(f_0 + f_1, g_0 + g_1) := (f_0, g_0)_0 + (f_1, g_1)_1.$
where $K$ is positive semi-definite. We consider first that $K$ is non-singular. As it can be verified by a simple substitution of $\alpha$ and $\beta$ in the first order conditions, the unique solution of (4) is obtained by solving

\[
\begin{pmatrix} K + n\gamma I & V \\ V^\top & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} y \\ 0 \end{pmatrix}.
\]

If $K$ is singular, then (4) can have several solutions $\alpha^*$ and $\beta^*$, which however yield the same in-sample estimator $\hat{z} = K\alpha^* + V\beta^*$ of the true function values $z_i = f(x_i)$ for $1 \leq i \leq n$. In that case, we select the solution corresponding to the coefficients obtained by solving (5).

### 3.2 Case study: The Gaussian kernel RKHS does not contain polynomials

Let $X \subset \mathbb{R}^d$ be any set with non-empty interior and let $\mathcal{H}_1$ be the RKHS of the Gaussian kernel

\[ k(x, x') = \exp(-\|x - x'\|^2/\sigma^2) \]

defined on $X \times X$. Under these assumptions, Theorem 2 in [34] states that $\mathcal{H}_1$ does not contain any polynomial on $X$, including the non-zero constant function. We can then solve the functional minimization problem (PLS) where $\mathcal{H}_0$ is a finite set of polynomials, since $\mathcal{H}_0 \cap \mathcal{H}_1 = \{0\}$.

**Example 2** (LS-SVM with the Gaussian kernel). In particular, the constant $p_1(x) = 1$ is not part of the RKHS of the Gaussian kernel. Therefore, Least-Squares Support Vector Machine (LS-SVM) [43] with the Gaussian kernel is also a particular case of the above discussion. Its dual optimization problem indeed reads $\min_{\alpha, b} \frac{1}{2}\|y - K\alpha - b1_n\|^2_2 + \gamma \alpha^\top K\alpha$, where the real $b$ is the so-called bias term.

We illustrate the use of semi-parametric regression with a Gaussian kernel on a toy example consisting out of a linear trend with two Gaussian bumps, i.e.,

\[ f(x) = x + 7 + 4\exp(-(x - 4)^2) - 4\exp(-(x + 4)^2) \]

The training points are sampled uniformly within the interval $[-10, 10]$ and the function samples are $y_i = f(x_i) + \epsilon_i$ where $\epsilon_i \sim N(0, 0.2)$ for $1 \leq i \leq n$ and $n = 40$. The test set consists of 1000 points sampled uniformly in the interval $[-11, 11]$. This allows to assess the estimated function to capture the linear trend of the ground truth.

Let $\mathcal{H}_1$ be the RKHS of the Gaussian kernel. We compare the results obtained by different choices of the space of polynomials $\mathcal{H}_0$. Namely, the following models are estimated: **Model 1**: $\hat{f}(x) = \beta_1 + \beta_2 x + \sum_i \alpha_i k(x, x_i)$ (semi-parametric), **Model 2**: $\hat{f}(x) = \beta_1 + \sum_i \alpha_i k(x, x_i)$ (LS-SVM) and **Model 3**: $\hat{f}(x) = \sum_i \alpha_i k(x, x_i)$ (KRR). For all the models drawn in Figure 14, the bandwidth is fixed to $\sigma = 1$ to match the width of the two Gaussians of the ground truth and the regularization parameter $\gamma$ is varied over an interval. For completeness, we also include the performance of the best model in Figure 14 (dashed line), where both the bandwidth and regularization parameter are determined by using cross-validation. The simulation is repeated 25 times and the error bars show the 97.5% confidence interval. The results of the simulation are visualized in Figure 13. When including the knowledge of the linear trend, the model is capable of correctly extrapolating in low density regions, as well as outside of the training interval. In Figure 14, the function prediction in low density regions of both model 2 and model 3 quickly moves to the bias. This is avoided by including a parametric linear part such as in model 1. We emphasize that the differences between the three models are reduced within the interval $[-10, 10]$ if the number of training samples becomes larger.

### 3.3 Case study: Conditionally positive semi-definite kernels and thin-plate splines

A well-known choice of penalty functional yielding to a linear system with a conditionally positive semi-definite kernel is associated to thin-plate splines, and is given by

\[ J^d_p(f) = \langle f, f \rangle_1 + \sum_{\alpha_1 + \cdots + \alpha_d = m} \frac{p!}{\alpha_1! \cdots \alpha_d!} \int_{\mathbb{R}^d} \frac{\partial^p f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} \frac{\partial^p g}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} dx_1 \cdots dx_d, \]

where $J^d_p(f)$ is a squared norm on $\{ f : J^d_p(f) < \infty \}$ for a large enough regularity index with respect to the dimension, i.e., for $2p > d$. Its null space $N_d$ consists of polynomials of maximal total order equal to $p - 1$. Following section 4.3.2 of [27], the penalty functional $J^d_p(f)$ satisfies

\[ J^d_p \left( \sum_{i=1}^n \alpha_i k(x_i, x_j) \right) = \sum_{i,j=1}^n \alpha_i \alpha_j k(x_i, x_j), \]

for all $\alpha \in \mathbb{R}^n$ such that $V^\top \alpha = 0$, where

\[ V = \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_d} \end{pmatrix}. \]
Figure 1: A Toy example of semi-parametric regression. Figure 1a shows the training points and the estimated function with $\sigma = 1$ and best performing $\gamma$. Only the semi-parametric model, i.e., model 1, predicts the linear trend in low density regions as well outside the training interval, contrary to model 2 (LS-SVM) and model 3 (KRR). The MSE of each model with bandwidth $\sigma = 1$ is visualized as a function of the regularization parameter in Figure 1b. The dashed line shows the best performance when cross-validating over both $\gamma$ and $\sigma$.

where $V$ is assumed to be full column rank and where the thin-plate spline kernel reads

$$k(x, x') = \begin{cases} \|x - x'\|^2 \log \|x - x'\| & \text{for even } d \\ \|x - x'\|^{2p-d} & \text{for odd } d. \end{cases}$$

The kernel $k(x, x')$ is a conditionally positive semi-definite, namely, $\sum_{i,j} c_i c_j k(x_i, x_j) \geq 0$, for all vectors satisfying $V^\top c = 0$. Again, $V$ is assumed to be full column rank. By an argument analogous to the previous section (see [27]), the solution of the least-squares penalized regression

$$\min_{\|f\|_d < \infty} \frac{1}{n} \sum_{i=1}^n (y_i - f(x_i))^2 + \gamma J_d(f),$$

is of the form $f(x) = \sum_{i=1}^n \alpha_i k(x, x_i) + \sum_{j=1}^p \beta_j p_j(x)$ with $V^\top \alpha = 0$. This result is proved in [18, Theorem 4 bis] in the case of optimal interpolation (i.e., $\gamma \to 0$). The substitution of $f(x)$ into the objective above yields a similar discrete minimization problem as (4) with the extra condition $V^\top \alpha = 0$. In particular, a solution of this minimization problem is given by the same system as (5) with the exception that, here, $K$ is conditionally positive semi-definite.

Let $V_{\perp}$ a matrix with orthonormal columns such that $P V_{\perp} = V_{\perp} V_{\perp}^\top$. The solution of this linear system is given as

$$\alpha^* = V_{\perp} (V_{\perp}^\top K V_{\perp} + n\gamma I_{n-p})^{-1} V_{\perp}^\top y,$$

$$\beta^* = (V^\top V)^{-1} V^\top (y - K\alpha),$$

where we used the fact that $V$ is full column rank and $P_{V_{\perp}} K P_{V_{\perp}} \succeq 0$. Notice that the full in-sample estimator is $\hat{z} = \tilde{K}(\tilde{K} + n\gamma I)^{-1} y + P_{V_{\perp}} y$. The RKHS associated to the thin-plate splines and a psd kernel built from the conditionally positive semi-definite kernel are determined in [27], where this problem is put in the form of (PLS). Then, the domain $\{f : J_d(f) < \infty\}$ is shown to be the direct sum of a RKHS and the space of polynomials of maximal total degree $p - 1$.

Furthermore, a discussion of optimal interpolation with conditionally positive semi-definite kernels, within the framework of Hilbertian subspaces of L. Schwartz, can be found in the PhD thesis [25]. Let us now consider the use of extended $L$-ensembles for obtaining designs in the context of optimal interpolations.

4 Implicit regularization of optimal interpolation with a determinantal design

In the context of applications mentioned in the introduction, we consider here the problem of interpolating function values given a small training data set. In this section, we assume that getting the $y_i$ values is expensive and therefore
A Gaussian kernel \( k \) performance is measured by the total MSE:
\[
\sum_{x} \| f(x) - \hat{f}_0(x, \mathcal{C}) \|_2^2
\]
on a number of UCI benchmark regression data sets: Boston Housing, Abalone and Parkinson. Let \( k_x = [k(x, x_1), \ldots, k(x, x_n)] \) \( \in \mathbb{R}^n \) and \( p_x = [p_1(x), \ldots, p_p(x)] \) \( \in \mathbb{R}^p \) for all \( x \in \mathbb{R}^d \). The estimated interpolator on a subset \( \mathcal{C} \) reads
\[
\hat{f}_0(x, \mathcal{C}) = (k_x^\top C) (p_x^\top V_c^{-1} (y_c - 0)).
\] (6)

If \( \mathcal{C} \sim \text{DPP}(K, V) \), notice that: (i) the square matrix on the RHS of (6) is non-singular almost surely, and (ii) \( V_c \) is full column rank almost surely, in the light of Lemma 3. One of our main results is that the system (6) is regularized on expectation when subsets \( \mathcal{C} \) are sampled according to a suitable DPP.

**Theorem 1.** Let \((K, V)\) be a NNP. Let \( u_0, v_0 \in \mathbb{R}^n \) and \( u_1, v_1 \in \mathbb{R}^p \). We have the identity
\[
E_{\mathcal{C} \sim \text{DPP}(K, V)} \left[ \begin{pmatrix} u_0 & u_1 \end{pmatrix}^\top \begin{pmatrix} K_{cc} & V_c \\ V_c^\top & 0 \end{pmatrix}^{-1} \begin{pmatrix} u_0 & v_0 \\ v_1 \end{pmatrix} \right] = \left( \begin{pmatrix} K + I & V \\ V^\top & 0 \end{pmatrix}^{-1} \begin{pmatrix} u_0 \\ v_1 \end{pmatrix} \right).
\]

This identity remains valid when \( K \) is replaced by \( \tilde{K} = \mathbb{P}_{V^\perp} K \mathbb{P}_{V^\perp} \).

Similarly to (5), the \( \gamma \)-regularized regressor on the full data set obtained by solving PLS is
\[
\hat{f}_\gamma(x) = (k_x^\top p_x) (K + n\gamma I)^{-1} (y_0)
\]

The upshot is that the interpolator obtained with this determinantal design is actually regularized on expectation, as a direct consequence of Theorem 1.

**Corollary 1.** Let \( \mathcal{C} \sim \text{DPP}(K/(\gamma n), V) \). We have \( E_{\mathcal{C}}[\hat{f}_0(x, \mathcal{C})] = \hat{f}_\gamma(x) \) for all \( x \in \mathbb{R}^d \).

A similar identity was given for kernel ridgeless regression in (14) while Corollary 1 extends it.

### 4.1 Illustration of determinantal design for thin-plate spline interpolation

We illustrate the effect of subsampling for thin-plate spline interpolation on Franke’s function, which is frequently used to demonstrate radial basis function interpolation problems. Franke’s function has two Gaussian peaks of different heights, and a smaller dip:
\[
f(x) = 0.75 \exp \left( -\frac{(9x_1 - 2)^2}{4} - \frac{(9x_2 - 2)^2}{4} \right) + 0.75 \exp \left( -\frac{(9x_1 + 1)^2}{49} - \frac{9x_2 + 1}{10} \right) + 0.5 \exp \left( -\frac{(9x_1 - 7)^2}{4} - \frac{(9x_2 - 3)^2}{4} \right) - 0.2 \exp \left( -\frac{(9x_1 - 4)^2}{4} - \frac{(9x_2 - 7)^2}{4} \right).
\]

The full training set consists of 5000 points sampled uniformly at random from \([0, 1]^2\), the test consists of 10000 points sampled from the same domain. The full interpolation problem is solved by (3) with \( \gamma = 0 \) and regression function \( f(x) = \sum_{i=1}^n b_i x_i + \sum_{i=1}^n \alpha_i \| x_i - x \|_2 \log \| x_i - x \|_2 \). The subsampled interpolation problem is solved by (9). In this simulation, we compare uniform sampling to the associated partial-projection DPP. The simulation is repeated for an increasing subset size, and the performance is measured by the mean squared error (MSE) on the test set. In the experiments, we each time sample a partial-projection \( k \)-DPP to finer control the number of sampled landmarks. Every sampling is repeated 10 times and the averaged results are visualized in Figure 2. Error bars correspond to the standard error of the mean. For a given subset size, the partial-projection DPP outperforms uniform sampling.

### 4.2 Empirical results for Gaussian kernel interpolation

We illustrate the effect of extended \( L \)-ensemble sampling versus uniform sampling for subsampled interpolation on a number of UCI benchmark regression data sets: Boston Housing, Abalone and Parkinson. Both the regressors and response are standardized, afterwards the data set is split into a 50% training and 50% test set, performance is measured by the total MSE: \( \sum_{i=1}^n (y_i - \hat{y}_i)^2 \). To obtain the regressor, we solve the system (3). A Gaussian kernel \( k(x, x') = \exp(-\|x - x\|_2^2/\sigma^2) \) is used with a linear regression component: \( V = [X \ y] \) where \( X = [x_1, \ldots, x_n] \). The squared bandwidth is determined by using the median heuristic (29), computed as:
\[
\hat{\sigma}^2 = \text{median}\{\| x_i - x \|_2^2 : 1 \leq i < j \leq n \}/2.
\]
Cross-validation is not possible as the full \( y \) is hidden from us in the experimental design setup. The simulation is repeated 25 times and the error bars show the standard error of the mean. The results are displayed in Figure 3. Extended DPP sampling improves the performance especially for smaller number of samples, compared to uniform sampling.
Figure 2a displays a mesh plot of the Franke’s function. The MSE on the test set in function of the subset size $|C|$ is given in Figure 2b.

Figure 3: The total loss (MSE) in function of the number of landmarks using uniform vs extended DPP sampling with the bandwidth estimated using the median heuristic.

5 Large scale regularized semi-parametric regression

In this section, we consider the setting where the training points $(x_i, y_i)$ with $1 \leq i \leq n$ are abundant. Penalized least-squares problems of the form (PLS) have solutions which are determined by $n + p$ parameters where $n$ is the number of training points and $p$ is the number of functions used in the parametric component. When $n$ is large, it can be interesting to reduce the number of parameters describing the estimated function, for instance, in order to allow for a faster out-of-sample prediction. To introduce the Nyström approximation of regularized semi-parametric regression, we firstly define the matrix version of Nyström approximation.

5.1 Matrix Nyström approximation

For a positive semi-definite kernel matrix $K$, its Nyström approximation reads $K_{cc}^{-1} K_{cc} C$. We extend here this definition to the case of conditionally positive semi-definite kernels. Firstly, we provide in Proposition 1 a simple expression for an analogue of $CK_{cc}^{-1} C^T$.

Proposition 1. Let $C \sim DPP(K, V)$ and let $B(C) \in \mathbb{R}^{k \times (k-p)}$ be a matrix whose columns are an orthonormal basis of $(V_c)^\perp$. Define $I(C) = CB(C) (B^T(C)K_{cc}B(C))^{-1} B^T(C)C^T \geq 0$. Then, we have

$$
\begin{pmatrix}
I(C) & 0 \\
0 & 0
\end{pmatrix} = \begin{pmatrix}
C & 0 \\
0 & 0
\end{pmatrix} \begin{pmatrix}
K_{cc} & 0 \\
0 & V_c
\end{pmatrix}^{-1} \begin{pmatrix}
C^T & 0 \\
0 & 0
\end{pmatrix},
$$

(7)

where $K_{cc}$ can be equivalently replaced by $\tilde{K}_{cc} = C^T \tilde{K} C$. 

Proof. Firstly, we prove this identity by directly solving the matrix linear system of (7). Indeed, the RHS of (7) is
\[
\begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} K_{CC} & V_C \\ V_C^T & 0 \end{pmatrix}^{-1} \begin{pmatrix} C^T & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} CA_{11} & CA_{12} \\ 0 & 0 \end{pmatrix},
\]
where the submatrices \(A_{11}\) and \(A_{12}\) are obtained by solving the linear system
\[
\begin{pmatrix} K_{CC} & V_C \\ V_C^T & 0 \end{pmatrix} \begin{pmatrix} A_{11} \\ A_{21} \end{pmatrix} = \begin{pmatrix} C^T & 0 \\ 0 & 0 \end{pmatrix}.
\]
A direct calculation gives \(A_{11} = B(C) (B^T(C)K_{CC}B(C))^{-1} B^T(C)C^T\) and \(A_{12} = 0\). This is due to the fact that
\(B^T(C)K_{CC}B(C)\) is non-singular. Indeed, since \(C \sim DPP(K,V)\) and, thanks to Lemma 3 in Appendix, we have
\[
0 \neq \det \begin{pmatrix} K_{CC} & V_C \\ V_C^T & 0 \end{pmatrix} = (-1)^p \det \begin{pmatrix} V_C^T V_C \end{pmatrix} \det \begin{pmatrix} B^T(C)K_{CC}B(C) \end{pmatrix}.
\]
Next, we show that \(I(C)\) admits a simpler expression. By definition, \(P_{V^\perp} = \mathbb{I} - QQ^T\) where \(Q\) has orthonormal columns and is obtained thanks to the QR-decomposition \(V = QR\). Then, we obtain \(B^T(C)V_C = 0 = B^T(C)Q_C\). Therefore, we find that \(B^T(C)K_{CC}B(C) = B^T(C)K_{CC}B(C)\) where we used that \(K_{CC} = (C^T - Q_C Q_C^T)K(C - Q Q_C^T)\), and \(B^T(C)Q_C = 0\). This completes the proof.

We can now formally proof the identity given in (3) in the introduction by leveraging the previous results.

**Proposition 2.** Let \(C \sim DPP(K,\lambda, V)\). It holds that
\[
\mathbb{E}_{C}[(C P_{V^\perp} C K_{CC} P_{V^\perp} C^T)^T] = P_{V^\perp}(\tilde{K} + \lambda I)^{-1} P_{V^\perp}.
\]

**Proof.** To fix the ideas, we put \(\lambda = 1\) whereas the general result can be found by a simple re-scaling. Firstly, we show that
\[
(C P_{V^\perp} C K_{CC} P_{V^\perp} C^T)^T = CB(C) (B^T(C)K_{CC}B(C))^{-1} B^T(C)C^T,
\]
with \(P_{V^\perp} = B(C)B^T(C)\), and where \(B(C) \in \mathbb{R}^{k \times (k-p)}\) is a matrix whose columns are orthonormal basis of \((V_C)^\perp\). This is done by checking the definition of the Moore-Penrose pseudo-inverse. Namely, define \(A = C P_{V^\perp} C K_{CC} P_{V^\perp} C^T\) for simplicity. Then, we have \(AA^T = A\) and \(A^T A = A^T\). Similarly, it holds that \(AA^T = C P_{V^\perp} C^T\) and \(A^T A = C P_{V^\perp} C^T\) are symmetric. Secondly, let \(I(C) = CB(C) (B^T(C)K_{CC}B(C))^{-1} B^T(C)C^T\). Then, by combining Proposition 1 and Theorem 1 we find, for \(C \sim DPP(K,V)\),
\[
\mathbb{E}_{C} \begin{pmatrix} u_0 \\ 0 \end{pmatrix}^T \begin{pmatrix} I(C) & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} v_0 \\ 0 \end{pmatrix} = \mathbb{E}_{C} \begin{pmatrix} u_0 \\ 0 \end{pmatrix}^T \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} K_{CC} & V_C \\ V_C^T & 0 \end{pmatrix}^{-1} \begin{pmatrix} C^T & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} v_0 \\ 0 \end{pmatrix} = \begin{pmatrix} u_0 \\ 0 \end{pmatrix}^T \begin{pmatrix} \tilde{K} + I \\ V^T \end{pmatrix}^{-1} \begin{pmatrix} v_0 \\ 0 \end{pmatrix},
\]
for all \(u_0, v_0 \in \mathbb{R}^n\). Then, by using the formula for the inverse of block matrices given in Lemma 3 in Appendix, we remark that
\[
(\tilde{K} + I)^{-1} V^T = (\tilde{K} + I)^{-1} P_V V (V^T V)^{-1} - (V^T V)^{-1},
\]
where we recall that \(\tilde{K} = P_{V^\perp} K P_{V^\perp}\). By a direct substitution, this gives the final result
\[
\mathbb{E}_{C} [CB(C) (B^T(C)K_{CC}B(C))^{-1} B^T(C)C^T] = (\tilde{K} + I)^{-1/2} P_{V^\perp} P_{V^\perp} (\tilde{K} + I)^{-1/2} = P_{V^\perp} (\tilde{K} + I)^{-1} P_{V^\perp}.
\]
Notice that \(P_{V^\perp}\) and \((\tilde{K} + I)^{-1}\) commute since they share the same eigenvectors.

In view of Proposition 2, we now define the projected Nyström approximation.

**Definition 4.** Let \((K,V)\) be a NNP and \(\tilde{K} = P_{V^\perp} K P_{V^\perp}\). Let \(C\) such that \(\text{Pr}(C) \neq 0\) for \(DPP(K,V)\). The projected Nyström approximation of \(\tilde{K}\) is
\[
\tilde{L}(C) = P_{V^\perp} K_{CC} B(C) (B^T(C)K_{CC}B(C))^{-1} B^T(C)K_{CC} P_{V^\perp},
\]
where \(B(C) \in \mathbb{R}^{k \times (k-p)}\) be a matrix whose columns are an orthonormal basis of \((V_C)^\perp\).
It is worth emphasizing that in Definition 3 the submatrices $K_C$ and $K_{CC}$ are sufficient to construct the projected Nyström approximation while $\tilde{K}$ should not be explicitly constructed. Therefore, the projected Nyström approximation is also promising in order to solve problems where the kernel matrix is too large compared to the computer memory. We leave this study for a future work.

As a consequence Theorem 1 Corollary 2 shows that the expected error of the approximation naturally decreases as the number of sampled landmarks increases.

**Corollary 2.** Let $\mathcal{C} \sim DPP(K/\lambda, V)$ with $\lambda > 0$. We have the identities

1. $0 \preceq \tilde{L}^{\top} = \tilde{K}_C D(C) \left( B^{\top}(C) \tilde{K}_{CC} B(C) \right)^{-1} B^{\top}(C) \tilde{K}_C \preceq \tilde{K},$

2. $\mathbb{E}[\tilde{K} - \tilde{L}^{\top}] = \lambda \tilde{K} (\tilde{K} + \lambda I)^{-1} \preceq \lambda I.$

**Proof.** (i) The first identity follows from the same argument as in the proof of Proposition 1. Define $\tilde{K}_C = \mathbb{E}[\tilde{K}^{\top} \mathbb{E}[\tilde{K} + \lambda I)^{-1}].$

To show that $\tilde{L}^{\top} \preceq \tilde{K}$, it is sufficient to show the following fact: for all $\epsilon > 0$,

$$\tilde{K}_C D(C) \left( B^{\top}(C) \tilde{K}_{CC} B(C) + \epsilon I \right)^{-1} B^{\top}(C) \tilde{K}_C \preceq \tilde{K},$$

since by taking the limit $\epsilon \to 0$, we obtain $\tilde{L}^{\top} \preceq \tilde{K}$. To prove the inequality (8), we define $\tilde{K} = A^{\top} A$ and, thanks to the push-through identity, we show that

$$A_C^{\top} B(C) \left( B^{\top}(C) A_C A_C^{\top} B(C) + \epsilon I \right)^{-1} B^{\top}(C) A_C = \left( A_C^{\top} B(C) B^{\top}(C) A_C + \epsilon I \right)^{-1} A_C^{\top} B(C) B^{\top}(C) A_C \preceq \mathbb{I}.$$

(ii) The second identity follows from Proposition 1 and Theorem 1. Consider first the case $\lambda = 1$ without loss of generality. Define

$$\tilde{M}(C) = \begin{pmatrix} \tilde{K}_C^{\top} & 0 \\ 0 & \tilde{K}_C \end{pmatrix} \begin{pmatrix} K_{CC} & V_c \\ V_c & 0 \end{pmatrix}^{-1} \begin{pmatrix} \tilde{K}_C & V_c \\ V_c & 0 \end{pmatrix}.$$

Then, by using $\tilde{K} V = 0$, we find

$$\mathbb{E}[\tilde{M}(C)] = \begin{pmatrix} \tilde{K}_C^{\top} & 0 \\ V_c^{\top} & 0 \end{pmatrix} \begin{pmatrix} \tilde{K} + I & V_c \\ V_c & 0 \end{pmatrix}^{-1} \begin{pmatrix} \tilde{K}_C & V_c \\ V_c & 0 \end{pmatrix} = \begin{pmatrix} \tilde{K} (\tilde{K} + I)^{-1} \tilde{K} & 0 \\ 0 & 0 \end{pmatrix},$$

where Lemma 4 in Appendix was used to compute the matrix inverse. This shows that the expectation of the projected Nyström approximation $\mathbb{E}[\tilde{L}^{\top}(C)] = \tilde{K} (\tilde{K} + I)^{-1} \tilde{K}$, which gives $\tilde{K} - \mathbb{E}[\tilde{L}^{\top}(C)] = \tilde{K} (\tilde{K} + I)^{-1}$. The final result is obtained by replacing $\tilde{K}$ by $\tilde{K}/\lambda$. $\square$

The Nyström approximation of the penalized regression problem can now be discussed by using the matrix Nyström approximation that we just introduced.

### 5.1.1 Empirical results for matrix Nyström approximation

We illustrate the effect of extended L-ensemble sampling versus uniform sampling for Nyström matrix approximation on the UCI benchmark data sets: Breast Cancer, Mushroom and Wine Quality. The data sets are standardized, performance is measured by the relative Frobenius norm of the error:

$$\| \tilde{K} - \tilde{L}(C) \|_F / \| \tilde{K} \|_F.$$

We again use a Gaussian kernel $k(x, x') = \exp(-\|x - x'\|^2/\sigma^2)$ and linear regression component: $V = [X \ 1_n]$ where $X = [x_1 \ldots x_n] \in \mathbb{R}^{n \times d}$. The bandwidth is determined using the median heuristic defined in Section 4.2. The simulation is repeated 10 times and the error bars show the standard error of the mean. The results are displayed in Figure 4. Extended DPP sampling gives a more accurate Nyström approximation.
notations. Let $\tilde{y}$ be a function of the number landmarks using uniform vs extended DPP sampling.

\section{Nyström approximation of regularized regression}

Given $C = \{i_1, \ldots, i_k\} \subset [n]$, the Nyström approximation allows to reduce the number of parameters from $n + p$ to $k + p$ without overlooking data points. To do so in the setting of this paper, we propose to solve a simplified problem which differs from \([PLS]\) by the domain of the minimization, i.e., we define the problem

$$\min_{f \in \mathcal{H}_N} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2 + \gamma J(f),$$

where $\mathcal{H}_N = \left\{ f(x) = \sum_{i=1}^{k} \alpha_i k(x, x_{i_1}) + \sum_{j=1}^{p} \beta_j p_j(x) \text{ s.t. } \sum_{i=1}^{k} \alpha_i p_j(x_{i_1}) = 0 \text{ for all } 1 \leq j \leq p \right\}$ where $k = |C|$ is the number of samples. The domain of the optimization problem now includes only finite linear combinations of $k(\cdot, x_{i_1})$ for $i_1 \in C$, with a specific condition on the coefficients, whereas the domain of the ‘full’ optimization problem \([PLS]\) includes possibly infinite linear combinations. In analogy with \([eq:regression1]\), this condition yields afterwards the constraint $V_C^\top \alpha' = 0$ where $\alpha' = [\alpha_{i_1} \ldots \alpha_{i_k}]^\top \in \mathbb{R}^k$. Here, $V = [p_1(x_i)]_{i}^{n}$ is a $n \times p$ matrix and $k = |C|$.

The solution of \([NysPLS]\) involves a $(k - p) \times (k - p)$ linear system that we write below, after introducing useful notations. Let $B(C) \in \mathbb{R}^{(k - p) \times p}$ be a matrix whose columns are an orthonormal basis of $(V_C)^\perp$, and that is such that $P_{V_C^\perp} = B(C)B(C)^\top$. Then, after elementary manipulations, the system yields

$$\alpha'^* = B(C) \left( B^\top(C)K_C \mathbb{1}_{V_C^\perp} K_C^\top B(C) + n \gamma K_C \mathbb{1}_{V_C^\perp} K_C^\top B(C) \right)^{-1} B^\top(C)K_C \mathbb{1}_{V_C^\perp} y$$

$$\beta'^* = (V^\top V)^{-1} V^\top \left( y - K_C \beta'^* \right)$$

The details of the derivation are given in Appendix. Also, it is straightforward to determine the in-sample estimator $\hat{z}_N = K_C^\top \alpha'^* + V^\top \beta'^*$, which is then given, in terms of the projected Nyström approximation, as follows

$$\hat{z}_N = \tilde{L}(C) \left( \tilde{L}(C) + n \gamma I_n \right)^{-1} \mathbb{1}_{V_C^\perp} y + \mathbb{1}_{V_C^\perp} y.$$

Importantly, this estimator is the estimator of the ‘full’ problem where $\tilde{K}$ is replace by $\tilde{L}(C)$.

\section{Bound on the expected risk}

We recall our data assumption $y_i = f(x_i) + \epsilon_i$ where $\epsilon_i$ denotes i.i.d. $N(0, \sigma^2)$ noise with $1 \leq i \leq n$. For convenience, define $z_i = f(x_i)$ for all $1 \leq i \leq n$. The expected risk of the full regression problem is $\mathcal{R}(\hat{z}) = \mathbb{E}_x \| \hat{z} - z \|^2$. We aim to find an upper bound for the expected risk obtained thanks to the projected Nyström approximation \([eq:regression2]\), i.e., $\mathcal{R}(\hat{z}_N) = \mathbb{E}_x \| \hat{z}_N - z \|^2$. In the spirit of the kernel ridge regression and Theorem 2.5 in \([23]\), we can prove the following stability bound on expectation.

\begin{theorem}
Let $C \sim DPP(K/\lambda, V)$ with $\lambda > 0$. Then, it holds that

$$\mathbb{E}_C \left[ \frac{\mathcal{R}(\hat{z}_N)}{\mathcal{R}(\hat{z})} \right] \leq 1 + \frac{\lambda}{n \gamma} d_{att}(\tilde{K}/\lambda), \text{ with } d_{att}(\tilde{K}/\lambda) = \text{Tr} \left( \tilde{K}(\tilde{K} + \lambda I_n)^{-1} \right).$$
\end{theorem}
This result indicates that using the Nyström approximation cannot dramatically degrade the risk on expectation. An analogous result for leverage scores sampling holding with high probability can found in [36] for kernel ridge regression. We remark that the effective dimension $d_{eff}(\tilde{K}/\lambda)$ is crucial in many sampling methods (see also, e.g. [19]). Typically, a small $\lambda > 0$ yields a large expected sample $E[|C|] = p + d_{eff}(\tilde{K}/\lambda)$ and therefore reduces the magnitude of the upper bound in Theorem 2.

**5.4 Application: non-linear time series using semi-parametric models**

A typical (embedded) application that requires a small number of parameters which is a problem of interest in engineering, for instance in the context of system identification, electromechanical systems or in the control of chemical processes. Within the framework of non-linear time series, a common approach consists in estimating a non-linear black-box model to produce accurate and fast forecasts starting from a set of observations. The user usually has some expert knowledge to incorporate into the estimation. This make the use of semi-parametric regression models especially appealing for systems and control [23, 21], while we refer to [24] for an overview of the various applications in finance, climate and environment sciences. Empirically, it is common to transform time series estimation or system identification problems into regression problems, such as PLS, as we explain hereafter. Therefore, we use this engineering application as a case study for the function estimation framework used in this paper. A recent theoretical analysis of this type of regression frameworks for time series can be found in [32].

The time cruciality of industrial applications necessitates models with a small number of parameters, as these have a profound impact on the memory requirements and prediction speed in real-time forecasting. We demonstrate the use of DPP sampling for Nyström based regression. We show that Nyström based regression (NysPLS) achieves a similar performance as the full system with a lower memory cost and prediction time.

In this simulation, we compare the performance of solving (PLS) and (NysPLS) by using either uniform or DPP sampling. Each model contains a linear parametric part corresponding to the system to be estimated and non-parametric part based on the Gaussian kernel. The non-parametric part can be viewed as a misspecification error. A simple observation given in Proposition 3 justifies a decomposition with a separation of variables between the linear and non-linear components.

**Proposition 3.** Let $v \in \mathbb{R}^d$ and let $P_{v,\perp}$ be the projector onto the orthogonal of $v$. Then, the kernel $k([P_{v,\perp}x, P_{v,\perp}x]) = \exp(-\|P_{v,\perp}(x - x')\|^2)$ is positive semi-definite on $\mathbb{R}^d$.

**Proof.** This can be shown thanks to the following result of [3]: $\exp(-g(x, x'))$ is positive semi-definite if and only if $g(x, x')$ is negative semi-definite with respect to 1. Clearly, $g(x, x') = \|P_{v,\perp}(x - x')\|^2$ satisfies $\sum_{i,j=1}^m \alpha_i \alpha_j \langle x_i, x_j \rangle \leq 0$ for all finite set of $x_i$ for $1 \leq i \leq m$ and $\alpha \in \mathbb{R}^m$ such that $\sum_{i=1}^m \alpha_i = 0$.

Then, the following systems are defined:

1. **System 1:** The first model is a static toy example that is given at time step $t$ with $1 \leq t \leq n$ by

   \[
y'(t) = a_2 z_i + a_1 + \sin(x_i' + x_j') + \epsilon',\]

   with $a_2 = 0.2$, $a_1 = 0.4$ and where superscript $t$ indicates a value obtained at time $t$. The real $y'$ is the output of the system at time step $t$, which is given by the combination of a linear combination of the real input $z'$ and a non-linear function of two other real inputs $x_i'$ and $x_j'$ at time $t$. The training set is obtained by considering a set of input-output pairs obtained for a sequence of integer time steps $1 \leq t \leq n$. The inputs are sampled independently as follows: $x_1$ and $x_2$ are $N(0, 2)$ random variables, whereas $z \sim N(0, 2.5)$, and $\epsilon \sim N(0, 0.05)$ is the noise. The training data for the penalized regression problem are $(x_i, y_i)$ with

   \[
x_i = [z_i' x_i' x_j' ]^\top \in \mathbb{R}^3 \text{ and } y_i = y'(i) \text{ for } 1 \leq i \leq n.
   \]

Notice that the time information is not considered here in order to transform the system identification problem into a regression problem, while non-static systems are given hereafter. Let $x = [z, x_1, x_2]^\top$. The estimated function is of the form

   \[
f(x) = \beta_1 p_1(x) + \beta_2 p_2(x) + \sum_{i=1}^n \alpha_i k(x, x_i),
   \]

Notice that a different font is used for the inputs and output, compared to the $(x_i, y_i)$ pairs.
where \( p_1(x) = 1 \) and \( p_2(x) = x_1 \), while the kernel is \( k(x, x') = \exp\left(-\frac{1}{\sigma^2} \left((x_2 - x'_2)^2 + (x_3 - x'_3)^2\right)\right) \), where \( x_k \) denotes the \( k \)-th component of \( x \) with \( 1 \leq k \leq 3 \). The estimation problem is then cast in the form of [PLS] since Proposition 3 indicates that \( k(x, x') \) is psd.

2. System 2: The second model is not static: for integer time steps \( 1 \leq t \leq n \), it reads

\[
y^t = a_1 + a_2 y^{t-1} + a_3 y^{t-2} + 2 \text{sinc} (x_1^t + x_2^t) + \varepsilon^t,
\]

where \( a_1 = 0.3 \), \( a_2 = 0.2 \), \( a_3 = 0.1 \). It is common to define \( y^0 = y^{-1} = 0 \). Also, we consider independent random variables \( x_1 \sim N(0, 2) \), \( x_2 \sim N(0, 2) \), and a noise \( \epsilon \sim N(0, 0.05) \). The training data for the penalized regression problem are \((x_i, y_i)\) for \( 1 \leq i \leq n \) with

\[
x_i = [x_1^i \ x_2^i \ y^{i-1} \ y^{i-2}]^\top \in \mathbb{R}^4 \quad \text{and} \quad y_i = y^i.
\]

Here, the time series is encoded into the regression problem in such a way that \( x_i \) contains the previous two time steps. Let \( x \in \mathbb{R}^4 \). The estimated function is of the form

\[
f(x) = \beta_1 p_1(x) + \beta_2 p_2(x) + \beta_3 p_3(x) + \sum_{i=1}^{n} \alpha_i k(x, x_i),
\]

where \( p_1(x) = 1 \), \( p_2(x) = x_3 \), \( p_3(x) = x_4 \) and \( k(x, x') = \exp\left(-\frac{1}{\sigma^2} \left((x_1 - x'_1)^2 + (x_2 - x'_2)^2\right)\right) \).

3. System 3: The third model is of the form:

\[
y^t = a_1 + a_2 y^{t-1} + a_3 y^{t-2} + b_1 \text{sinc} (u^{t-1}) + b_2 \text{sinc} (u^{t-2}) + \varepsilon^t,
\]

with \( a_1 = 0.6 \), \( a_2 = 0.4 \), \( a_3 = 0.2 \), \( b_1 = 0.7 \), \( b_2 = 0.6 \), \( u \sim N(0, 4) \), and the noise \( \epsilon \sim N(0, 0.05) \). We also have \( y^0 = y^{-1} = 0 \) and \( u^0 = u^{-1} = 0 \) by definition. The training data for the penalized regression problem are \((x_i, y_i)\) for \( 1 \leq i \leq n \) with

\[
x_i = [u^{i-1} \ u^{i-2} \ y^{i-1} \ y^{i-2}]^\top \in \mathbb{R}^4 \quad \text{and} \quad y_i = y^i
\]

Let \( x \in \mathbb{R}^4 \). The estimated function is of the form

\[
f(x) = \beta_1 p_1(x) + \beta_2 p_2(x) + \beta_3 p_3(x) + \sum_{i=1}^{n} \alpha_i k(x, x_i),
\]

where \( p_1(x) = 1 \), \( p_2(x) = x_3 \), \( p_3(x) = x_4 \) and \( k(x, x') = \exp\left(-\frac{1}{\sigma^2} \left((x_1 - x'_1)^2 + (x_2 - x'_2)^2\right)\right) \).

We take \( n = 1000 \) time steps, afterwards the data set is split into a 50/25/25 train, validation and test split. The validation set is used to determine the regularization parameter \( \gamma \) and bandwidth \( \sigma \). For each model, we measure the parameter identification error, i.e., the mean squared error between the true coefficients \( a_1, a_2, \ldots \) of the parametric component and their estimates \( \beta_1, \beta_2, \ldots \). More importantly, we calculate the prediction error on the test set: \((1/n_{\text{test}}) \sum_{t=1}^{n_{\text{test}}} (y_t - \hat{y}_t)^2\). The simulation is repeated 10 times. The results are visualized in Figures 5 and 6 where the error bars shown the 97.5% confidence interval. Both sampling algorithms are capable of correctly identifying the linear part of the model. Given a number of landmark points, DPP sampling shows better performance than uniform sampling for the prediction error which is the task of practical interest.

![Figure 5: The parameter identification error in function of the number landmarks \(|C|\) using uniform vs extended \(L\)-ensemble sampling. Here, the total number of training points is \( n = 500\).](image-url)
6 Discussion and conclusion

Although the extended $L$-ensembles are particularly suited for sampling in the context of semi-parametric regression, the sampling cost in practice might be high if an exact DPP sampling algorithm is used. We acknowledge this difficulty and point the reader towards the recent advances in DPP sampling algorithm which have achieved an improved scalability, especially, if the number of sampled landmarks is not large [10]. Sampling a fixed-size DPP without looking at all items was also studied in [7], which provides theoretical guarantees. We expect the methods of [10, 7] to be also applicable for partial-projection DPPs, while further approximate DPP sampling algorithms can be developed in the future.

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Appendix

6.1 Solution of the penalized least-squares regression

**Theorem 3** (Existence, Thm 2.9 in [27]). Suppose $L(f)$ is a continuous and convex functional in a Hilbert space $H$ and $J(f)$ is a square (semi) norm in $H$ with a null space $N_J$, of finite dimension. If $L(f)$ has a unique minimizer in $N_J$, then $L(f) + \gamma J(f)$ has a minimizer in $H$.

6.2 Useful identities and results

Firstly, we mention an instrumental result given in [29].

**Lemma 1** (Theorem 2.1 in [29]). Let $A \subseteq [n]$ and $M \in \mathbb{R}^{n \times n}$. Let $\mathbb{1}_A$ be the diagonal matrix with ones in the diagonal positions corresponding to elements of $A = [n] \setminus A$, and zeros otherwise. Then, it holds that $\sum_{C: A \subseteq C} \det M_{CC} = \det(M + \mathbb{1}_A)$.

Secondly, we provide useful formulae to calculate the determinant of matrices with the special structure of extended $L$-ensembles.
Lemma 2 (Lemma 3.12 in [1]). Let \((M, V)\) is a NNP such as in Definition 1. Let \(\widetilde{M} = P_{V^\perp} M P_{V^\perp}\in \mathbb{R}^{n \times n}\) and \(V = QR \in \mathbb{R}^{n \times p}\) where \(Q \in \mathbb{R}^{n \times p}\) has orthonormal columns and \(R\) is upper triangular. Then, we have

\[
\det \left( \frac{\widetilde{M} \ Q}{\ Q \ 0} \right) = (-1)^p[t^p] \det \left( \frac{\widetilde{M} + tQQ^\top}{\ Q \ 0} \right)
\]

where \([t^p]\) denotes the coefficient of the term \(t^p\).

Lemma 3 (Lemma 3.11 [1]). Let \(M \in \mathbb{R}^{n \times n}\) and \(V \in \mathbb{R}^{n \times p}\). Then, we have

\[
\det \left( \frac{M \ V}{\ V \ 0} \right) = (-1)^p \det(V^\top V) \det(Q_\perp M Q_\perp),
\]

where \(Q_\perp \in \mathbb{R}^{n \times (n-p)}\) has orthonormal columns and is such that \(V^\top Q_\perp = 0\).

For the sake of completeness, we derive an equivalent expression for the normalization appearing in Definition 3 by extensively using proof techniques of [1]. The proof of Proposition 3 is in Section 6.3.

Proposition 4 (Normalization factors). Let \((L, V)\) is a NNP such as in Definition 2. We have the following identity

\[
(-1)^p \det(\mathbb{I} + \tilde{L}) \det(V^\top V) = \det \left( \frac{L + \mathbb{I}}{\ V^\top \ 0} \right).
\]

Finally, we quote a formula for the inversion of a specific block matrix.

Lemma 4 (Inverse of a specific block matrix).

\[
\left( \begin{array}{cc}
A & V \\
V^\top & 0
\end{array} \right)^{-1} = \left( \begin{array}{cc}
A^{-1} - A^{-1}V(V^\top A^{-1}V)^{-1}V^\top A^{-1} & A^{-1}V(V^\top A^{-1}V)^{-1} - (V^\top A^{-1}V)^{-1}A^{-1}V \\
(V^\top A^{-1}V)^{-1}V^\top A^{-1} & -(V^\top A^{-1}V)^{-1}
\end{array} \right).
\]

6.3 Deferred proofs

Proof of Proposition 4 [1] Let \(V = QR\) thanks to the QR-decomposition of \(V\), with \(Q \in \mathbb{R}^{n \times n}\). Let \(Q_\perp \in \mathbb{R}^{n \times (n-p)}\) be a matrix with orthonormal columns so that \(P_{V^\perp} = Q_\perp Q_\perp^\top\). Then, \(\tilde{L} = Q_\perp L Q_\perp^\top\). This gives the following decomposition

\[
\mathbb{I} + \tilde{L} = QQ^\top + Q_\perp \left( \mathbb{I}_{(n-p) \times (n-p)} + Q_\perp L Q_\perp^\top \right) Q_\perp^\top,
\]

(10)

where we used \(\mathbb{I} = Q_\perp Q_\perp^\top + QQ^\top\). Let us define the eigendecomposition \(Q_\perp L Q_\perp^\top + \mathbb{I}_{(n-p) \times (n-p)} = U \Lambda U^\top\), with \(U \in \mathbb{R}^{(n-p) \times (n-p)}\) an orthogonal matrix and \(\Lambda \in \mathbb{R}^{(n-p) \times (n-p)}\) a diagonal matrix. Therefore, in view of (10), we find \(\det(\mathbb{I} + \tilde{L}) = \det(\Lambda)\). Now, we use the following identity, which results from Lemma 2.6 in [1],

\[
\det \left( \frac{L + \mathbb{I}}{\ V^\top \ 0} \right) = \det \left( \frac{\tilde{L} + \mathbb{I}}{\ V^\top \ 0} \right),
\]

(11)

with \(\mathbb{I} = P_{V^\perp}\) and \(\tilde{L} = P_{V^\perp} L P_{V^\perp}\). Next, by using the decomposition of \(V = QR\), we find

\[
\det \left( \frac{\tilde{L} + \mathbb{I}}{\ V^\top \ 0} \right) = \det(R^\top R) \det \left( \frac{\tilde{L} + \mathbb{I}}{\ V^\top \ 0} \right) = \det(V^\top V) \det \left( \frac{\tilde{L} + \mathbb{I}}{\ V^\top \ 0} \right),
\]

(12)

where the equality \(\ast\) uses Lemma 3. Then, we use Lemma 2 to express the last factor of the RHS of (12),

\[
\det \left( \frac{\tilde{L} + \mathbb{I}}{\ V^\top \ 0} \right) = (-1)^p [t^p] \det \left( \frac{\tilde{L} + \mathbb{I} + tQQ^\top}{\ V^\top \ 0} \right),
\]

(13)

where \([t^p]\) denotes the coefficient of the term \(t^p\) in the polynomial \(p(t)\). Next, by using the above eigendecomposition, we find

\[
[t^p] \det \left( \frac{\tilde{L} + \mathbb{I} + tQQ^\top}{\ V^\top \ 0} \right) = [t^p] \det \left( \frac{Q}{\ U} \left( \begin{array}{cc}
t_0^p & 0 \\
0 & \Lambda
\end{array} \right) \right) = \det(\Lambda) = \det(\mathbb{I} + \tilde{L}),
\]

(14)

where we used that \((Q \ U) \in \mathbb{R}^{n \times n}\) is an orthogonal matrix. Finally, we combine (11), (12), (13) and (14) to give

\[
\det \left( \frac{L + \mathbb{I}}{\ V^\top \ 0} \right) = \det(V^\top V) (-1)^p \det(\mathbb{I} + \tilde{L}),
\]

which is the desired result. \(\square\)
Proof of Theorem 4. Let \( \mathbf{u}, \mathbf{v} \in \mathbb{R}^{n+p} \). Firstly, we notice first that, for all \( K \in \mathbb{R}^{n \times n} \), we have
\[
\begin{pmatrix}
    C^T KC & C^T V \\
    V^T C & 0
\end{pmatrix} = 
\begin{pmatrix}
    C^T & 0 \\
    0 & 1
\end{pmatrix} 
\begin{pmatrix}
    K & V \\
    V^T & 0
\end{pmatrix} 
\begin{pmatrix}
    C & 0 \\
    0 & 1
\end{pmatrix} = \tilde{C}^T \begin{pmatrix}
    K & V \\
    V^T & 0
\end{pmatrix} \tilde{C},
\]
where \( \tilde{C} \) is a sampling matrix corresponding to a subset of \( \{1, \ldots, n+p\} \), namely \( \tilde{C} \) is associated to the set \( \tilde{C} = C \cup A \) with \( A = \{n+1, \ldots, n+p\} \). Therefore, by using Lemma 4, we obtain
\[
\sum_c \det \begin{pmatrix}
    C^T KC & C^T V \\
    V^T C & 0
\end{pmatrix} = \det \begin{pmatrix}
    K+1 & V \\
    V^T & 0
\end{pmatrix}.
\]
(15)

Take \( Q = \begin{pmatrix}
    K & V \\
    V^T & 0
\end{pmatrix} \), then the desired expectation can be written as follows
\[
N^{-1} \sum_c \det(\tilde{C}^T Q \tilde{C}) \times \mathbf{u}^T \tilde{C} \begin{pmatrix}
    C^T & V \\
    V^T C & 0
\end{pmatrix}^{-1} \tilde{C}^T \mathbf{v} = N^{-1} \left( \sum_c \det(\tilde{C}^T Q \tilde{C}) - \sum_c \det(\tilde{C}^T (Q - \mathbf{v} \mathbf{u}^T) \tilde{C}) \right),
\]
thanks to the matrix determinant lemma, and where the normalization \( N \) is given by (15). Then, we find
\[
(I) = \det \begin{pmatrix}
    K+1 & V \\
    V^T & 0
\end{pmatrix} = \det(Q + \mathbb{I}_{[n]} = N,
\]
where \( \mathbb{I}_{[n]} \) is the diagonal matrix with ones in the diagonal positions corresponding to elements of the set \( \mathcal{B} \), and zeros otherwise. Let \( \mathbf{u} = [\mathbf{u}_0, \mathbf{v}_1]^\top \) and \( \mathbf{v} = [\mathbf{v}_0, \mathbf{v}_1]^\top \), with \( \mathbf{u}_0, \mathbf{v}_0 \in \mathbb{R}^n \) and \( \mathbf{u}_1, \mathbf{v}_1 \in \mathbb{R}^p \). Similarly, we have also
\[
(II) = \sum_c \det \begin{pmatrix}
    C^T(K - \mathbf{v}_0 \mathbf{u}_0^\top) & C^T(V - \mathbf{v}_0 \mathbf{u}_1^\top) \\
    (V^T - \mathbf{v}_1 \mathbf{u}_0^\top) & -\mathbf{v}_1 \mathbf{u}_1^\top
\end{pmatrix} = \det \begin{pmatrix}
    (K + \mathbb{I} - \mathbf{v}_0 \mathbf{u}_0^\top) & V - \mathbf{v}_0 \mathbf{u}_1^\top \\
    V^T - \mathbf{v}_1 \mathbf{u}_0^\top & -\mathbf{v}_1 \mathbf{u}_1^\top
\end{pmatrix}
\]
\[
= \det(Q + \mathbb{I}_{[n]} - \mathbf{v} \mathbf{u}^\top).
\]
Hence, we obtain another expression for the desired expectation
\[
\mathbb{E}_{\mathcal{C} \sim \text{DPP}(K,V)} \begin{pmatrix}
    \mathbf{u}^\top \\
    C^T & V \\
    V^T C & 0
\end{pmatrix}^{-1} \mathbf{v} = \frac{\det(Q + \mathbb{I}_{[n]}) - \det(Q + \mathbb{I}_{[n]} - \mathbf{v} \mathbf{u}^\top)}{\det(Q + \mathbb{I}_{[n]})} \mathbf{u}^\top (Q + \mathbb{I}_{[n]})^{-1} \mathbf{v},
\]
where we used the matrix determinant lemma in \( \star \). This completes the proof.

6.4 Details of the derivation of the large scale system of Section 5.2

After elementary manipulations, we obtain the following system
\[
\begin{pmatrix}
    \mathbb{P}_V \hat{C} \mathbb{P}_V \perp K \mathbb{P}_V \perp K \mathbb{P}_V \perp C \mathbb{P}_V \perp + n \gamma \mathbb{P}_V \perp K \mathbb{P}_C \mathbb{P}_V \perp C \mathbb{P}_V \perp \\
    (\mathbb{P}_V \perp)^\top V \mathbb{P}_V \perp \mathbf{y} - K \mathbb{P}_V \perp \mathbf{u}^\prime
\end{pmatrix} \mathbf{u}^\prime = \mathbb{P}_V \perp K \mathbb{P}_V \perp \mathbf{y}
\]
\[
\mathbf{b}^\prime = (V^\top V)^{-1} V^\top (\mathbf{y} - K \mathbb{P}_V \perp \mathbf{u}^\prime)
\]
\[
\mathbb{P}_V \perp \mathbf{u}^\prime = 0.
\]
Let \( B(C) \in \mathbb{R}^{k \times (k-p)} \) be a matrix whose columns are an orthonormal basis of \( (V\mathcal{C})^\perp \), and that is such that \( \mathbb{P}_{V\mathcal{C}} = B(C)B^\top(C) \). Define \( N = B^\top(C)K\mathbb{P}_C B(C) \), which is non-singular almost surely, as shown in the proof of Proposition 4. Then, the first equation of the system yields
\[
\mathbf{u}^\prime = B(C) \left( B^\top(C)K\mathbb{P}_V \perp K \mathbb{P}_V \perp B(C) + n \gamma B^\top(C)K\mathbb{P}_C B(C) \right)^{-1} B^\top(C)K\mathbb{P}_V \perp \mathbf{y}
\]
\[
= B(C)N^{-1/2} \left( N^{-1/2}B^\top(C)K\mathbb{P}_V \perp K \mathbb{P}_V \perp B(C)N^{-1/2} + n \gamma \mathbb{I}_{k-p} \right)^{-1} N^{-1/2}B^\top(C)K\mathbb{P}_V \perp \mathbf{y}
\]
\[
\mathbf{b}^\prime = B(C)N^{-1/2} B^\top(C)K\mathbb{P}_V \perp \left( \mathbb{P}_V \perp K \mathbb{P}_C B(C)N^{-1}B^\top(C)K\mathbb{P}_V \perp + n \gamma \mathbb{I}_n \right)^{-1} \mathbb{P}_V \perp \mathbf{y},
\]
where we used in \( \star \) the push-through identity \((XY + \mathbb{I})^{-1}X = X(YX + \mathbb{I})^{-1}\) with \( X = N^{-1/2}B^\top(C)K\mathbb{P}_V \perp, Y = X^\top \) and \( \mathbb{P}_V \perp = \mathbb{P}_V \perp \). As detailed above, an equivalent expression for \( N = B^\top(C)K\mathbb{P}_C B(C) \) is \( N = B^\top(C)K\mathbb{P}_C B(C) \). The in-sample estimator \( \hat{z}_N = K \hat{C} \mathbf{u}^\prime + \mathbb{V}^\top \mathbf{b}^\prime \) is then given, in terms of the projected Nyström approximation, as follows
\[
\hat{z}_N = \hat{L}(\tilde{C}) \left( \hat{L}(\tilde{C}) + n \gamma \mathbb{I}_n \right)^{-1} \mathbb{P}_V \perp \mathbf{y} + \mathbb{P}_V \mathbf{y},
\]
which is the result stated in Section 5.2.
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