Scattered data approximation

Lecture Notes

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Prologue

This lecture has been taught for the first time in the Master of Computational Science at the Università della Svizzera italiana as a 3 ECTS course. It is mainly based on the text book "Meshfree Approximation Methods with MATLAB" by G. E. Fasshauer. The chapter on numerical methods focuses on low-rank approximation ideas and draws upon current literature in the field, while the chapter on support vector machines follows the lecture notes of a similar lecture from H. Harbrecht at the University of Basel.

1. Introduction

In many applications, we are given a set of *data values*, for example, measurements or samples, and *data sites* for which these data were obtained. We then want to come up with a *model* s_f that matches the data with regard to a certain criterion. Conceptionally, we distinguish two different settings depending on if the underlying data generating process f is known or unknown. If f is unknown, we want to derive a model s_f, which allows us to extrapolate the data for unseen data sites. The "goodness" of fit can be defined in several different ways here. If f is known, for example, as solution operator of a partial differential equation, the goal is to derive a surrogate model s_f, that is cheaper to evaluate than f itself. In either case, if the data are not located on a uniform grid, we speak of *scattered data approximation*.

We start from the data interpolation problem, which aims at exactly matching a given set of data. The data sites are always labelled by $\boldsymbol{x}_i,\ i = 1, \dots, N$ and we introduce the set

$$X := \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset \Omega$$

for some region $\Omega \subset \mathbb{R}^d$. We focus on scalar data values and denote them by $y_i \in \mathbb{R}$, $i = 1, \dots, N$.

Problem 1.1 (Scattered data interpolation) Given data $(\boldsymbol{x}_i, y_i),\ i = 1, \dots, N$, with $\boldsymbol{x}_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$, find a continuous function s_f such that

$$s_f(\boldsymbol{x}_i) = y_i \quad \text{for } i = 1, \dots, N. \tag{1.1}$$

A common solution to (1.1) is to assume that s_f is a linear combination of certain functions φ_j, i.e.,

$$s_f(\boldsymbol{x}) = \sum_{j=1}^{N} c_j \varphi_j(\boldsymbol{x}) \quad \text{for all } \boldsymbol{x} \in \mathbb{R}^d. \tag{1.2}$$

Inserting the interpolation condition (1.1), yields the linear system

$$\boldsymbol{A}\boldsymbol{c} = \boldsymbol{y},$$

where the *generalized Vandermonde matrix* is given by

$$\boldsymbol{A} := [\varphi_j(\boldsymbol{x}_i)]_{i,j=1}^{N} \in \mathbb{R}^{N \times N}.$$

Further, we set $\boldsymbol{c} := [c_j]_{j=1}^{N} \in \mathbb{R}^N$ and $\boldsymbol{y} := [y_i]_{i=1}^{N} \in \mathbb{R}^N$.

Problem 1.1 is *well-posed*, i.e., a solution exists and is unique, iff $\boldsymbol{A}$ is non-singular.

Example 1.2 Given $x_1, \dots, x_N \in \mathbb{R}$ and $y_1, \dots, y_N \in \mathbb{R}$, we are looking for a polynomial $p \in \Pi_{N-1} := \operatorname{span}\{1, x, \dots, x^{N-1}\}$ such that $p(x_i) = y_i$ for $i = 1, \dots, N$. With respect to the monomial basis, the Vandermonde matrix is given by

$$\boldsymbol{A} = \begin{bmatrix} 1 & x_1 & \cdots & x_1^{N-1} \\ \vdots & \vdots & & \vdots \\ 1 & x_N & \cdots & x_N^{N-1} \end{bmatrix} \in \mathbb{R}^{N \times N}.$$

It can be shown that its determinant satisfies

$$\det \boldsymbol{A} = \prod_{0 < i < j \leq N} (x_j - x_i).$$

Therefore, we have $\det \boldsymbol{A} \neq 0$ whenever $x_i \neq x_j$ for $i \neq j$, which directly implies the existence and uniqueness of a solution to (1.1) and, hence, the well-posedness of the polynomial interpolation problem. △

Generalizing the ideas of polynomial interpolation yields the concept of *Haar spaces*.

Definition 1.3 Let $V \subset C(\Omega)$ be a finite-dimensional function space with basis $\varphi_1, \dots, \varphi_N$. The space V is a *Haar space*, iff $\det \boldsymbol{A} \neq 0$ for every set of mutually distinct points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N \in \Omega$, where $\boldsymbol{A}$ is the generalized Vandermonde matrix from (1.1).

The immediate question issuing from the previous definition is: Are there examples of Haar spaces in higher dimensions? We have the following negative result.

Theorem 1.4 (Mairhuber-Curtis) If $\Omega \subset \mathbb{R}^d$, $d > 1$ contains an interior point, then there exist no Haar spaces except for one-dimensional ones.

Proof. Let $d > 1$ and assume that $V \subset C(\Omega)$ is a Haar space with basis $\varphi_1, \dots \varphi_N$ with $N > 1$. We prove the claim by contradiction. Let $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N \in \Omega$ be a set of mutually distinct interior points. By assumption there holds $\det \boldsymbol{A} \neq 0$. Now consider a simple closed path p connecting only $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$. We can interchange the positions of $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$, effectively swapping the first two rows of $\boldsymbol{A}$ by continuously moving along p. This in turn changes the sign of $\det \boldsymbol{A}$. Since φ_1, φ_2, p as well as det are continuous functions, this means that there must exist values $\tilde{\boldsymbol{x}}_1, \tilde{\boldsymbol{x}}_2$ along p, such that $\det \tilde{\boldsymbol{A}} = 0$ for the corresponding generalized Vandermonde matrix. This is a contradiction. □

The theorem tells us that, if we want to have a well-posed multivariate scattered data interpolation problem, we can no longer fix the basis in advance, as we did in Example 1.2. Instead, the basis should depend on the data locations.

Example 1.5 (Interpolation by distance matrices) Given data sites $x_1 \dots, x_N \in \mathbb{R}$ and values $y_1, \dots, y_N \in \mathbb{R}$, we make the ansatz

$$s_f(x) = \sum_{j=1}^{N} c_j |x - x_j|,$$

which amounts to the linear spline interpolant (prove!) if we solve (1.1).

For $d > 1$, this approach can be generalized by employing the euclidean norm:

$$s_f(\boldsymbol{x}) = \sum_{j=1}^{N} c_j \|\boldsymbol{x} - \boldsymbol{x}_j\|_2.$$

△

We call the functions $\phi_j(\boldsymbol{x}) = \|\boldsymbol{x} - \boldsymbol{x}_j\|_2$, $j = 1, \ldots, N$, *radial basis functions*, since ϕ_j only depends on the distance of $\boldsymbol{x}$ from the data site $\boldsymbol{x}_j$.

Definition 1.6 A function $K\colon \mathbb{R}^d \to \mathbb{R}$ is called *radial*, iff there exists a univariate function $k\colon [0, \infty) \to \mathbb{R}$ such that $K(\boldsymbol{x}) = k(r)$, where $r := \|\boldsymbol{x}\|$ and $\|\cdot\|$ is any norm on $\mathbb{R}^d$. We say that K is a *basic function* and that $\varphi_j(\boldsymbol{x}) = K(\boldsymbol{x} - \boldsymbol{x}_j)$, $j = 1, \ldots, N$, are *radial basis functions*.

We finish this chapter by introducing a class of radial functions that always give rise to well-posed problems.

Definition 1.7 A function $K\colon \mathbb{R}^d \to \mathbb{R}$ is *positive semidefinite*, iff the generalized Vandermonde matrix $\boldsymbol{A} = [\varphi_j(\boldsymbol{x}_i)]_{i,j=1}^N := [K(\boldsymbol{x}_i - \boldsymbol{x}_j)]_{i,j=1}^N$ is symmetric positive semidefinite for any mutually distinct $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \mathbb{R}^d$ and any $N \in \mathbb{N}$. It is *positive definite*, iff $\boldsymbol{A}$ is symmetric positive definite.

Example 1.8 The *Matérn kernels*

$$k_\nu(r) := \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu} r}{\ell} \right)^{\nu} B_\nu \left(\frac{\sqrt{2\nu} r}{\ell} \right), \quad \nu, \ell > 0,$$

where B_ν is the modified Bessel function of the second kind of order ν, are positive definite. In particular, there holds

$$k_{1/2}(r) = e^{-\frac{r}{\ell}} \quad \text{and} \quad k_\infty = e^{-\frac{r^2}{2\ell^2}}.$$

△

Fact 1.9

1. If $K_1, \ldots, K_n$ are positive semidefinite and $c_i \geq 0$ for $i = 1, \ldots, n$, then $K = \sum_{i=1}^n c_i K_i$ is also positive semidefinite. If at least one K_i is positive definite and $c_i > 0$, then K is positive definite.
2. If K is positive semidefinite, then $K(\boldsymbol{0}) \geq 0$.
3. If K is positive semidefinite, then $K(\boldsymbol{x}) = K(-\boldsymbol{x})$.
4. Any positive semidefinite function is bounded, i.e., $|K(\boldsymbol{x})| \leq K(\boldsymbol{0})$.
5. If K is positive semidefinite with $K(\boldsymbol{0}) = 0$, then $K \equiv 0$.
6. The product of positive (semi-)definite functions is positive (semi-)definite.

2. Scattered data interpolation with polynomial precision

In many applications, it is desirable that an approximation can represent polynomials exactly. As we have seen in Theorem 1.4, in this case the interpolation points need to be carefully chosen.

Definition 2.1 We call a set $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset \mathbb{R}^d$ *q-unisolvent*, iff the only polynomial $p \in \mathcal{P}_q := \operatorname{span}\{\boldsymbol{x}^{\boldsymbol{\alpha}} : \boldsymbol{\alpha} \in \mathbb{N}^d, \|\boldsymbol{\alpha}\|_1 \leq q\}$ interpolating zero data on X is $p \equiv 0$. This means that the matrix $\boldsymbol{P} := [\boldsymbol{x}_i^{\boldsymbol{\alpha}}]_{i=1,\dots,N,\|\boldsymbol{\alpha}\|_1 \leq q}$ has full column rank $m_q := \dim \mathcal{P}_q = \binom{q+d}{d}$

Taking polynomials into account for the approximation gives rise to a specific version of Problem 1.1 according to

$$s_f(\boldsymbol{x}) = \sum_{j=1}^{N} c_j \varphi_j(\boldsymbol{x}) + \sum_{k=1}^{m_q} d_k p_k(\boldsymbol{x}) \tag{2.1}$$

for a basis $\{p_1, \dots, p_{m_q}\}$ of $\mathcal{P}_q$ and $q \geq 0$.
Enforcing the interpolation conditions $s_f(\boldsymbol{x}_i) = y_i$ for $i = 1, \dots, N$ leads to a linear system of N equations for $N + m_q$ unknowns. To determine the remaining m_q coefficients, we add the additional conditions

$$\sum_{j=1}^{N} c_j p_k(\boldsymbol{x}_j) = 0 \quad \text{for } k = 1, \dots, m_q. \tag{2.2}$$

Introducing the matrices

$$\boldsymbol{A} := [\varphi_j(\boldsymbol{x}_i)]_{i,j=1}^{N} \in \mathbb{R}^{N \times N} \quad \text{and} \quad \boldsymbol{P} := [p_j(\boldsymbol{x}_i)]_{\substack{i=1,\dots,N \\ j=1,\dots,m_q}} \in \mathbb{R}^{N \times m_q}$$

as well as the vectors $\boldsymbol{c} := [c_1, \dots, c_N]^\intercal$, $\boldsymbol{d} := [d_1, \dots, d_{m_q}]^\intercal$ yields the saddle point system

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{P} \\ \boldsymbol{P}^\intercal & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{c} \\ \boldsymbol{d} \end{bmatrix} = \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{0} \end{bmatrix}. \tag{2.3}$$

In view of (2.1), we can weaken the conditions on the positive definiteness of the basic function and still obtain a well-posed problem.

Definition 2.2 A function $K\colon \mathbb{R}^d \to \mathbb{R}$ is *conditionally positive semidefinite* of order $(q+1)$, iff for any mutually distinct points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N \in \mathbb{R}^d$ and any $N \in \mathbb{N}$ the generalized Vandermonde matrix $\boldsymbol{A} := [K(\boldsymbol{x}_i - \boldsymbol{x}_j)]_{i,j=1}^N$ satisfies

$$\boldsymbol{c}^\intercal \boldsymbol{A}\boldsymbol{c} \geq 0 \quad \text{for any } \boldsymbol{c} \in \operatorname{kern} \boldsymbol{P}^\intercal, \tag{2.4}$$

where $\boldsymbol{P} := \left[\boldsymbol{x}_i^{\boldsymbol{\alpha}}\right]_{\substack{i=1,\dots,n \\ \|\boldsymbol{\alpha}\|_1 \leq q}}$.
It is *conditionally positive definite*, iff equality in (2.4) only holds for $\boldsymbol{c} = \boldsymbol{0}$.

We have the following relation between conditionally positive definite functions.

Fact 2.3 A function that is conditionally positive (semi-)definite of order $(q+1)$ is also conditionally positive (semi-)definite of any higher order. In particular, a function that is conditionally positive (semi-)definite of order 1 is conditionally positive (semi-)definite of any order.

The next theorem guarantees the solvability of (2.3) in case of conditionally positive basic functions.

Theorem 2.4 Let $K\colon \mathbb{R}^d \to \mathbb{R}$ be conditionally positive definite of order $(q+1)$ and let $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N$ be q-unisolvent. Then, the linear system (2.3) is uniquely solvable.

Proof. To prove the assertion, we show that the kernel of the matrix in (2.3) is trivial. To this end, let $[\boldsymbol{c}, \boldsymbol{d}]^\intercal$ be a solution to the homogenous system, i.e., a solution for $\boldsymbol{y} = \boldsymbol{0}$. We show that $[\boldsymbol{c}, \boldsymbol{d}]^\intercal = \boldsymbol{0}$ is the only solution. Multiplying the top block of (2.3) by $\boldsymbol{c}^\intercal$ yields

$$\boldsymbol{c}^\intercal \boldsymbol{A}\boldsymbol{c} + \boldsymbol{c}^\intercal \boldsymbol{P}\boldsymbol{d} = 0.$$

From the bottom block, we have $\boldsymbol{P}^\intercal \boldsymbol{c} = \boldsymbol{0}$ or $\boldsymbol{c}^\intercal \boldsymbol{P} = \boldsymbol{0}^\intercal$. Consequently, we infer $\boldsymbol{c}^\intercal \boldsymbol{A}\boldsymbol{c} = 0$. Since K is conditionally positive definite of oder $(q+1)$, this implies $\boldsymbol{c} = \boldsymbol{0}$.
By the unisolvency of $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N$, the matrix $\boldsymbol{P}$ has full column rank. Therefore, $\boldsymbol{d} = \boldsymbol{0}$ is the only solution to

$$\boldsymbol{P}\boldsymbol{d} = \boldsymbol{A}\boldsymbol{c} + \boldsymbol{P}\boldsymbol{d} = \boldsymbol{0}$$

of the top block of (2.3). This completes the proof. □

Remark Definition 2.2 and Theorem 2.4 are a special, finite dimensional, instance of the inf-sup- or *Ladyzhenskaya-Babuška-Brezzi* (LBB) condition, which guarantees the well-posedness of (infinite dimensional) saddle point problems. △

Example 2.5 The *generalized multiquadrics* $K(\boldsymbol{x}) := (1 + \|\boldsymbol{x}\|^2)^\beta$, $0 < \beta \notin \mathbb{N}$, are conditionally positive definite of order $\lceil \beta \rceil$.
The *radial powers* $K(\boldsymbol{x}) := \|\boldsymbol{x}\|^\beta$, $0 < \beta \notin 2\mathbb{N}$ are conditionally positive definite of order $\lceil \beta/2 \rceil$. This means that the distance functions from Example 1.5 are conditionally positive definite of order 1.
Duchon's thin plate splines $K(\boldsymbol{x}) := \|\boldsymbol{x}\|^{2\beta} \log \|\boldsymbol{x}\|$, $\beta \in \mathbb{N}^*$, are conditionally positive definite of order $\beta + 1$. △

3. Reproducing kernel Hilbert spaces

Definition 3.1 Let $(\mathcal{H}, \langle\cdot,\cdot\rangle_{\mathcal{H}})$ be a real Hilbert space of functions $f\colon \Omega \to \mathbb{R}$. A function $K\colon \Omega \times \Omega \to \mathbb{R}$ is a *reproducing kernel* for $\mathcal{H}$, iff

1. $K(\boldsymbol{x},\cdot) \in \mathcal{H}$ for all $\boldsymbol{x} \in \Omega$,
2. $\langle K(\boldsymbol{x},\cdot), f\rangle_{\mathcal{H}} = f(\boldsymbol{x})$ for all $f \in \mathcal{H},\ \boldsymbol{x} \in \Omega$.

If $\mathcal{H}$ exhibits a reproducing kernel, we call it a *reproducing kernel Hilbert space* (RKHS).

The question if the reproducing kernel is unique is answered by the following

Fact 3.2 The reproducing kernel of an RKHS is unique.

The existence of a reproducing kernel is equivalent to the point evaluation functional $\delta_{\boldsymbol{x}}$ being continuous for every $\boldsymbol{x} \in \Omega$, i.e., there exists $M_{\boldsymbol{x}} > 0$ such that

$$|\delta_{\boldsymbol{x}} f| = |f(\boldsymbol{x})| \leq M_{\boldsymbol{x}} \|f\|_{\mathcal{H}} \quad \text{for all } f \in \mathcal{H}.$$

This means that $\delta_{\boldsymbol{x}}$ is contained in the dual space $\mathcal{H}'$ of $\mathcal{H}$ for any $\boldsymbol{x} \in \Omega$. By the Riesz representation theorem, there exists $(J\delta_{\boldsymbol{x}}) \in \mathcal{H}$ such that $\langle (J\delta_{\boldsymbol{x}}), f\rangle_{\mathcal{H}} = f(\boldsymbol{x})$ for all $f \in \mathcal{H}$, i.e., $(J\delta_{\boldsymbol{x}})(\boldsymbol{y})$ is the reproducing kernel.
The next theorem establishes some properties of a reproducing kernel.

Theorem 3.3 Let $(\mathcal{H}, \langle\cdot,\cdot\rangle_{\mathcal{H}})$ be an RKHS. Then, there hold the following statements:

1. $K(\boldsymbol{x},\boldsymbol{y}) = \langle K(\boldsymbol{y},\cdot), K(\boldsymbol{x},\cdot)\rangle_{\mathcal{H}}$ for all $\boldsymbol{x},\boldsymbol{y} \in \Omega$.
2. $K(\boldsymbol{x},\boldsymbol{y}) = K(\boldsymbol{y},\boldsymbol{x})$ for all $\boldsymbol{x},\boldsymbol{y} \in \Omega$.
3. Convergence in $\mathcal{H}$ implies pointwise convergence, i.e., if $\|f_n - f\|_{\mathcal{H}} \to 0$ for $n \to \infty$, then $|f_n(\boldsymbol{x}) - f(\boldsymbol{x})| \to 0$ for all $\boldsymbol{x} \in \Omega$.

Proof. By Definition 3.1.1., we have $K(\boldsymbol{y},\cdot), K(\boldsymbol{x},\cdot) \in \mathcal{H}$. Therefore, the reproducing property Definition 3.1.2. yields

$$\langle K(\boldsymbol{y},\cdot), K(\boldsymbol{x},\cdot)\rangle_{\mathcal{H}} = K(\boldsymbol{x},\boldsymbol{y}) \quad \text{for all } \boldsymbol{x},\boldsymbol{y} \in \Omega.$$

This proves the first item of the theorem.
The symmetry of the kernel is a direct consequence of the symmetry of the inner product $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ and the first item.

Finally, the third item is obtained by the Cauchy-Schwarz inequality according to

$$|f_n(\boldsymbol{x}) - f(\boldsymbol{x})| = |\langle K(\boldsymbol{x}, \cdot), f_n - f\rangle_{\mathcal{H}}| \leq \|K(\boldsymbol{x}, \cdot)\|_{\mathcal{H}} \|f_n - f\|_{\mathcal{H}}.$$

□

Remark There holds $\|K(\boldsymbol{x}, \cdot)\|_{\mathcal{H}} = \sqrt{K(\boldsymbol{x}, \boldsymbol{x})}$. △

The reproducing kernel of an RKHS is positive semidefinite in the sense of Definition 1.7, if we replace everywhere $K(\boldsymbol{x}_i - \boldsymbol{x}_j)$ by $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$.

Definition 3.4 Let $K \colon \Omega \times \Omega \to \mathbb{R}$ be a kernel. We say that K is *positive semidefinite*, iff the *kernel matrix*

$$\boldsymbol{K} := [K(\boldsymbol{x}_i, \boldsymbol{x}_j)]_{i,j=1}^{N} \tag{3.1}$$

is positive semidefinite for any choice of mutually distinct points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ and any $N \in \mathbb{N}$. It is *positive definite* if the kernel matrix is positive definite.

The following lemma is a direct consequence of the reproducing property and characterizes the kernel matrix.

Lemma 3.5 Suppose that $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ is an RKHS with reproducing kernel $K \colon \Omega \times \Omega \to \mathbb{R}$. Given a set of mutually distinct points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$, there holds

$$\boldsymbol{K} = \langle \boldsymbol{\Phi}, \boldsymbol{\Phi}^\intercal \rangle_{\mathcal{H}} := \begin{bmatrix} \langle \varphi_1, \varphi_1 \rangle_{\mathcal{H}} & \cdots & \langle \varphi_1, \varphi_N \rangle_{\mathcal{H}} \\ \vdots & \ddots & \vdots \\ \langle \varphi_N, \varphi_1 \rangle_{\mathcal{H}} & \cdots & \langle \varphi_N, \varphi_N \rangle_{\mathcal{H}} \end{bmatrix},$$

where we set $\varphi_i := \Phi(\boldsymbol{x}_i) \in \mathcal{H}$ for the *canonical feature map* $\Phi \colon \Omega \to \mathcal{H},\ \boldsymbol{x} \mapsto K(\boldsymbol{x}, \cdot)$. The vector $\boldsymbol{\Phi} := [\varphi_1, \ldots, \varphi_N]^\intercal \in \mathcal{H}^N$ is called *canonical feature vector*.

Reproducing kernels are particularly positive semidefinite function. This is addressed by the following

Theorem 3.6 Suppose that $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$ is an RKHS with reproducing kernel $K \colon \Omega \times \Omega \to \mathbb{R}$. Then K is positive semidefinite. Moreover, K is positive definite, iff $\delta_{\boldsymbol{x}_1}, \ldots, \delta_{\boldsymbol{x}_N}$ are linearly independent for any choice of mutually distinct points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \Omega$ and any $N \in \mathbb{N}$.

Proof. Let $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \Omega$ be mutually distinct and let $\boldsymbol{c} \in \mathbb{R}^N$ with $\boldsymbol{c} \neq 0$. There holds for the kernel matrix, cp. (3.1), that

$$\boldsymbol{c}^\intercal \boldsymbol{K} \boldsymbol{c} = \boldsymbol{c}^\intercal \langle \boldsymbol{\Phi}, \boldsymbol{\Phi}^\intercal \rangle_{\mathcal{H}} \boldsymbol{c} = \langle \boldsymbol{c}^\intercal \boldsymbol{\Phi}, \boldsymbol{\Phi}^\intercal \boldsymbol{c} \rangle_{\mathcal{H}} = \langle \boldsymbol{\Phi}^\intercal \boldsymbol{c}, \boldsymbol{\Phi}^\intercal \boldsymbol{c} \rangle_{\mathcal{H}} = \|\boldsymbol{\Phi}^\intercal \boldsymbol{c}\|_{\mathcal{H}}^2 \geq 0.$$

This proves the positive semidefiniteness.

To prove the second claim, assume that K is not positive definite. Hence, there exists a vector $\boldsymbol{c} \neq \boldsymbol{0}$ such that $\boldsymbol{c}^\intercal \boldsymbol{K} \boldsymbol{c} = 0$. From the first part, we infer $\boldsymbol{\Phi}^\intercal \boldsymbol{c} = 0$. Thus, for every $f \in \mathcal{H}$, we obtain

$$0 = \langle f, \boldsymbol{\Phi}^\intercal \boldsymbol{c} \rangle_{\mathcal{H}} = \left\langle f, \sum_{i=1}^{N} c_i K(\boldsymbol{x}_i, \cdot) \right\rangle_{\mathcal{H}} = \sum_{i=1}^{N} c_i \langle f, K(\boldsymbol{x}_i, \cdot) \rangle_{\mathcal{H}} = \sum_{i=1}^{N} c_i \delta_{\boldsymbol{x}_i}(f)$$

by the Riesz representation theorem. Consquently, we have

$$\left\| \sum_{i=1}^{N} c_i \delta_{\boldsymbol{x}_i} \right\|_{\mathcal{H}'} = \sup_{0 \neq f \in \mathcal{H}} \frac{\left| \sum_{i=1}^{N} c_i \delta_{\boldsymbol{x}_i}(f) \right|}{\|f\|_{\mathcal{H}}} = 0,$$

which implies the linear dependence of $\delta_{\boldsymbol{x}_1}, \ldots, \delta_{\boldsymbol{x}_N}$.
The other implication is shown analogously. □

The reverse statement of Theorem 3.6 is also correct: Each positive definite kernel can be associated to an RKHS, its *native space*. Motivated by the fact that for $f = \sum_{i=1}^{N} c_i K(\boldsymbol{x}_i, \cdot)$ holds

$$\|f\|_{\mathcal{H}}^2 = \boldsymbol{c}^\intercal \boldsymbol{K} \boldsymbol{c},$$

we define the linear space

$$H_K(\Omega) := \left\{ \sum_{i=1}^{N} c_i K(\boldsymbol{x}_i, \cdot) : c_i \in \mathbb{R}, \boldsymbol{x}_i \in \Omega \text{ for } i = 1, \ldots, N,\ N \in \mathbb{N} \right\}.$$

On $H_K(\Omega)$, we introduce the bilinear form

$$(f, g)_K = \left(\sum_{i=1}^{N} c_i K(\boldsymbol{x}_i, \cdot), \sum_{j=1}^{M} d_j K(\boldsymbol{y}_j, \cdot) \right)_K := \boldsymbol{c}^\intercal [K(\boldsymbol{x}_i, \boldsymbol{y}_j)]_{\substack{i=1,\ldots,N \\ j=1,\ldots,M}} \boldsymbol{d},$$

where $M = N = \infty$ is possible.

Theorem 3.7 If $K \colon \Omega \times \Omega \to \mathbb{R}$ is symmetric and positive definite, then the bilinear form $(\cdot, \cdot)_K$ defines an inner product on $H_K(\Omega)$. Moreover, $H_K(\Omega)$ is a pre-Hilbert space with reproducing kernel K.

Proof. The bilinear form $(\cdot, \cdot)_K$ is symmetric due to

$$\begin{aligned}(f, g)_K &= \boldsymbol{c}^\intercal [K(\boldsymbol{x}_i, \boldsymbol{y}_j)]_{\substack{i=1,\ldots,N \\ j=1,\ldots,M}} \boldsymbol{d} = \left([K(\boldsymbol{x}_i, \boldsymbol{y}_j)]_{\substack{i=1,\ldots,N \\ j=1,\ldots,M}} \boldsymbol{d} \right)^\intercal \boldsymbol{c} \\ &= \boldsymbol{d}^\intercal [K(\boldsymbol{x}_i, \boldsymbol{y}_j)]_{\substack{i=1,\ldots,N \\ j=1,\ldots,M}}^\intercal \boldsymbol{c} = \boldsymbol{d}^\intercal [K(\boldsymbol{y}_j, \boldsymbol{x}_i)]_{\substack{j=1,\ldots,M \\ i=1,\ldots,N}} \boldsymbol{c} = (g, f)_K,\end{aligned}$$

which directly follows from the symmetry of K. The definiteness follows from the positive definiteness of K according

$$(f, f)_K = \boldsymbol{c}^\intercal \boldsymbol{K} \boldsymbol{c} > 0$$

for all $f = \boldsymbol{\Phi}^\intercal \boldsymbol{c} \neq 0$.
Finally, the reproducing property is obtained by

$$\big(K(\boldsymbol{x}, \cdot), f\big)_K = 1[K(\boldsymbol{x}, \boldsymbol{x}_j)]_{j=1,\ldots,N} \boldsymbol{c} = \sum_{j=1}^{n} c_j K(\boldsymbol{x}, \boldsymbol{x}_j) = \sum_{j=1}^{n} c_j K(\boldsymbol{x}_j, \boldsymbol{x}) = f(\boldsymbol{x}).$$

□

The theorem provides that $\big(H_K(\Omega), (\cdot, \cdot)_K\big)$ is a pre-Hilbert space, hence it is not necessarily complete. However, the next theorem guarantees that each normed vector space exhibits a *completion* that is unique up to isometry.

Theorem 3.8 Let $(V, \|\cdot\|_V)$ denote a normed vector space. There exists a Banach space $(\overline{V}, \|\cdot\|_{\overline{V}})$ called *completion* of V and an injective mapping $J\colon V \to \overline{V}$ such that

$$J(v+w) = J(v) + J(w), \quad J(\alpha \cdot v) = \alpha \cdot J(v), \quad \text{and } \|v\|_V = \|J(v)\|_{\overline{V}}$$

for all $v \in V$. The completion is uniquely determined up to isometry.

Proof. We consider the vector space of all Cauchy sequences on V, which we denote by

$$\tilde{V} := \{\tilde{v} = (v_n)_{n\in\mathbb{N}} \subset V : (v_n)_{n\in\mathbb{N}} \text{ is a Cauchy sequence}\}.$$

On $\tilde{V}$ we introduce the *equivalence relation*

$$(v_n)_{n\in\mathbb{N}} \sim (w_n)_{n\in\mathbb{N}} \quad \text{iff} \quad \|v_n - w_n\|_V \text{ is a null sequence in } \mathbb{R}$$

and define the *equivalence classes* $[\tilde{v}] := \{w \in \tilde{V} : v \sim w\}$. With the addition and scalar multiplication for Cauchy sequences, the set $\overline{V} := \{[\tilde{v}] : \tilde{v} \in \tilde{V}\}$ becomes a vector space. Since $|\|v_n\|_V - \|v_m\|_V| \le \|v_n - v_m\|_V$ for any Cauchy sequence $(v_n)_{n\in\mathbb{N}}$, $\lim_{n\to\infty} \|v_n\|_V$ exists in $\mathbb{R}$ and we define

$$\|[\tilde{v}]\|_{\overline{V}} := \lim_{n\to\infty} \|v_n\|_V.$$

The mapping $J\colon V \to \overline{V}$ is given by $J(v) = [(v)_{n\in\mathbb{N}}]$, i.e., the equivalence class which contains the constant sequence with value v. The linearity of the mapping J is a consequence of the fact that $\overline{V}$ is a vector space. Moreover J is injective, since $v \neq w$ obviously implies $J(v) \neq J(w)$. Further, it holds $\|J(v)\|_{\overline{V}} = \lim_{n\to\infty} \|v\|_V = \|v\|_V$.
It remains to show that the space $(\overline{V}, \|\cdot\|_{\overline{V}})$ is indeed a Banach space. To that end, let $\big([\tilde{v}]_k\big)_{k\in\mathbb{N}} \subset \overline{V}$ be a Cauchy sequence. We denote the n-th element of some representer of $[\tilde{v}]_k$ by $v_{k,n}$. For each k we can now choose n_k such that

$$\|v_{k,m} - v_{k,n_k}\|_V \le k^{-1} \quad \text{if } m > n_k. \tag{3.2}$$

We show that the sequence

$$\tilde{v}^\star := \big(v_{1,n_1}, v_{2,n_2}, \dots, v_{k,n_k}, \dots\big) \subset V \tag{3.3}$$

is a Cauchy sequence and that $\big([\tilde{v}]_k\big)_{k\in\mathbb{N}}$ converges towards $[\tilde{v}^\star]$. We have

$$\|[\tilde{v}]_k - J(v_{k,n_k})\|_{\overline{V}} = \lim_{m\to\infty} \|v_{k,m} - v_{k,n_k}\|_V \le k^{-1}$$

due to (3.2). Note that the limit exists, since the sum of two Cauchy sequences forms a Cauchy sequence. Further, we derive

$$\begin{aligned} \|v_{k,n_k} - v_{m,n_m}\|_V &= \|J(v_{k,n_k}) - J(v_{m,n_m})\|_{\overline{V}} \\ &\le \|[\tilde{v}]_k - J(v_{k,n_k})\|_{\overline{V}} + \|[\tilde{v}]_m - J(v_{m,n_m})\|_{\overline{V}} + \|[\tilde{v}]_k - [\tilde{v}]_m\|_{\overline{V}} \\ &\le k^{-1} + m^{-1} + \|[\tilde{v}]_k - [\tilde{v}]_m\|_{\overline{V}}. \end{aligned} \tag{3.4}$$

This implies that (3.3) is a Cauchy sequence. We find

$$\begin{aligned} \|[\tilde{v}^\star] - [\tilde{v}]_k\|_{\overline{V}} &\le \|[\tilde{v}^\star] - J(v_{k,n_k})\|_{\overline{V}} + \|J(v_{k,n_k}) - [\tilde{v}]_k\|_{\overline{V}} \\ &\le \|[\tilde{v}^\star] - J(v_{k,n_k})\|_{\overline{V}} + k^{-1}. \end{aligned}$$

The first term on the right hand side can be bounded with the help of (3.4) in accordance with

$$\begin{aligned}\|[\tilde{v}^\star] - J(v_{k,n_k})\|_{\overline{V}} &= \lim_{m\to\infty} \|v_{m,n_m} - v_{k,n_k}\|_V \\ &\leq \lim_{m\to\infty} \left(k^{-1} + m^{-1} + \|[\tilde{v}]_k - [\tilde{v}]_m\|_{\overline{V}}\right) \\ &= \lim_{m\to\infty} \|[\tilde{v}]_k - [\tilde{v}]_m\|_{\overline{V}} + k^{-1}.\end{aligned}$$

Again the limit exists and is bounded by some ϵ_k, as $([\tilde{v}]_k)_{k\in\mathbb{N}}$ is a Cauchy sequence and it holds $\epsilon_k \to 0$ for $k \to \infty$. Combining the two estimates yields

$$\lim_{k\to\infty} \|[\tilde{v}^\star] - [\tilde{v}]_k\|_{\overline{V}} = 0,$$

which implies the completeness of $\overline{V}$. □

Definition 3.9 The completion $\mathcal{N}_K(\Omega) := \overline{H_K(\Omega)}^{\|\cdot\|_K}$ with respect to the norm $\|f\|_K := \sqrt{(f,f)_K}$ is called *native space* of K.

Another characterization of the native space is given by the eigenfunctions of the linear operator

$$T_K \colon L^2(\Omega) \to L^2(\Omega), \quad (T_K v)(\boldsymbol{x}) := \int_\Omega K(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}.$$

Fact 3.10 (Mercer) Let $K \in C(\Omega\times\Omega)$ be a continuous and positive definite kernel. Then, there holds

$$K(\boldsymbol{x},\boldsymbol{y}) = \sum_{i=1}^\infty \lambda_i \phi_i(\boldsymbol{x})\phi_i(\boldsymbol{y}),$$

where $\{(\lambda_i,\phi_i)\}_{i=1}^\infty$ are the eigen-pairs of the compact operator T_K.

The previous fact allows for a spectral characterization of the native space. To this end, we endow

$$\mathcal{H} := \left\{ f\colon \Omega\to\mathbb{R} : f = \sum_{i=1}^\infty c_i\phi_i, c_i \in \mathbb{R} \right\}$$

with the inner product

$$\langle f,g\rangle_{\mathcal{H}} = \left\langle \sum_{i=1}^\infty c_i\phi_i, \sum_{i=1}^\infty d_i\phi_i \right\rangle_{\mathcal{H}} := \sum_{i=1}^\infty \frac{c_i d_i}{\lambda_i} = \sum_{i=1}^\infty \frac{(f,\phi_i)_{L^2(\Omega)}(g,\phi_i)_{L^2(\Omega)}}{\lambda_i}.$$

There holds

$$\begin{aligned}\langle K(\boldsymbol{x},\cdot), f\rangle_{\mathcal{H}} &= \sum_{i=1}^\infty \frac{\big(K(\boldsymbol{x},\cdot),\phi_i\big)_{L^2(\Omega)}(f,\phi_i)_{L^2(\Omega)}}{\lambda_i} \\ &= \sum_{i=1}^\infty \frac{\big(\sum_{j=1}^\infty \lambda_j\phi_j(\boldsymbol{x})\phi_j(\cdot),\phi_i\big)_{L^2(\Omega)}(f,\phi_i)_{L^2(\Omega)}}{\lambda_i} \\ &= \sum_{i=1}^\infty \frac{\lambda_i\phi_i(\boldsymbol{x})(f,\phi_i)_{L^2(\Omega)}}{\lambda_i} = \sum_{i=1}^\infty c_i\phi_i(\boldsymbol{x}) = f(\boldsymbol{x}).\end{aligned}$$

Consequently, we may set $\langle\cdot,\cdot\rangle_{\mathcal{N}_K(\Omega)} := \langle\cdot,\cdot\rangle_{\mathcal{H}}$ and obtain

$$\mathcal{N}_K(\Omega) = \{f \in L^2(\Omega) : \langle f,f\rangle_{\mathcal{N}_K(\Omega)} < \infty\}.$$

4. Approximation results

In this chapter, we derive approximation results based on the *fill-distance*.

Definition 4.1 Given $\Omega \subset \mathbb{R}^d$ and $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset \Omega$, we introduce the *fill distance*

$$h_{X,\Omega} := \sup_{\boldsymbol{x}\in\Omega} \min_{\boldsymbol{x}_i \in X} \|\boldsymbol{x} - \boldsymbol{x}_i\|_2. \tag{4.1}$$

and the *separation distance*

$$q_X := \min_{\boldsymbol{x}_i \neq \boldsymbol{x}_j} \|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2. \tag{4.2}$$

We call X *quasi-uniform*, iff there exists a constant $c \geq 1$ such that $q_X/c \leq h_{X,\Omega} \leq cq_X$.

We start by introducing the concept of *Lagrange bases*. To this end, we recall the kernel matrix

$$\boldsymbol{K} = [K(\boldsymbol{x}_i, \boldsymbol{x}_j)]_{i,j=1}^N$$

and the canonical feature vector

$$\boldsymbol{\Phi}(\boldsymbol{x}) = [K(\boldsymbol{x}_i, \boldsymbol{x})]_{i=1}^N = [\varphi_1(\boldsymbol{x}), \dots, \varphi_N(\boldsymbol{x})]^\intercal.$$

Further, we denote the canonical basis in $\mathbb{R}^N$ by $\boldsymbol{e}_1, \dots, \boldsymbol{e}_N$.

Theorem 4.2 Let K be a positive definite kernel. Then, for any mutually distinct points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N$, the *Lagrange basis* is given by

$$\ell_j(\boldsymbol{x}) := \sum_{k=1}^N c_k^{(j)} K(\boldsymbol{x}_k, \boldsymbol{x}) = \boldsymbol{c}^{(j)} \boldsymbol{\Phi}(\boldsymbol{x})$$

with $\boldsymbol{c}^{(j)} := \boldsymbol{e}_j^\intercal \boldsymbol{K}^{-1}$, $j = 1, \dots, N$, i.e., the functions ℓ_j satisfy $\ell_j(\boldsymbol{x}_i) = \delta_{i,j}$.

Proof. There holds

$$\ell_j(\boldsymbol{x}_i) = \sum_{k=1}^N c_k^{(j)} K(\boldsymbol{x}_k, \boldsymbol{x}_i) = \boldsymbol{e}_j^\intercal \boldsymbol{K}^{-1} \boldsymbol{\Phi}(\boldsymbol{x}_i) = \boldsymbol{e}_j^\intercal \boldsymbol{e}_i = \delta_{i,j},$$

since $\boldsymbol{\Phi}(\boldsymbol{x}_i)$ is the i-th column of $\boldsymbol{K}$. □

Given a function $f\colon \Omega \to \mathbb{R}$ we can write its interpolant according to

$$s_f(\boldsymbol{x}) = \sum_{j=1}^N f(\boldsymbol{x}_j) \ell_j(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega.$$

To derive an error estimate in terms of the fill-distance, an important tool is the *power function*.

Definition 4.3 Let $\Omega \subset \mathbb{R}^d$ and $K\colon \Omega \times \Omega \to \mathbb{R}$ a continuous and positive definite kernel. Given any set $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ of mutually distinct points, the *power function* is defined as

$$P_{K,X}(\boldsymbol{x}) := \left\| K(\boldsymbol{x}, \cdot) - \sum_{j=1}^{N} \ell_j(\boldsymbol{x}) K(\boldsymbol{x}_j, \cdot) \right\|_{\mathcal{N}_K(\Omega)}, \quad \boldsymbol{x} \in \Omega.$$

A direct calculation yields the following

Fact 4.4 Let $\Omega \subset \mathbb{R}^d$ and $K\colon \Omega \times \Omega \to \mathbb{R}$ a continuous and positive definite kernel. Given any set $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ of mutually distinct points, there holds

$$P_{K,X}(\boldsymbol{x}) = \sqrt{K(\boldsymbol{x}, \boldsymbol{x}) - \boldsymbol{\Phi}^{\intercal}(\boldsymbol{x}) \boldsymbol{K}^{-1} \boldsymbol{\Phi}(\boldsymbol{x})}, \quad \boldsymbol{x} \in \Omega,$$

and, hence, $0 \leq P_{K,X}(\boldsymbol{x}) \leq \sqrt{K(\boldsymbol{x}, \boldsymbol{x})}$.

The point-wise approximation error can be bounded by the power function.

Theorem 4.5 Let $\Omega \subset \mathbb{R}^d$ and $K\colon \Omega \times \Omega \to \mathbb{R}$ a continuous and positive definite kernel and $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ be a set of mutually distinct points. Then, there holds for every $f \in \mathcal{N}_K(\Omega)$ that

$$|f(\boldsymbol{x}) - s_f(\boldsymbol{x})| \leq P_{K,X}(\boldsymbol{x}) \|f\|_{\mathcal{N}_K(\Omega)}, \quad \boldsymbol{x} \in \Omega.$$

Proof. We have

$$s_f(\boldsymbol{x}) = \sum_{j=1}^{N} f(\boldsymbol{x}_j) \ell_j(\boldsymbol{x}) = \sum_{j=1}^{N} \langle K(\boldsymbol{x}_j, \cdot), f \rangle_{\mathcal{N}_K(\Omega)} \ell_j(\boldsymbol{x}) = \left\langle \sum_{j=1}^{N} \ell_j(\boldsymbol{x}) K(\boldsymbol{x}_j, \cdot), f \right\rangle_{\mathcal{N}_K(\Omega)}$$

by the reproducing property. Consequently, we obtain

$$\begin{aligned} |f(\boldsymbol{x}) - s_f(\boldsymbol{x})| &= \left| \left\langle K(\boldsymbol{x}, \cdot) - \sum_{j=1}^{N} \ell_j(\boldsymbol{x}) K(\boldsymbol{x}_j, \cdot), f \right\rangle_{\mathcal{N}_K(\Omega)} \right| \\ &\leq P_{K,X}(\boldsymbol{x}) \|f\|_{\mathcal{N}_K(\Omega)} \end{aligned}$$

by the Cauchy-Schwarz inequality. □

Fact 4.6 Let $\Omega \in \mathbb{R}^d$ satisfy an interior cone condition, i.e., there exists an angle $\alpha > 0$ such that the interior angle at every corner of Ω is bigger than α. Moreover, let $K \in C^{2k}(\Omega \times \Omega)$ be a positive definite kernel. Then, there exist constants $C_K, h_0 > 0$ such that

$$P_{K,X}(\boldsymbol{x}) \leq C_K h_{X,\Omega}^k$$

whenever $h_{X,\Omega} \leq h_0$.

Combining Theorem 4.5 with the preceding fact yields the final error estimate.

Theorem 4.7 Let $\Omega \in \mathbb{R}^d$ satisfy an interior cone condition. Moreover, let $K \in C^{2k}(\Omega \times \Omega)$ be a positive definite kernel and let $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ be a set of mutually distinct points. Then, there holds for every $f \in \mathcal{N}_K(\Omega)$ that

$$|f(\boldsymbol{x}) - s_f(\boldsymbol{x})| \leq C_K h_{X,\Omega}^k \|f\|_{\mathcal{N}_K(\Omega)}, \quad \boldsymbol{x} \in \Omega,$$

whenever $h_{X,\Omega} \leq h_0$.

5. Numerical methods

In this chapter, we focus on the situation where the basic or kernel function under consideration is positive definite. As a consequence, the generalized Vandermonde or kernel matrix $\boldsymbol{K} = [K(\boldsymbol{x}_i, \boldsymbol{x}_j)]_{i,j=1}^N \in \mathbb{R}^{N\times N}$ is positive semi-definite. We need the following result.

Lemma 5.1 Let $\boldsymbol{A}$ be a symmetric and positive semi-definite matrix. Then, the *Schur complement* $\boldsymbol{S} := \boldsymbol{A}_{2,2} - \boldsymbol{A}_{2,1}\boldsymbol{A}_{1,1}^{-1}\boldsymbol{A}_{1,2}$ is well defined for any block partitioning of

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{A}_{1,1} & \boldsymbol{A}_{1,2} \\ \boldsymbol{A}_{2,1} & \boldsymbol{A}_{2,2} \end{bmatrix}$$

for which $\boldsymbol{A}_{1,1}^{-1}$ exists. Moreover, $\boldsymbol{A}_{1,1}$ is always symmetric and positive semi-definite, while $\boldsymbol{S}$ is symmetric and positive definite.

Proof. Let $\left[\begin{smallmatrix}\boldsymbol{x}\\ \boldsymbol{y}\end{smallmatrix}\right] \in \mathbb{R}^N$ be partitioned similarly to $\boldsymbol{A}$. Since

$$\begin{bmatrix} \boldsymbol{A}_{1,1} & \boldsymbol{A}_{1,2} \\ \boldsymbol{A}_{2,1} & \boldsymbol{A}_{2,2} \end{bmatrix} = \boldsymbol{A} = \boldsymbol{A}^\intercal = \begin{bmatrix} \boldsymbol{A}_{1,1}^\intercal & \boldsymbol{A}_{2,1}^\intercal \\ \boldsymbol{A}_{1,2}^\intercal & \boldsymbol{A}_{2,2}^\intercal \end{bmatrix},$$

we obtain

$$\boldsymbol{A}_{1,1} = \boldsymbol{A}_{1,1}^\intercal, \qquad \boldsymbol{A}_{2,2} = \boldsymbol{A}_{2,2}^\intercal, \qquad \boldsymbol{A}_{1,2} = \boldsymbol{A}_{2,1}^\intercal.$$

Consequently, $\boldsymbol{A}_{1,1}$ is symmetric and there holds

$$0 \le \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{0} \end{bmatrix}^\intercal \boldsymbol{A} \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{0} \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{0} \end{bmatrix}^\intercal \begin{bmatrix} \boldsymbol{A}_{1,1}\boldsymbol{x} \\ \boldsymbol{A}_{2,1}\boldsymbol{x} \end{bmatrix} = \boldsymbol{x}^\intercal \boldsymbol{A}_{1,1}\boldsymbol{x}.$$

Therefore, $\boldsymbol{A}_{1,1}$ is positive semi-definite. In fact, it is even positive definite as $\boldsymbol{A}_{1,1}^{-1}$ exists by assumption.
Furthermore, there holds

$$\boldsymbol{S}^\intercal = \boldsymbol{A}_{2,2}^\intercal - \boldsymbol{A}_{1,2}^\intercal \boldsymbol{A}_{1,1}^{-\intercal} \boldsymbol{A}_{2,1}^\intercal = \boldsymbol{A}_{2,2} - \boldsymbol{A}_{2,1}\boldsymbol{A}_{1,1}^{-1}\boldsymbol{A}_{1,2} = \boldsymbol{S}.$$

Finally, we consider $\left[\begin{smallmatrix}\boldsymbol{x}\\ \boldsymbol{y}\end{smallmatrix}\right]$ with $\boldsymbol{x} = -\boldsymbol{A}_{1,1}^{-1}\boldsymbol{A}_{1,2}\boldsymbol{y}$. This yields

$$\begin{aligned} 0 \le \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix}^\intercal \boldsymbol{A} \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix} &= \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix}^\intercal \begin{bmatrix} \boldsymbol{A}_{1,1}\boldsymbol{x} + \boldsymbol{A}_{1,2}\boldsymbol{y} \\ \boldsymbol{A}_{2,1}\boldsymbol{x} + \boldsymbol{A}_{2,2}\boldsymbol{y} \end{bmatrix} = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix}^\intercal \begin{bmatrix} -\boldsymbol{A}_{1,2}\boldsymbol{y} + \boldsymbol{A}_{1,2}\boldsymbol{y} \\ -\boldsymbol{A}_{2,1}\boldsymbol{A}_{1,1}^{-1}\boldsymbol{A}_{1,2}\boldsymbol{y} + \boldsymbol{A}_{2,2}\boldsymbol{y} \end{bmatrix} \\ &= \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{bmatrix}^\intercal \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{S}\boldsymbol{y} \end{bmatrix} = \boldsymbol{y}^\intercal \boldsymbol{S}\boldsymbol{y}, \end{aligned}$$

which yields the semi-definiteness of $\boldsymbol{S}$. □

Given a positive semi-definite matrix $\boldsymbol{A}$, successively reducing the Schur complement by setting

$$\boldsymbol{A}_1 := \boldsymbol{A}, \quad \boldsymbol{\ell}_i := \frac{1}{\sqrt{a^{(i)}_{\pi(i),\pi(i)}}} \boldsymbol{a}^{(i)}_{:,\pi(i)}, \quad \boldsymbol{A}_{i+1} := \boldsymbol{A}_i - \boldsymbol{\ell}_i \boldsymbol{\ell}_i^\intercal$$

for a permutation π of the set $\{1, \dots N\}$ leads to a representation

$$\boldsymbol{A} = \sum_{i=1}^{\operatorname{rank}(\boldsymbol{A})} \boldsymbol{\ell}_i \boldsymbol{\ell}_i^\intercal,$$

given that all pivots $a^{(i)}_{\pi(i),\pi(i)}$ are non-zero. In this case, also all matrices $\boldsymbol{A}_i$, $i = 1, \dots, \operatorname{rank}(\boldsymbol{A})$ are positive semi-definite. This can be seen by introducing the permutation matrix $\boldsymbol{P} := [\boldsymbol{e}_{\pi(1)}, \dots, \boldsymbol{e}_{\pi(N)}]^\intercal$ and considering the matrix $\boldsymbol{P}\boldsymbol{A}\boldsymbol{P}^\intercal$ in Lemma 5.1.

Remark For $\pi(i) = i$, we obtain the well known Cholesky decomposition. △

Lemma 5.2 Let $\boldsymbol{A}$ be a symmetric and positive semi-definite matrix. Then, there holds

$$|a_{i,j}| \leq \sqrt{a_{i,i} a_{j,j}} \quad \text{for all } i, j = 1, \dots, N.$$

Proof. The positive semi-definiteness of the Schur complement established by Lemma 5.1 holds true for any pivot element $a_{i,i}$, $i = 1, \dots, N$. In particular, all diagonal elements of the Schur complement have to be non-negative, which implies

$$0 \leq a_{j,j} - \frac{a_{i,j}^2}{a_{i,i}} \quad \text{or} \quad |a_{i,j}| \leq \sqrt{a_{i,i} a_{j,j}}$$

as claimed. □

A direct consequence of the previous lemma is that the largest element of a positive semi-definite matrix is always located on the diagonal, i.e.,

$$|a_{i,j}| \leq \sqrt{a_{i,i} a_{j,j}} \leq \frac{a_{i,i} + a_{j,j}}{2} \leq \max_{i=1,\dots,N} a_{i,i}.$$

Therefore, if all diagonal elements are zero, the matrix has to be the zero matrix. This motivates the following pivoted version of the Cholesky decomposition, which greedily removes the largest element from the Schur complement.

Algorithm 5.3 (Pivoted Cholesky Decomposition)
input: symmetric and positive semidefinite matrix $\boldsymbol{K} \in \mathbb{R}^{N\times N}$, $\varepsilon \geq 0$
output: low-rank approximation $\boldsymbol{K} \approx \boldsymbol{L}\boldsymbol{L}^\top$
and biorthogonal basis $\boldsymbol{B}$ such that $\boldsymbol{B}^\top \boldsymbol{L} = \boldsymbol{I}_m$

1: Initialization: set $m := 1$, $\boldsymbol{d} := \operatorname{diag}(\boldsymbol{K})$, $\boldsymbol{L} := [\,]$, $\boldsymbol{B} := [\,]$, err $:= \|\boldsymbol{d}\|_1$
2: **while** err $> \varepsilon$
3: determine $\pi(m) := \arg\max_{1\leq i\leq N} d_i$
4: compute

$$\boldsymbol{\ell}_m := \frac{1}{\sqrt{d_{\pi(m)}}}\Big(\boldsymbol{K} - \boldsymbol{L}\boldsymbol{L}^\top\Big)\boldsymbol{e}_{\pi(m)} \quad \text{and} \quad \boldsymbol{b}_m := \frac{1}{\sqrt{d_{\pi(m)}}}\Big(\boldsymbol{I} - \boldsymbol{B}\boldsymbol{L}^\top\Big)\boldsymbol{e}_{\pi(m)}$$

5: set $\boldsymbol{L} := [\boldsymbol{L}, \boldsymbol{\ell}_m]$, $\boldsymbol{B} := [\boldsymbol{B}, \boldsymbol{b}_m]$
6: set $\boldsymbol{d} := \boldsymbol{d} - \boldsymbol{\ell}_m \odot \boldsymbol{\ell}_m$, where $\odot$ denotes the Hadamard product
7: set err $:= \|\boldsymbol{d}\|_1$, $m := m + 1$

By the previous considerations, the pivoting strategy in Algorithm 5.3 amounts to a total pivoting, which always eliminates the largest entry of the Schur complement. Moreover, the algorithm computes also the biorthogonal basis associated to $\boldsymbol{L}$.

Theorem 5.4 For any $\varepsilon \geq 0$, Algorithm 5.3 computes $N \times m$-matrices $\boldsymbol{B}$ and $\boldsymbol{L}$ with $m \leq \operatorname{rank}\boldsymbol{K}$ such that $\boldsymbol{K} - \boldsymbol{L}\boldsymbol{L}^\intercal$ is positive semi-definite and

$$\begin{aligned} \operatorname{trace}\left(\boldsymbol{K} - \boldsymbol{L}\boldsymbol{L}^\intercal\right) &\leq \varepsilon, \\ \boldsymbol{B}^\intercal\boldsymbol{L} &= \boldsymbol{I}, \\ \boldsymbol{K}\boldsymbol{B} &= \boldsymbol{L}. \end{aligned}$$

Proof. Without loss of generality, we assume that always $\pi(m) = m$ for $m \leq \operatorname{rank}\boldsymbol{K}$. Otherwise, perform the proof with the accordingly permuted matrix $\boldsymbol{K}$. The error bound is directly inferred from the truncation criterion.

To prove the other claims, we observe that $\boldsymbol{L}_m$ is a lower-triangular matrix. From line 4 of the algorithm, it follows that $\boldsymbol{b}_i \in \operatorname{span}\{\boldsymbol{e}_1, \ldots, \boldsymbol{e}_i\}$ for $i \leq m$, i.e. $\boldsymbol{B}_m$ is upper triangular. We prove inductively that $\boldsymbol{B}_m^\intercal\boldsymbol{L}_m = \boldsymbol{I}_m$. For $m = 1$, there holds

$$\boldsymbol{B}_1^\intercal\boldsymbol{L}_1 = \boldsymbol{b}_1^\intercal\boldsymbol{\ell}_1 = \frac{1}{\sqrt{d_1}}\boldsymbol{e}_1^\intercal\boldsymbol{\ell}_1 = [1] = \boldsymbol{I}_1,$$

since $\ell_{1,1} = \sqrt{d_1}$. Now, let the induction hypothesis hold for $m-1$ and consider the block matrix

$$\boldsymbol{B}_m^\intercal\boldsymbol{L}_m = [\boldsymbol{B}_{m-1}, \boldsymbol{b}_m]^\intercal[\boldsymbol{L}_{m-1}, \boldsymbol{\ell}_m] = \begin{bmatrix} \boldsymbol{B}_{m-1}^\intercal\boldsymbol{L}_{m-1} & \boldsymbol{B}_{m-1}^\intercal\boldsymbol{\ell}_m \\ \boldsymbol{b}_m^\intercal\boldsymbol{L}_{m-1} & \boldsymbol{b}_m^\intercal\boldsymbol{\ell}_m \end{bmatrix} \tag{5.1}$$

By the induction hypothesis, there holds $\boldsymbol{B}_{m-1}^\intercal\boldsymbol{L}_{m-1} = \boldsymbol{I}_{m-1}$. Thus, since $\boldsymbol{L}_m$ is lower triangular, we obtain

$$\boldsymbol{B}_{m-1}^\intercal\boldsymbol{\ell}_m = \boldsymbol{0} \in \mathbb{R}^{(m-1)\times 1}, \tag{5.2}$$

and it remains to show that $\boldsymbol{b}_m^\intercal\boldsymbol{L}_m = \boldsymbol{b}_m^\intercal[\boldsymbol{L}_{m-1}, \boldsymbol{\ell}_m] = [0, \ldots, 0, 1] \in \mathbb{R}^{1\times m}$. From the

induction hypothesis and (5.2) it follows that $\boldsymbol{B}_{m-1}^\intercal \boldsymbol{L}_m = [\boldsymbol{I}_{(m-1)}, \boldsymbol{0}]$. Hence, we infer

$$\begin{aligned}\boldsymbol{b}_m^\intercal \boldsymbol{L}_m &= \frac{1}{\sqrt{d_m}}\big(\boldsymbol{e}_m - \boldsymbol{B}_{m-1}\boldsymbol{L}_{m-1}^\intercal \boldsymbol{e}_m\big)^\intercal \boldsymbol{L}_m = \frac{1}{\sqrt{d_m}}\big(\boldsymbol{e}_m^\intercal \boldsymbol{L}_m - \boldsymbol{e}_m^\intercal \boldsymbol{L}_{m-1}\boldsymbol{B}_{m-1}^\intercal \boldsymbol{L}_m\big)\\ &= \frac{1}{\sqrt{d_m}}\boldsymbol{e}_m^\intercal\big(\boldsymbol{L}_m - \boldsymbol{L}_{m-1}[\boldsymbol{I}_{(m-1)}, \boldsymbol{0}]\big) = \frac{1}{\sqrt{d_m}}\boldsymbol{e}_m^\intercal[\boldsymbol{0}, \boldsymbol{\ell}_m].\end{aligned}$$

In view of $\ell_{m,m} = \sqrt{d_m}$, we arrive at $\boldsymbol{b}_m^\intercal \boldsymbol{L}_m = \frac{1}{\sqrt{d_m}}\boldsymbol{e}_k^\intercal[\boldsymbol{0}, \boldsymbol{\ell}_m] = [0, \dots, 0, 1] \in \mathbb{R}^{1\times m}$. Inserting this into (5.1) proves $\boldsymbol{B}_m^\intercal \boldsymbol{L}_m = \boldsymbol{I}_m$. With $r := \operatorname{rank} \boldsymbol{K}$, we finally have

$$\boldsymbol{K}\boldsymbol{B}_m = \boldsymbol{L}_r\boldsymbol{L}_r^\intercal \boldsymbol{B}_m = \boldsymbol{L}_r \begin{bmatrix}\boldsymbol{I}_m \\ \boldsymbol{0}\end{bmatrix} = \boldsymbol{L}_m \quad \text{for all } m \le r.$$

This completes the proof. □

Corollary 5.5 Let $\boldsymbol{U} = [\boldsymbol{b}_{\pi(1),:}^\intercal, \dots, \boldsymbol{b}_{\pi(m),:}^\intercal]^\intercal$. There holds $\boldsymbol{U}\boldsymbol{U}^\intercal = [k_{\pi(i),\pi(j)}]_{i,j=1,\dots,m}^{-1}$.

Proof. Without loss of generality, we assume $\pi(m) = m$. Let

$$\boldsymbol{K} = \begin{bmatrix}\boldsymbol{K}_{1,1} & \boldsymbol{K}_{1,2} \\ \boldsymbol{K}_{2,1} & \boldsymbol{K}_{2,2}\end{bmatrix} \quad \text{and} \quad \boldsymbol{L} = \begin{bmatrix}\boldsymbol{L}_{1,1} \\ \boldsymbol{L}_{1,2}\end{bmatrix},$$

where $\boldsymbol{K}_{1,1}, \boldsymbol{L}_{1,1} \in \mathbb{R}^{m\times m}$. There particularly holds $\boldsymbol{K}_{1,1} = \boldsymbol{L}_{1,1}\boldsymbol{L}_{1,1}^\intercal$. Furthermore, the theorem yields

$$\boldsymbol{B}^\intercal \boldsymbol{L} = \begin{bmatrix}\boldsymbol{U} \\ \boldsymbol{0}\end{bmatrix}^\intercal \begin{bmatrix}\boldsymbol{L}_{1,1} \\ \boldsymbol{L}_{1,2}\end{bmatrix} = \boldsymbol{U}^\intercal \boldsymbol{L}_{1,1} = \boldsymbol{I},$$

which shows $\boldsymbol{U}^\intercal = \boldsymbol{L}_{1,1}^{-1}$ or $\boldsymbol{U} = \boldsymbol{L}_{1,1}^{-\intercal}$. Combining this with the previous argument yields

$$\boldsymbol{K}_{1,1}^{-1} = \big(\boldsymbol{L}_{1,1}\boldsymbol{L}_{1,1}^\intercal\big)^{-1} = \boldsymbol{L}_{1,1}^{-\intercal}\boldsymbol{L}_{1,1}^{-1} = \boldsymbol{U}\boldsymbol{U}^\intercal.$$

□

Remark The well known Nyström method for the low-rank approximation of kernel matrices randomly selects data sites $\boldsymbol{x}_{\pi(1)}, \dots, \boldsymbol{x}_{\pi(m)}$ and computes the approximation

$$\boldsymbol{K} \approx [K(\boldsymbol{x}_i, \boldsymbol{x}_{\pi(j)})]_{\substack{i=1,\dots,n\\ j=1,\dots,m}} [K(\boldsymbol{x}_{\pi(i)}, \boldsymbol{x}_{\pi(j)})]_{i,j=1,\dots,m}^{-1} [K(\boldsymbol{x}_{\pi(i)}, \boldsymbol{x}_j)]_{\substack{i=1,\dots,m\\ j=1,\dots,n}}.$$

The previous corollary shows that this is equivalent to a pivoted Cholesky decomposition with pivots $\pi(1), \dots, \pi(m)$. △

Corollary 5.6 Let $(\mathcal{H}, \langle\cdot,\cdot\rangle_{\mathcal{H}})$ be an RKHS. Given the canonical feature vector $\boldsymbol{\Phi}(\boldsymbol{x}) := [K(\boldsymbol{x}_i, \boldsymbol{x})]_{i=1}^N$, the *Newton basis* $\boldsymbol{N}(\boldsymbol{x}) := \boldsymbol{B}^\intercal \boldsymbol{\Phi}(\boldsymbol{x})$ forms an orthonormal system in $\mathcal{H}$, i.e., $\langle N_i, N_j\rangle_{\mathcal{H}} = \delta_{i,j}$ for $i, j = 1, \dots, m$, where $m = \operatorname{rank} \boldsymbol{B}$.

Proof. There holds

$$\langle \boldsymbol{N}, \boldsymbol{N}^\intercal\rangle_{\mathcal{H}} = \boldsymbol{B}^\intercal \langle \boldsymbol{\Phi}, \boldsymbol{\Phi}^\intercal\rangle_{\mathcal{H}} \boldsymbol{B} = \boldsymbol{B}^\intercal \boldsymbol{K}\boldsymbol{B} = \boldsymbol{B}^\intercal \boldsymbol{L} = \boldsymbol{I}_m$$

by the third part of the previous theorem. □

Remark There holds

$$\operatorname{span}\{N_1, \dots, N_m\} = \operatorname{span}\{K(\boldsymbol{x}_{\pi(1)}, \cdot), \dots, K(\boldsymbol{x}_{\pi(m)}, \cdot)\} \subset \operatorname{span}\{\varphi_1, \dots, \varphi_N\}.$$

△

The orthogonal projection of a function $f \in \mathcal{H}$ onto the subspace spanned by $N_1, \dots, N_m$ is easily computed by

$$Pf := \sum_{i=1}^{m} N_i \langle N_i, f \rangle_{\mathcal{H}} = \boldsymbol{N}^\intercal \boldsymbol{B}^\intercal \boldsymbol{f} = \boldsymbol{\Phi}^\intercal \boldsymbol{B} \boldsymbol{B}^\intercal \boldsymbol{f}.$$

In particular, there holds

$$[(Pf)(\boldsymbol{x}_i)]_{i=1}^N = \boldsymbol{K} \boldsymbol{B} \boldsymbol{B}^\intercal \boldsymbol{f} = \boldsymbol{L} \boldsymbol{B}^\intercal \boldsymbol{f}.$$

Given a (low-rank) factorization of the kernel matrix $\boldsymbol{K}$, we can directly compute the least square solution to the linear system

$$\boldsymbol{K} \boldsymbol{c} = \boldsymbol{f}.$$

Theorem 5.7 Let $\boldsymbol{K} \approx \boldsymbol{L}\boldsymbol{L}^\intercal$ be the pivoted Cholesky decomposition of the kernel matrix $\boldsymbol{K}$. A minimum norm solution of the problem

$$\|\boldsymbol{L}\boldsymbol{L}^\intercal \boldsymbol{x} - \boldsymbol{f}\|_2 \to \min$$

is given by

$$\boldsymbol{x}^\dagger = \boldsymbol{L}(\boldsymbol{L}^\intercal \boldsymbol{L})^{-2} \boldsymbol{L}^\intercal \boldsymbol{f}.$$

The cost for the computation of the solution is $\mathcal{O}(Nm^2)$, where $m = \operatorname{rank} \boldsymbol{L}$.

Proof. The Gaussian normal equations read

$$\boldsymbol{L}\boldsymbol{L}^\intercal \boldsymbol{L}\boldsymbol{L}^\intercal \boldsymbol{x} = \boldsymbol{L}\boldsymbol{L}^\intercal \boldsymbol{b}.$$

Inserting $\boldsymbol{x}^\dagger = \boldsymbol{L}(\boldsymbol{L}^\intercal \boldsymbol{L})^{-2} \boldsymbol{L}^\intercal \boldsymbol{b}$ into the normal equations yields

$$\boldsymbol{L}\boldsymbol{L}^\intercal \boldsymbol{L}\boldsymbol{L}^\intercal \boldsymbol{L}(\boldsymbol{L}^\intercal \boldsymbol{L})^{-2} \boldsymbol{L}^\intercal \boldsymbol{b} = \boldsymbol{L}\boldsymbol{L}^\intercal \boldsymbol{b}.$$

Therefore, $\boldsymbol{x}^\dagger$ solves the Gaussian normal equations and is consequently a minimum norm solution. □

Remark The matrix $(\boldsymbol{L}^\intercal \boldsymbol{L})^{-2}$ has condition number $(\operatorname{cond} \boldsymbol{L})^4$ and therefore easily becomes ill-conditioned. To mitigate this, one may compute the QR-decomposition $\boldsymbol{Q}\boldsymbol{R} = \boldsymbol{L}$. Then, there holds $\boldsymbol{L}^\intercal \boldsymbol{L} = \boldsymbol{R}^\intercal \boldsymbol{Q}^\intercal \boldsymbol{Q} \boldsymbol{R} = \boldsymbol{R}^\intercal \boldsymbol{R}$. The action of $(\boldsymbol{L}^\intercal \boldsymbol{L})^{-2}$ can thus be computed by solving two linear systems using forward- and backward-substitution. △

6. Optimal recovery

We consider the following

Problem 6.1 (Optimal recovery) Given values $f_1 := \lambda_1(f), \dots f_N := \lambda_N(f) \in \mathbb{R}$, where $\{\lambda_1, \dots, \lambda_N\}$ is a set of linearly independent linear functionals (called *information functionals*), how can we best approximate the value $\lambda(f)$ of a known functional λ for an unknown function f?

In the Hilbert space setting, the solution to this problem is given by the *minimum-norm interpolant*, i.e., the function $g^\star \in \mathcal{H}$ with

$$\lambda_i(g^\star) = \lambda_i(f), \quad i = 1, \dots, N \tag{6.1}$$

and

$$\|g^\star\|_{\mathcal{H}} = \min_{g \in \mathcal{H}:(6.1)} \|g\|_{\mathcal{H}}$$

We present three corresponding optimality results for radial basis function interpolation. As a preparation, we require two Lemmata.

Lemma 6.2 Let K be a strictly positive definite kernel. Then, there holds

$$\langle s_f, s_f - g \rangle_{\mathcal{N}_K(\Omega)} = 0$$

for all interpolants $g \in \mathcal{N}_K(\Omega)$ with $g(\boldsymbol{x}_i) = f(\boldsymbol{x}_i)$ for $i = 1, \dots, N$.

Proof. There holds

$$\begin{aligned}\langle s_f, s_f - g \rangle_{\mathcal{N}_K(\Omega)} &= \left\langle \sum_{j=1}^N c_j K(\boldsymbol{x}_j, \cdot), s_f - g \right\rangle_{\mathcal{N}_K(\Omega)} = \sum_{j=1}^N c_j \langle K(\boldsymbol{x}_j, \cdot), s_f - g \rangle_{\mathcal{N}_K(\Omega)} \\ &= \sum_{j=1}^N c_j \big(s_f(\boldsymbol{x}_j) - g(\boldsymbol{x}_j)\big) = 0,\end{aligned}$$

since s_f and g both interpolate f. □

Lemma 6.3 Let K be a strictly positive definite kernel. Then, there holds

$$\langle f - s_f, h \rangle_{\mathcal{N}_K(\Omega)} = 0 \quad \text{for all } h \in \operatorname{span}\{\varphi_1, \dots, \varphi_N\}.$$

Proof. Exercise! □

A straightforward consequence is a Pythagorean theorem.

Corollary 6.4 There holds

$$\|f\|^2_{\mathcal{N}_K(\Omega)} = \|f - s_f\|^2_{\mathcal{N}_K(\Omega)} + \|s_f\|^2_{\mathcal{N}_K(\Omega)}.$$

Proof. Exercise! □

Theorem 6.5 (Optimality I) Let K be a strictly positive definite kernel. Then, given the values $f_1, \dots, f_N$, the interpolant s_f is the minimum-norm interpolant, i.e.,

$$\|s_f\|_{\mathcal{N}_K(\Omega)} = \min_{g \in \mathcal{N}_K(\Omega) : g(\boldsymbol{x}_j) = f_j} \|g\|_{\mathcal{N}_K(\Omega)}.$$

Proof. From Lemma 6.2, we have

$$\langle s_f, s_f - g \rangle_{\mathcal{N}_K(\Omega)} = 0.$$

This yields

$$\|s_f\|^2_{\mathcal{N}_K(\Omega)} = \langle s_f, s_f - g + g \rangle_{\mathcal{N}_K(\Omega)}. = \langle s_f, g \rangle_{\mathcal{N}_K(\Omega)}$$

for any interpolant.
By the Cauchy-Schwarz inequality, we finally at

$$\|s_f\|^2_{\mathcal{N}_K(\Omega)} \leq \|s_f\|_{\mathcal{N}_K(\Omega)} \|g\|_{\mathcal{N}_K(\Omega)}.$$

Dividing by $\|s_f\|_{\mathcal{N}_K(\Omega)}$ yields the assertion. □

The next optimality theorem is a version of Céa's lemma.

Theorem 6.6 (Optimality II) Let K be a strictly positive definite kernel. Then, s_f is the best approximation to $f \in \mathcal{N}_K(\Omega)$ within $\operatorname{span}\{\varphi_1, \dots, \varphi_N\}$, i.e.,

$$\|f - s_f\|_{\mathcal{N}_K(\Omega)} \leq \|f - g\|_{\mathcal{N}_K(\Omega)} \quad \text{for all } g \in \operatorname{span}\{\varphi_1, \dots, \varphi_N\}.$$

Proof. There holds by the orthogonality from Lemma 6.3 and the Cauchy-Schwarz inequality that

$$\|f - s_f\|^2_{\mathcal{N}_K(\Omega)} = \langle f - s_f, f - s_f \rangle_{\mathcal{N}_K(\Omega)} = \langle f - s_f, f - g \rangle_{\mathcal{N}_K(\Omega)} \leq \|f - s_f\|_{\mathcal{N}_K(\Omega)} \|f - g\|_{\mathcal{N}_K(\Omega)}.$$

Dividing by $\|f - s_f\|_{\mathcal{N}_K(\Omega)}$ yields the assertion. □

Remark The previous two optimality theorems also hold for strictly conditionally positive definite kernels, given that the point set $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$ is unisolvent. △

We state the last optimality theorem in the context of quasi-interpolation without proof. It states that the kernel interpolant is better than any linear combination of function values in the pointwise sense.

Theorem 6.7 (Optimality III) Let K be strictly conditionally positive definite with respect to $P \subset C(\Omega)$ and assume that X is P-unisolvent. Then there holds

$$\left| f(\boldsymbol{x}) - \sum_{j=1}^{N} f(\boldsymbol{x}_j)\ell_j(\boldsymbol{x}) \right| \leq \left| f(\boldsymbol{x}) - \sum_{j=1}^{N} f(\boldsymbol{x}_j)c_j \right|$$

for any choice $c_1, \ldots, c_N \subset \mathbb{R}$ with $\boldsymbol{c}^\intercal \boldsymbol{P} = \boldsymbol{0}$.

7. Least squares approximation

As we have shown in the previous chapter, the kernel interpolation solves a constraint optimization problem. We adopt this perspective here, but make the more general assumption that our ansatz is of the form

$$s_{f,m} := \sum_{j=1}^{m} c_j K(\tilde{\boldsymbol{x}}_j, \cdot),$$

where $\tilde{\boldsymbol{x}}_1, \ldots, \tilde{\boldsymbol{x}}_m$ are not necessarily contained in X. Then, we are looking for a vector $\boldsymbol{c} \in \mathbb{R}^m$ which minimizes the quadratic form

$$\frac{1}{2}\boldsymbol{c}^\intercal \boldsymbol{Q}\boldsymbol{c}$$

for some symmetric and positive definite matrix $\boldsymbol{Q}$, subject to the linear constraints

$$\boldsymbol{A}\boldsymbol{c} = \boldsymbol{f}$$

with the generalized Vandermonde matrix $\boldsymbol{A} \in \mathbb{R}^{N\times m}$. This constraint optimization problem is solved by minimizing

$$\mathcal{L}(\boldsymbol{c}, \boldsymbol{\lambda}) := \frac{1}{2}\boldsymbol{c}^\intercal \boldsymbol{Q}\boldsymbol{c} - \boldsymbol{\lambda}^\intercal(\boldsymbol{A}\boldsymbol{c} - \boldsymbol{f})$$

with the *Lagrange multipliers* $\boldsymbol{\lambda} \in \mathbb{R}^N$. The unique minimum of $\mathcal{L}(\boldsymbol{c}, \boldsymbol{\lambda})$ is obtained from the solution of the saddle point formulation

$$\begin{bmatrix} \boldsymbol{Q} & -\boldsymbol{A}^\intercal \\ \boldsymbol{A} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{c} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \boldsymbol{0} \\ \boldsymbol{f} \end{bmatrix}.$$

The solution is obtained by block Gaussian elimination in accordance with

$$\begin{aligned} \boldsymbol{\lambda} &= (\boldsymbol{A}\boldsymbol{Q}^{-1}\boldsymbol{A}^\intercal)^\dagger \boldsymbol{f}, \\ \boldsymbol{c} &= \boldsymbol{Q}^{-1}\boldsymbol{A}^\intercal \boldsymbol{\lambda}. \end{aligned}$$

In the particular case that $m = N$, $\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i$, and $\boldsymbol{A} = \boldsymbol{Q} = \boldsymbol{K}$, we find

$$\boldsymbol{c} = \boldsymbol{\lambda} = \boldsymbol{K}^{-1}\boldsymbol{f},$$

as in the previous chapter. However, the presented approach is more general as it also considers the cases $N < m$ (underdetermined least squares) and $N > m$ (overdetermined least squares), where the matrix $\boldsymbol{Q}$ takes the role of a *regularization term*.

In the case that $\boldsymbol{Q} = [K(\tilde{\boldsymbol{x}}_i, \tilde{\boldsymbol{x}}_j)]_{i,j=1}^m$ represents the native space norm of the interpolant, we obtain the least-squares problem

$$\min_{\boldsymbol{c}\in\mathbb{R}^m} \frac{1}{2}\|\boldsymbol{A}\boldsymbol{c} - \boldsymbol{f}\|_2^2 + \frac{\omega}{2}\|s_{f,m}\|_{\mathcal{N}_K(\Omega)}^2.$$

The *ridge parameter* ω controls the tradeoff between the smoothness and the fit of $s_{f,m}$. Finally, if we choose $m = N$, $\tilde{\boldsymbol{x}}_i = \boldsymbol{x}_i$, and $\boldsymbol{A} = \boldsymbol{Q} = \boldsymbol{K}$, this minimization problem becomes

$$\min_{\boldsymbol{c}\in\mathbb{R}^N} \frac{1}{2}\|\boldsymbol{K}\boldsymbol{c} - \boldsymbol{f}\|_2^2 + \frac{\omega}{2}\boldsymbol{c}^\intercal\boldsymbol{K}\boldsymbol{c}.$$

The first order optimality condition reads

$$\boldsymbol{K}^2\boldsymbol{c} + \omega\boldsymbol{K}\boldsymbol{c} = \boldsymbol{K}(\boldsymbol{K} + \omega\boldsymbol{I})\boldsymbol{c} = \boldsymbol{K}\boldsymbol{f}$$

If $\boldsymbol{K}$ has a trivial kernel, this equation is satisfied iff

$$(\boldsymbol{K} + \omega\boldsymbol{I})\boldsymbol{c} = \boldsymbol{f}.$$

8. Support vector machines

Given N points $X = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\} \subset \mathbb{R}^d$ and *labels* $y_i \in \{-1, 1\}$ for $i = 1, \dots, N$, we introduce the sets

$$\begin{aligned} X_+ &:= \{\boldsymbol{x}_i \in X : y_i = 1\}, \\ X_- &:= \{\boldsymbol{x}_i \in X : y_i = -1\}. \end{aligned} \tag{8.1}$$

We are interested in solving the following *classification problem*.

Problem 8.1 (Binary classification problem) Given the two sets X_+ and X_- from (8.1), find a function $f\colon \mathbb{R}^d \to \mathbb{R}$ such that $f(\boldsymbol{x}) > 0$ for all $\boldsymbol{x} \in X_+$ and $f(\boldsymbol{x}) < 0$ for all $\boldsymbol{x} \in X_-$.

In the easiest case, the two sets can be split by a *separating hyper-plane*.

Definition 8.2 The sets X_+ and X_- are called *linearly separable*, iff there exists a *separating hyper-plane* $H = \{\boldsymbol{x} \in \mathbb{R}^d : \boldsymbol{n}^\intercal \boldsymbol{x} = m\}$ such that $\boldsymbol{n}^\intercal \boldsymbol{x} > m$ iff $\boldsymbol{x} \in X_+$ and $\boldsymbol{n}^\intercal \boldsymbol{x} \leq m$ iff $\boldsymbol{x} \in X_-$.

If X_+ and X_- are linearly separable, it is sufficient to determine an affine map

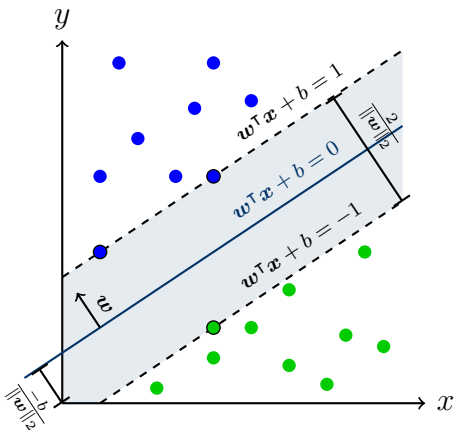
$$f(\boldsymbol{x}) = \boldsymbol{w}^\intercal \boldsymbol{x} + b,$$

whose zero levelset $\mathcal{S} := \{\boldsymbol{x} \in \mathbb{R}^d : f(\boldsymbol{x}) = 0\}$ serves as *separator*. More precisely, we wish to determine a vector $\boldsymbol{w} \in \mathbb{R}^d$ and a threshold b such that the following two separation conditions are satisfied:

$$\begin{aligned} \boldsymbol{w}^\intercal \boldsymbol{x}_i + b &\geq 1, \quad \text{if } y_i = 1, \\ \boldsymbol{w}^\intercal \boldsymbol{x}_i + b &\leq -1, \quad \text{if } y_i = -1. \end{aligned}$$

These conditions can be summarized according to

$$y_i(\boldsymbol{w}^\intercal \boldsymbol{x}_i + b) \geq 1 \quad \text{for all } i = 1, \dots, N.$$



Given that X_+ and X_- are linearly separable, typically there exists more than one solution. Therefore, we aim to find a separator that maximizes the distance from X_+ and X_- (*maximal margin*). In this case, there exist points $\boldsymbol{x}_+ \in X_+$, $\boldsymbol{x}_- \in X_-$, such that

$$\boldsymbol{w}^\intercal\boldsymbol{x}_+ + b = 1, \quad \boldsymbol{w}^\intercal\boldsymbol{x}_- + b = -1,$$

which are called *support vectors*. Taking any pair of such points, we have

$$\boldsymbol{w}^\intercal(\boldsymbol{x}_+ - \boldsymbol{x}_-) = 2.$$

From this, we obtain the separator by solving the maximization problem

$$\frac{1}{\|\boldsymbol{w}\|_2}\boldsymbol{w}^\intercal(\boldsymbol{x}_+ - \boldsymbol{x}_-) = \frac{2}{\|\boldsymbol{w}\|_2} \to \max.$$

The latter es equivalent to the minimization problem

$$\frac{1}{2}\|\boldsymbol{w}\|_2^2 = \frac{1}{2}\sum_{i=1}^{d} w_i^2 \to \min.$$

Imposing the separation conditions finally yields the constrained optimzation problem

$$\min_{[\boldsymbol{w},b]^\intercal\in\mathbb{R}^{d+1}} \frac{1}{2}\sum_{i=1}^{d} w_i^2, \quad \text{such that } y_i(\boldsymbol{w}^\intercal\boldsymbol{x}_i + b) \geq 1 \quad \text{for all } i = 1,\dots,N. \tag{8.2}$$

A solution $[\boldsymbol{w}^\star, b^\star]^\intercal$ to (8.2) gives rise to the *hard margin SVM classifier* according to

$$c(\boldsymbol{x}) = \operatorname{sign}(\boldsymbol{w}^\intercal\boldsymbol{x} + b). \tag{8.3}$$

We have the following

Fact 8.3 Let $X = \{\boldsymbol{x}_1,\dots,\boldsymbol{x}_N\} \subset \mathbb{R}^d$ with labels $y_i \in \{-1,1\}$ for $i = 1,\dots,N$ be given. If the sets X_+ and X_- are non-empty and linearly separable, then the optimization problem (8.2) has a unique solution $[\boldsymbol{w}^\star, b^\star]^\intercal$ with $\boldsymbol{w}^\star \neq \boldsymbol{0}$.

To solve the optimization problem (8.2), we introduce the N non-negative Lagrange multipliers λ_i, $i = 1,\dots,N$ and consider the Lagrange functional

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\lambda}) = \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_{i=1}^{N} \lambda_i\big(y_i(\boldsymbol{w}^\intercal\boldsymbol{x}_i + b) - 1\big). \tag{8.4}$$

The constrained optimization problem (8.2) is now eqivalent to the unconstrained one

$$\min_{[\boldsymbol{w},b]^\intercal \in \mathbb{R}^{d+1}} \max_{\boldsymbol{\lambda} \in \mathbb{R}^N} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\lambda}),$$

which is called the *primal problem*.
Minimizing $\mathcal{L}$ with respect to $\boldsymbol{w}$ and b yields the first order optimality conditions

$$\begin{aligned} \frac{\partial}{\partial \boldsymbol{w}} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\lambda}) &= \boldsymbol{w} - \sum_{i=1}^N \lambda_i y_i \boldsymbol{x}_i = \boldsymbol{0}, \\ \frac{\partial}{\partial b} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\lambda}) &= -\sum_{i=1}^N \lambda_i y_i = 0. \end{aligned} \tag{8.5}$$

In addition, we have to satisfy the *complementarity conditions*

$$\lambda_i \geq 0, \quad y_i(\boldsymbol{w}^\intercal \boldsymbol{x}_i + b) - 1 \geq 0, \quad \lambda_i \big(y_i(\boldsymbol{w}^\intercal \boldsymbol{x}_i + b) - 1 \big) = 0, \quad i = 1, \ldots, N. \tag{8.6}$$

Equations (8.5) and (8.6) are known as *Karush-Kuhn-Tucker conditions* (KKT). They are necessary and sufficient for the existence of an optimal solution. Particularly, (8.6) ensures that either $\boldsymbol{x}_i$ is lying on the hyperplane $y_i(\boldsymbol{w}^\intercal \boldsymbol{x}_i + b) = 1$ or $\lambda_i = 0$.
Inserting (8.5) into (8.4) eliminates the variables $\boldsymbol{w}, b$ according to

$$\mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\lambda}) = \sum_{i=1}^N \lambda_i - \frac{1}{2} \sum_{i,j=1}^N \lambda_i \lambda_j y_i y_j \boldsymbol{x}_i^\intercal \boldsymbol{x}_j =: -f(\boldsymbol{\lambda}).$$

The optimization problem

$$\min_{\boldsymbol{\lambda} \in \mathbb{R}^N} f(\boldsymbol{\lambda}), \quad \text{such that } \sum_{i=1}^N \lambda_i y_i = 0, \quad \lambda_i \geq 0, \quad i = 1, \ldots, N \tag{8.7}$$

is called the *dual problem* to (8.2).
Vice versa, wa can solve (8.2) by solving (8.7) and inserting (8.5). Therefore, we have the following

Theorem 8.4 Let $\boldsymbol{\lambda}^\star \in \mathbb{R}^N$ be a solution to the dual problem (8.7). Setting

$$\boldsymbol{w}^\star := \sum_{i=1}^N \lambda_i^\star y_i \boldsymbol{x}_i$$

and choosing $b^\star$ such that $y_i\big((\boldsymbol{w}^\star)^\intercal \boldsymbol{x}_i + b\big) = 1$ for any $i \in \{1, \ldots, N\}$ with $\lambda_i \neq 0$ yields the solution $[\boldsymbol{w}^\star, b^\star]^\intercal$ to (8.2).

A solution to the dual problem exists whenever the conditions of Fact 8.3 are satisfied.

Remark Since f in (8.7) is not strictly convex, the solution may not be unique. The optimization problem can efficiently be solved by the *active set method*. △

We finish this chapter by considering the situation that the sets X_+ and X_-, cp. (8.1), are not linearly separable. In this case, we replace the inner product $\boldsymbol{x}^\intercal \boldsymbol{y}$ in (8.3) by the inner product of the canonical feature map, i.e., $\langle K(\boldsymbol{x},\cdot), K(\boldsymbol{y},\cdot)\rangle_{\mathcal{H}} = K(\boldsymbol{x},\boldsymbol{y})$ for all $\boldsymbol{x},\boldsymbol{y} \in X$. In what follows, we assume that the data (φ_i, y_i), $i = 1,\dots,N$, is linearly separable in the RKHS $\mathcal{H}$. Then there exist

$$w \in \mathcal{H}_X := \operatorname{span}\{K(\boldsymbol{x}_1,\cdot),\dots,K(\boldsymbol{x}_N,\cdot)\} \subset \mathcal{H}, \quad b \in \mathbb{R}$$

such that

$$y_i\big(\langle w, K(\boldsymbol{x}_i,\cdot)\rangle_{\mathcal{H}} + b\big) \geq 1 \quad \text{for all } i = 1,\dots,N. \tag{8.8}$$

Remark The kernel interpolant

$$w(\boldsymbol{x}) = \sum_{i=1}^{N} y_i \ell_i(\boldsymbol{x})$$

obviously satisfies $w(\boldsymbol{x}_i) = y_i$ for $i = 1,\dots,N$ and, hence, (8.8) for $b = 0$. Therefore, the existence of a solution is guaranteed whenever the kernel is strictly positive definite. △

Analogously to the linear case, the weight is obtained by solving the optimization problem

$$\min_{(w,b)\in\mathcal{H}_X\times\mathbb{R}} \frac{1}{2}\|w\|_{\mathcal{H}}^2, \tag{8.9}$$

such that the constraints (8.8) are satisfied. The existence and uniqueness of a solution is obtained analogously to Fact 8.3. Considering the dual problem yields the optimization problem

$$\min_{\boldsymbol{\lambda}\in\mathbb{R}^N} \frac{1}{2}\sum_{i,j=1}^{N} \lambda_i\lambda_j y_i y_j K(\boldsymbol{x}_i,\boldsymbol{x}_j) - \sum_{i=1}^{N}\lambda_i$$

with the constraints

$$\sum_{i=1}^{N} \lambda_i y_i = 0, \quad \lambda_i \geq 0, \quad i = 1,\dots,N.$$

Given a solution $\boldsymbol{\lambda}^\star$, we retrieve $w^\star$ via

$$w^\star = \sum_{i=1}^{N} \lambda_i^\star y_i K(\boldsymbol{x}_i,\cdot)$$

and $b^\star$ by a choice such that

$$y_i\big(\langle w, K(\boldsymbol{x}_i,\cdot)\rangle_{\mathcal{H}} + b^\star\big) = 1$$

for any $i \in \{1,\dots,N\}$ with $\lambda_i \neq 0$. The classifier is then finally given by

$$c(\boldsymbol{x}) = \operatorname{sign}\left(\sum_{i=1}^{N} \lambda_i^\star y_i K(\boldsymbol{x}_i,\boldsymbol{x}) + b^\star\right).$$

Recommended Literature

[Fas] G. E. Fasshauer. Meshfree Approximation Methods with MATLAB.
[Wen] H. Wendland. Scattered Data Approximation.