Lecture notes on Scientific Computing 2

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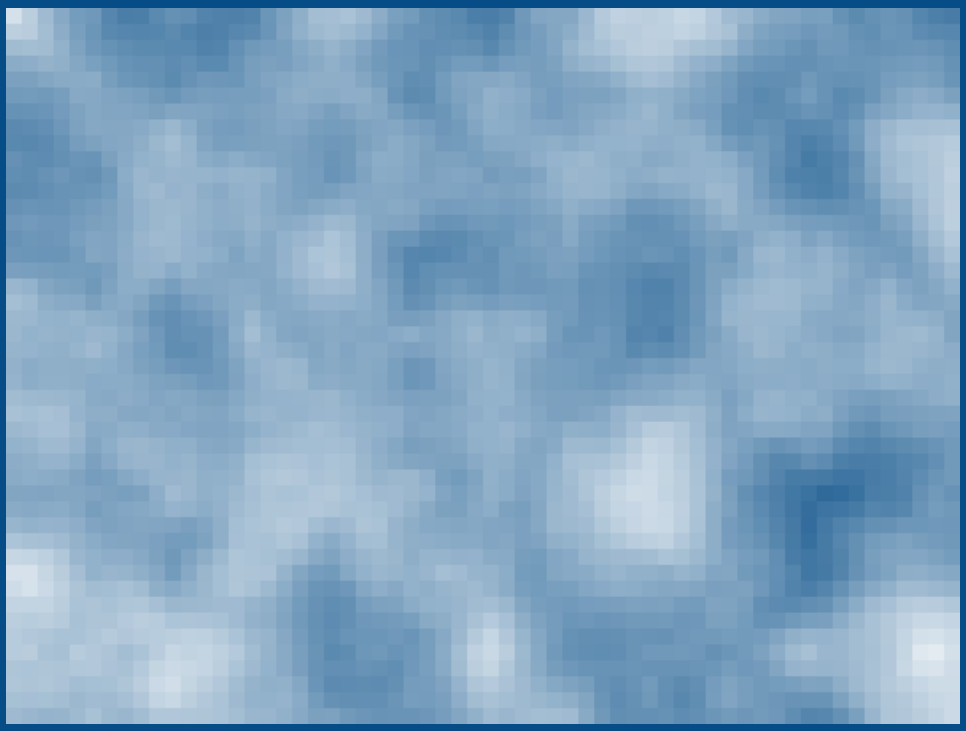

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Chapter 0:
Manuel's notes and introduction

Warning

These are unofficial lecture notes written by a student. They are messy, will almost surely contain errors, typos and misunderstandings and may not be kept up to date! I do however try my best and use these notes to prepare for my exams. Feel free to email me any corrections to mh@mssh.dev or s6mlhinz@uni-bonn.de.
Happy learning!

General Information

- Ecampus: Ecampus link
- Basis: Basis link
- Website: https://ins.uni-bonn.de/teachings/ss-2024-440-v3e2-wissenschaftlich/
- Time slot(s): Tuesday 10-12 and Thursday 08-10
- Exams: Oral, unless more than 50 people take the exam
- Deadlines: tbd
- Two topics:
  - Kernel based methods for function approximation
  - Nonlinear dimensionality reduction / manifold learning / latent space embeddings
- Official lecture notes for most of the lectures
- Exercises are a mix of theory (proofs, (counter-)examples) and programming tasks

Start of lecture 01 (09.04.23)

0.1 Overview

We begin with a quick overview of the two parts of the lecture:

0.1.1 Function approximation / Interpolation

Consider $x_i \in \mathbb{R}^d, \hat{f}_i \in \mathbb{R}$:

$$\{(x_i, \hat{f}_i)\}_{i=1}^N.$$

Aim: Find a "good" function f such that

$$f(x_i) = \hat{f}_i, \ i = 1, \dots, N$$

Lagrangian Interpolation does not work great for a lot of points and higher dimensions

To compute f, we can make use of a discrete representation of f using **Ansatzfunctions** $\{b_j\}_{j=1}^N$:

$$f(x) = \sum_{j=1}^{N} c_j b_j(x).$$

Here we assume the same number of data and functions b_j.
For interpolation, we can solve this via:

$$BC = \hat{F}$$

Kernel functions that are centered at the locations x_j turn out to be a good choice:

$$b_j(x) = k(x_j, x)$$

which gives

$$f(x) = \sum_{j=1}^{N} c_j k(x_j, x).$$

We will also consider approximation instead of interpolation

$$f(x_i) \approx \hat{f}_i.$$

This is in particular relevant in machine learning, where one usually assumes, and actually has noise and measurement errors in the given data.
Example: Asses credit risk
Example: Chemistry / energy of molecules. This needs a kernel on graphs
Example: Time series. This needs a kernel on time series

Careful not to discriminate, credit risk should be independent of neighbourhood for example!

Remark. *We will also see that kernels relate to similarity measures and therefore to distances (dissimilarity).*

Topics in part 1:

- What are kernels and their properties
- Reproducing Kernel Hilbert spaces as the function space in which we are working
- Function interpolation and their approximation properties
- Generalized interpolation for solving partial differential equations
- Kernel methods for prediction in machine learning, representer theorem and regularization
- Gaussian Process Regression and Support Vector Machines

0.1.2 Dimensionality reduction

Distances and similarities are a key aspect of the second topic of the course:

Dimensionality reduction for high-dimensional data

The key idea is to find a "good" low dimensional representation (called embedding), such that chosen properties in high dimensions are approximately preserved.

- Linear dimensionality reduction (numerical linear algebra)
- Nonlinear dimensionality reduction (numerical linear algebra with Non-euclidean geometry)
- Dimensionality reduction with neural networks and other nonlinear function representations

Chapter 1:
Kernel based methods

1.1 Kernels

Definition (Gaussian kernel)**.** *The **gaussian kernel** is a prime example of a kernel:*

$$k(x,y) \coloneqq \exp\left(-\alpha\|x-y\|_2^2\right) = \phi(\|x-y\|_2)$$

for all $x, y \in \mathbb{R}^d$ where α is a scaling parameter.

Definition 1.1. *Let Ω be an arbitrary nonempty set. A function $k : \Omega \times \Omega \to \mathbb{R}$ is called **kernel** on Ω. We call k a **symmetric kernel** if*

$$k(x,y) = k(y,x)$$

for all $x, y \in \Omega$.

Definition 1.2. *A function $\Phi : \mathbb{R}^d \to \mathbb{R}$ is said to be **radial** if there exists a function $\phi : [0,\infty] \to \mathbb{R}$ such that*

$$\Phi(x) = \phi(\|x\|_2)$$

*for all $x \in \mathbb{R}^d$. Such a function is traditionally called a **radial basis function (rbf)**.*

1.1.1 Examples

Example ((Inverse) multiquadratics)**.** ***Multiquadratics** are of the form*

$$\phi(r) = (1+\alpha r^2)^\beta$$

*for positive β, while **inverse multiquadratics** have a $\beta < 0$.*

Example (Polyharmonic kernels)**.** ***Polyharmonic kernels** are of the form*

$$\phi(r) = r^\beta \log(|r|)$$

where $\beta \in 2\mathbb{Z}$.
*The special case $\beta = 2$ is the so-called **thin-plate spline**. It relates to the partial differential equation that describes the bending of thin plates.*

While the previous examples were monotone kernels (as a function of r), these are not!

Example (Wendland's kernels)**.** ***Wendland's kernels** are of the form*

$$\phi_{a,1} \coloneqq (1-r)_+^{(a+1)}(1+(a+1)r)$$

*with the **cut-off function***

$$(x)_+ \coloneqq \begin{cases} x & x \geq 0 \\ 0 & x < 0 \end{cases}$$

Remark. *There are also non radial kernels:*
Translation-invariant *or* ***stationary*** *kernels are functions of differences:*

$$k(x, y) = \Phi(x - y).$$

For periodic setups, we have the ***Dirichlet kernel*** *as an example:*

$$D(\phi) \coloneqq \frac{1}{2} + \sum_{j=1}^{N} \cos(j\varphi) = \frac{\sin\left(\left(n + \frac{1}{2}\right)\phi\right)}{2\sin\left(\frac{\phi}{2}\right)}.$$

This is applied to differences $\phi = \alpha - \beta$ of angles or 2π-periodic arguments and is an important tool for Fourier series theory.
There are so called ***zonal kernels****, for working on a sphere, where the kernel can be represented as a function of an angle. An example are functions of inner products, such as*

$$k(x, y) = \exp(x^{\perp} y).$$

Remember, $x^{\perp} y$ is the (scaled) cosine of the angle between the two vectors.

Remark. *We wil see that a kernel k on Ω defines a function $k(x, \cdot)$ for all fixed $x \in \Omega$. The space*

$$\mathcal{K}_0 \coloneqq span\{k(x, \cdot) \mid x \in \Omega\}$$

can for example be used as a so called trial space in meshless methods for solving partial differential equations.

Remark. *Kernels can always be restricted to subsets without losing essential properties. This easily allows kernels on embedded manifolds, e.g. the sphere.*

Remark. *Most of this works for complex kernels too.*

1.1.2 Kernels in machine learning

In machine learning the data $x \in \Omega$ can be quite diverse and without (much) structure on first glance. For example consider images, text documents, customers, graphs, ...
Here, one views the kernel as a **similarity measure**, i.e.

In $\mathbb{R}^d$, we can work with the standard scalar product

$$k : \Omega \times \Omega \to \mathbb{R}$$

return a number $k(x, y)$ describing the similarity of two patterns x and y.
To work with general data, we first need to represent it in a Hilbert space $\mathcal{F}$, the so-called **feature space**. One considers the (application dependent) **feature map**

Reminder: A Hilbert space is a complete vector space with a scalar product

$$\Phi : \Omega \to \mathcal{F}.$$

The map describes each $x \in \Omega$ by a collection of **features** which are characteristic for a x and capture the essentials of elements of Ω. Since we are now in $\mathcal{F}$ we can work with linear techniques. In particular we can use the scalar product in $\mathcal{F}$ of two elements of Ω represented by their features:

$$\langle \Phi(x), \Phi(y) \rangle_{\mathcal{F}} =: k(x, y)$$

and define a kernel that way.

Remark. *Given a kernel, neither the feature map nor the feature space are unique, as the following example shows:*

Example. *Let $\Omega = \mathbb{R}, k(x, y) = x \cdot y$. A feature map, with feature space $\mathcal{F} = \mathbb{R}$ is given by the identity map.*

Such a construction can be made for any arbitrary kernel, therefore every kernel has many different feature spaces

But,the map $\Phi : \Omega \to \mathbb{R}^2$ defined by

$$\Phi(x) \coloneqq (x/\sqrt{2}, x/\sqrt{2})$$

is also a feature map given the same k!

The following two examples show how one can handle non-euclidean origin spaces:

Example (Kernels on a set of documents)**.** *Consider a collection of documents. We represent each document as a* ***bag of words*** *and describe a bag as a vector in a space in which each dimension is associated with a term from the set of words, i.e. the dictionary. The feature map is*

that is a set of frequencies of (chosen) words

$$\Phi(t) \coloneqq (wf(w_1, t), wf(w_2, t), \ldots, wf(w_d, t)) \in \mathbb{R}^d$$

where $wf(w_i, t)$ is the frequency of word w_i in document t.
A simple kernel is the vector space kernel

$$k(t_1, t_2) = \langle \Phi(t_1), \Phi(t_2) \rangle = \sum_{j=1}^{d} wf(w_j, t_1) wf(w_j, t_2).$$

Natural extensions to this kernel take e.g. word order, relevance or semantics into account, which can be achieved by using matrices in the scalar product:

$$k(t_1, t_2) = \langle S\Phi(t_1), S\Phi(t_2) \rangle = \Phi^{\perp}(t_1) S^{\perp} S \Phi(t_2.)$$

Example (Graph kernels)**.** *Another non-euclidean data object are graphs, where the class of* ***random walk kernels*** *can be defined. These are based on the idea that given a pair of graphs, one performs random walks on both and counts the number of matching walks. With $\tilde{A}_\times$ the adjacency matrix of the* ***direct product graph*** *of the two involved graphs, one defines:*

$$k(G, H) \coloneqq \sum_{j=1}^{N_G} \sum_{k=1}^{N_H} \sum_{l=1}^{\infty} \lambda_l [\tilde{A}_\times^l]_{j,k}.$$

More generally, one can define a ***random walk graph kernel*** *k as*

$$k(G, H) \coloneqq \sum_{k=0}^{\infty} \lambda_k q_\times^T W_\times^k p_\times,$$

where $W_\times$ is the ***weight matrix*** *of the direct product graph, $q_\times^T$ is the* ***stopping probability*** *on the direct product graph, and $p_\times$ is the initial product distribution on the direct product graph.*

1.1.3 Mercer kernels

More generally, one can consider kernels of the **Hilbert-Schmidt** or **Mercer** form

$$k(x, y) = \sum_{i \in I} \lambda_i \varphi_i(x) \varphi_i(y),$$

with certain functions $\varphi_i : \Omega \to \mathbb{R}$, certain positive **weights** λ_i and an index set I such that the following **summability condition** holds for all $x \in \Omega$:

$$k(x, y) = \sum_{i \in I} \lambda_i \varphi_i(x)^2 < \infty \tag{1}$$

Remark. *Such kernels arise in machine learning if the functions φ_i each describe a feature of x and the feature space is the weighted l_2-space of sequences with indices in I:*

$$l_{2,I,\lambda} \coloneqq \left\{ \{\xi_i\}_{i \in I} : \sum_{i \in I} \lambda_i \xi_i^2 < \infty \right\}.$$

This expansion also occurs when kernels generating positive operators are expanded into eigenfunctions on Ω. Such kernels can be views as arising from generalized convolutions. Generally kernels have three major application fields:

- Convolutions
- Trial spaces
- Covariances

We are mainly concerned with the last two.

Start of lecture 02 (11.04.24)

1.1.4 Properties of kernels

Consider an arbitrary set $X = \{x_1, \dots, x_N\}$ of N **distinct** elements of Ω and a symmetric Kernel K on $\Omega \times \Omega$.

N is the number of data points (always!)

$$f(x) = \sum_{j=1}^{N} a_j k(x_j, x), x \in \Omega$$

Remark. *The set of $k(x_j, \cdot)$ might not be linear independent!*

For X we construct the symmetric $N \times N$ Kernel matrix

$$K = K_{X,X} = (k(x_j, x_k))_{1 \le j,k \le N}$$

and obtain the interpolation problem

$$\hat{f}_k = f(x_k) = \sum_{j=1}^{N} a_j k(x_j, x_k)$$

in matrix form

$$K_{X,X} a = \hat{F}$$

Remark. *With kernels, we will see that this is indeed solvable, because our matrix is symmetric and positive definite.*

Definition 1.3. *A Kernel on $\Omega \times \Omega$ is **symmetric and positive semidefinite** , if all Kernel matrices for all finite sets of distinct elements of Ω are symmetric and positive definite*

semidefinite and definite have conflicting definitions in the literature!

Theorem 1.4. *1. Kernels arising from **feature maps** via*

$$k(x, y) = \langle \Phi(x), \Phi(y) \rangle$$

are positive semidefinite.

*2. **Hilbert-Schmidt** or **Mercer Kernels***

$$k(x, y) = \sum_{i \in I} \varphi_i(x) \varphi_i(y)$$

are positive semidefinite.

Proof. 1. K is a **Gram(-ian)** matrix

A Gram matrix, is a matrix whose entries are given by inner products $K_{i,j} = \langle v_i, v_j \rangle$

2.

$$a^\perp K a = \sum_{j,k=1}^{N} a_j a_k k(x_j, x_k) = \sum_{j,k=1}^{N} a_j a_k \sum_{i \in I} \varphi_i(x) \varphi_i(y)$$

$$= \sum_{i \in I} \lambda_i \sum_{j=1}^{N} a_j \varphi_i(x_j) \sum_{k=1}^{N} a_k \varphi_i(x_k) = \sum_{i \in I} \lambda_i \left(\sum_{j=1}^{N} a_j \phi_i(x_j) \right)^2 \ge 0$$

□

Theorem 1.5. *Let K be a symmetric positive semidefinite (spsd) Kernel on Ω. Then*

1. *$k(x,x) \geq 0$ for all $x \in \Omega$*
2. *$|k(x,y)|^2 \leq k(x,x)k(y,y)$ for all $x, y \in \Omega$*
3. *$2|k(x,y)|^2 \leq k(x,x)^2 + k(y,y)^2$ for all $x, y \in \Omega$*
4. *Any finite linear combination spsd Kernels with nonnegative coefficients gives a spsd Kernel. If any of these kernels is positive definite, and its coefficient is positive, then the combination of kernels is positive definite.*
5. *The product of two spsd kernels is spsd.*
6. *The product of two spd kernels is spd.*

Proof. 1.: Use the set $\{x\}$ in Definition 1.3.
2.: Consider K of $\{x, y\}$. The determinant of such a positve semidefinite matrix is nonnegative, therefore

$$k(x,x)k(y,y) - k(x,y)^2 \geq 0$$

3.: $2ab \leq a^2 + b^2$ for all $a, b \in \mathbb{R}_0^+$. Therefore this follows from 2.
4.: Expand $a^\perp K a$ to see this.
5.: Follows from Lemma 1.6.
6.: Follows from Lemma 1.6 and a bit more linear algebra. □

Lemma 1.6 (Schur's Lemma)**.** *For two matrices A, B, the matrix C with elements*

$$C_{jk} = A_{jk}B_{jk}$$

*is called the **Schur product** or **Hardarmard product**. The Schur product of two psd matrices is psd.*

Proof. Decompose $A = S^\perp DS$ with S an orthogonal matrix and $D = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ a diagonal matrix with $\lambda_i \geq 0$ the eigenvalues of A.
For all $q \in \mathbb{R}^N$ we look at

$$\begin{aligned} q^\perp Cq &= \sum_{j,k} q_j q_k a_{jk} b_{jk} = \sum_{j,k=1}^{N} q_j q_k \sum_{m=1}^{N} \lambda_m S_{jm} S_{km} \\ &= \sum_{m=1}^{N} \lambda_m \sum_{j,k=1}^{N} \underbrace{q_j S_{jm}}_{P_{k,m}} \underbrace{q_k S_{km}}_{P_{km}} b_{jk} = \sum_{m=1}^{N} \sum_{j,k=1}^{N} \underbrace{P_{jm} P_{km} b_{jk}}_{\geq 0 \text{ since } B \text{ is psd}} \geq 0 \end{aligned}$$

□

Remark. *Note that we only considered symmetric matrices, the above also holds if one of the matrices is not symmetric, but positive definite instead.*

Remark. *Our overall aim is to go from kernels to a **Reproducing Kernel Hilbert space (RKHS)**. Therefore we define candidate spaces and a bilinear form in a way we would expec them.*

Definition. *For spsd K we define*

$$H := span\{k(x, \cdot) \mid x \in \Omega\}.$$

In the same way

$$L := span\{\delta_x \mid x \in \Omega, \delta_x : H \to \mathbb{R}\}$$

the linear space of all finite linear combinations of pointevaluation functionals actions on functions of H, where

$$\delta_x(f) = f(x).$$

It is important that elements of L act on elements of H! These two spaces are paired in some sense.

We can, by definition, write all Elements from L and H as

$$\lambda_{a,X} \coloneqq \sum_{j=1}^{N} a_j \delta_{x_j}$$

$$f_{a,X} \coloneqq \sum_{j=1}^{N} a_j k(x_j, x) = \lambda_{a,X}^{(y)} k(x,y)$$

with $a \in \mathbb{R}^n, X = \{x_1, \dots, x_N\} \subset \Omega$ any arbitrary finite subset of Ω.

Remark. *From $f_{a,X} = 0$ or $\lambda_{a,X} = 0$ it does not follow that $a = 0$!*

There might be different representations of elements in L, H. While the representation is not unique, the element is

We now define a bilinear form on L

$$\langle \lambda_{a,X}, \lambda_{b,Y} \rangle_L \coloneqq \sum_{j=1}^{M} \sum_{k=1}^{N} a_j b_k k(x_j, x_k) = \lambda_{a,X}^{(x)} \lambda_{b,Y}^{(y)} k(x,y) = \lambda_{a,X}(f_b, Y)$$

Added remark. *One has to be a bit careful here: $\lambda_{a,X}^{(x)} \lambda_{b,Y}^{(y)} k(x,y)$ does not mean point wise multiplication, but concatenation:*

$$\lambda_{a,X}^{(x)} \lambda_{b,Y}^{(y)} k(x,y) = \lambda_{a,X}^{(x)} (\lambda_{b,Y}^{(y)} k(x,y))$$

This is well-defined, since it is based on the actions of the functional and not the specific representation.
We can observe that the bilinear form is psd, since the kernel matrices have this property.

$$|\lambda_{a,X}(f_{b,Y})| = |\langle \lambda_{a,X}, \lambda_{b,Y} \rangle_L| \leq \|\lambda_{a,X}\|_L \|\lambda_{b,Y}\|_L \ (\star)$$

Theorem 1.7. *If K is spsd Kernel on Ω, the bilinear form $\langle \cdot, \cdot \rangle_L$ is positive definite in the space L of functionals defined on H. This L is a pre-Hilbert-space.*

Proof. $0 = \langle \lambda_{a,X}, \lambda_{a,X} \rangle_L$ for $a \in \mathbb{R}^n, X = \{x_1, \dots, x_N\} \subset \Omega$.
Then by $(\star)$ we have $\lambda_{a,X} = 0$ as a functional on H. □

Here we use that the functionals in L are restricted to functions in H

Theorem 1.8. *The mapping $R : \lambda_{a,X} \mapsto f_{a,X} = \lambda_{a,X}(k(\cdot, y))$ is linear and bijective from L onto H. Thus*

$$\langle f_{a,X}, f_{b,Y} \rangle_H \coloneqq \langle \lambda_{a,X}, \lambda_{b,Y} \rangle_L = \langle R(\lambda_{a,X}), R(\lambda_{b,Y}) \rangle_H$$

is an inner product on H. R acts as the Riesz map.

Proof. Linearity is obvious. If $f_{b,Y} = R(\lambda_{b,Y}) \in H$ vanishes, the definition of $\langle \cdot, \cdot \rangle_L$ implies that $\lambda_{b,Y}$ is orthogonal to all of L. Due to Theorem 1.7 it is zero. The Riesz property comes from the definition of $\langle \cdot, \cdot \rangle_L$:

$$\lambda_{a,X}(f_{b,Y}) = \langle \lambda_{a,X}, \lambda_{b,Y} \rangle_L = \langle f_{a,X}, f_{b,Y} \rangle_H = \langle R(\lambda_{a,X}), f_{b,Y} \rangle$$

□

Specializing to $\lambda_{1,x}$, i.e. to a point $x \in \Omega$, we get:

$$\begin{aligned} \langle \lambda_{1,x}, \lambda_{b,Y} \rangle_L = \lambda_{1,x}(f_{b,Y}) = \delta_x(f_{b,Y}) = f_{b,Y}(x) \\ = \langle R(\lambda_{1,x}), R(\lambda_{b,Y}) \rangle_H = \langle R(\lambda_{1,x}), f_{b,Y} \rangle_H = \langle k(x, \cdot), f_{b,Y} \rangle_H \end{aligned}$$

In other words, for all $f \in H$, $x \in \Omega$, we have

$$f(x) = \underline{\delta_x(f)} = \langle f, R(\delta_x) \rangle_H = \underline{\langle f, k(x, \cdot) \rangle_H}$$

which is the so-called **reproduction equation** for values of functions from the inner product.

Start of lecture 03 (16.04.24)

Added remark. *In this lecture* $(\star)$ *refers to the reproduction equation.*

For $f = k(\cdot, y)$, we set $k(x, y) = \langle k(x, \cdot), k(y, \cdot)\rangle_H$. We furthermore can observe $\forall f \in H, x \in \Omega$:

$$|\delta_x(f)| = |f(x)| = |\langle f, k(x, \cdot)\rangle_H| \leq \|f\|_H \|k(x, \cdot)\|_H = \|f\|_H \sqrt{K(x, x)}$$

and

$$\langle \delta_x, \delta_y\rangle_L = \langle k(x, \cdot), k(y, \cdot)\rangle_H = k(x, y) \forall x, y \in \Omega$$

$$\|\delta_x - \delta_y\|_L^2 = \|\delta_x\|_L^2 - 2\langle \delta_x, \delta_y\rangle + \|\delta_y\|_L^2 = k(x, x) - 2\langle k(x, \cdot), k(y, \cdot)\rangle_H + k(y, y)$$

is a **distance** on Ω:

$$\text{dist}(x, y) := \|\delta_x - \delta_y\|_L = \sqrt{k(x, x) - 2\langle k(x, \cdot), k(y, \cdot)\rangle_H + k(y, y)}.$$

We see that for all $x, y \in \Omega$

$$|f(x)f(y)| \leq \|f\|_H \|\delta_x - \delta_y\|_L = \|f\|_H \text{dist}(x, y)$$

and therefore all functions in H are continuous with respect to this distance.

Theorem 1.9. *Each symmetric positive definite kernel k on a set Ω is the* ***reproducing kernel*** *of a Hilbert space called the* ***native space*** *$\mathcal{H} = \mathcal{N}_k$ of the kernel. This Hilbert space is unique and it is a space of functions on Ω. The kernel k fulfills*

$$\langle f, k(x, \cdot)\rangle_{\mathcal{H}} = f(x) \tag{2}$$

$\mathcal{H}$ can be constructed as the closure of H

Proof. Citation: The existence of native spaces follows from standard Hilbert space arguments, see e.g. chapter 11 from the lecture notes of Schaback. □

Added remark. *The good ideas are from Schaback, the errors are from me, Prof. Garcke*

The erros in this script are largely due to me :)

Proof of uniqueness:
If k is a reproducing kernel in a different Hilbert space T, we observe

$$\langle k(x, \cdot), k(y, \cdot)\rangle_{\mathcal{H}} = k(x, y) = \langle k(x, \cdot), k(y, \cdot)\rangle_T$$

which shows that the inner products coincide on H. Since T is a Hilbert space, it must contain the closure $\mathcal{N}_k$ of H as a closed subspace. For T to be larger than $\mathcal{H}$ non-zero element $f \in T$ must exist that is orthogonal to $\mathcal{N}_k$ and in particular to H. We observe

$$f(x) = \langle f, k(x, \cdot)\rangle_T = 0 \qquad \forall x \in \Omega.$$

which is a contradiction to $f \neq 0$, because of (2) for T.
Dual spaces:
$\delta_x : \mathcal{N}_k \to \mathbb{R}, f \mapsto f(x)$ for all $f \in \mathcal{N}_k, x \in \Omega$.
The dual space $\mathcal{N}_k^*$ of $\mathcal{N}_k$ is again a Hilbert space.

$$\begin{aligned} R :& \mathcal{N}_k^* \to \mathcal{N}_k \\ \lambda(f) =& \langle f, R(\lambda)\rangle_{\mathcal{N}_k} \forall f \in \mathcal{N}_k \lambda \in \mathcal{N}_k^* \\ \langle \lambda, \mu\rangle_{\mathcal{N}_k^*} =& \langle R(\lambda), R(\mu)\rangle_{\mathcal{N}_k} \forall \lambda, \mu \in \mathcal{N}_k^* \end{aligned}$$

Also via the reproducing equation 2

$$\delta_x(f) = \langle f, k(x, \cdot)\rangle_{\mathcal{N}_k} \forall f \in \mathcal{N}_k, x \in \Omega.$$

So $k(x, \cdot)$ is the **Riesz representer** $R(\delta_x)$ of δ_x

$$\begin{aligned} \langle \delta_x, \delta_y\rangle_{\mathcal{N}_k^*} = \langle R(\delta_x), R(\delta_y)\rangle_{\mathcal{N}_k} = k(x, y) & \qquad \forall x, y \in \Omega \\ \|\delta_x\|_{\mathcal{N}_k^*} = \|k(x, \cdot)\|_{\mathcal{N}_k} = \sqrt{k(x, x)} & \qquad \forall x \in \Omega \\ \lambda(f) = \langle f, \lambda^* k(x, \cdot)\rangle_{\mathcal{N}_k} & \qquad \forall f \in \mathcal{N}_k, \lambda \in \mathcal{N}_k^* \end{aligned}$$

so that $\lambda^* k(x, \cdot)$ is the Riesz representer of λ.

1.2 Reproducing Kernel Hilbert Space (RKHS)

Definition 1.10. *A Hilbert space $\mathcal{H}$ of functions on a set Ω with an inner product $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ is called **RKHS** if there is a kernel function $k : \Omega\times\Omega \to \mathbb{R}$ with $k(x,\cdot) \in \mathcal{H}$ forall $x \in \Omega$ and the reproducing kernel property*

$$f(x) = \langle f, k(x,\cdot)\rangle_{\mathcal{H}} \qquad \forall x \in \Omega, f \in \mathcal{H}$$

This directly implies

$$k(y,x) = \langle k(y,\cdot), k(x,\cdot)\rangle_{\mathcal{H}} = \langle k(x,\cdot), k(y,\cdot)\rangle_{\mathcal{H}} = k(x,y).$$

For positive semi-definiteness one can use a Gram matrix argument or take any $X = \{x_1,\dots,x_N\} \subset \Omega$ and $a \in \mathbb{R}^n$

$$\begin{aligned}\sum_{j,k=1}^{N} a_j a_k k(x_j,x_k) &= \sum_{j,k=1}^{N} a_j a_k \langle k(x,\cdot), k(y,\cdot)\rangle_{\mathcal{H}} \\ &= \langle \sum_{j=1}^{N} a_j k(x_j,\cdot), \sum_{k=1}^{N} a_k k(x_k,\cdot)\rangle_{\mathcal{H}} \\ &= \| \sum_{j=1}^{N} a_j k(x,\cdot)\|_{\mathcal{H}}^2 \geq 0\end{aligned}$$

Theorem 1.11. *Each Hilbert space $\mathcal{H}$ of real valued functions on some set Ω with point evaluation functionals*

$$\delta_x : f \mapsto f(x) \qquad \forall f \in \mathcal{H}$$

is a RKHS with a unique positive definite kernel k on Ω. The kernel is uniquely defined by providing the Riesz representers of the (continuous) point evaluation functionals. The space $\mathcal{H}$ is the native space of the kernel.

Proof. Under the given hypothesis, there must be a Riesz representer of δ_x. By the definition of th Riesz map it takes the form $k(x,\cdot) \in \mathcal{H}$ satisfying the reproduction equation 2.
In other words, any such Hilbert space has a symmetric positive definite kernel.
The final statement follows from theorem 1.9, because the native space and $\mathcal{H}$ are Hilbert spaces that contain all $k(x,y)$. □

Theorem 1.12. *If a Hilbert (sub-)space of functions on Ω has a finite orthogonal basis $v_1,\dots,v_N$ the reproducing kernel is*

$$k_N(x,\cdot)\sum_{j=1}^{N} v_j(x)v_j(\cdot) \qquad \forall x \in \Omega$$

In case of a subspace we have

$$\sum_{j=1}^{N} |v_j(x)|^2 = k_N(x,x) \leq k(x,x) \qquad \forall x \in \Omega$$

Which in some sense means that larger dimensions of the subspace can't add too much to the norm

Proof. The kernel must have a representation in the ONB

$$k_N(x,\cdot) = \sum_{j=1}^{N} \langle k_N(x,\cdot), v_j\rangle_{\mathcal{H}} v_j(\cdot) \overset{(2)}{=} \sum_{j=1}^{N} v_j(x)v_j(\cdot)$$

For the subspace,

$$\begin{aligned}k_N(x,x) &= \langle k_N(x,\cdot), k_N(x,\cdot)\rangle_{\mathcal{H}} \\ &\overset{\text{Hilbert subspace}}{=} \langle k_N(x,\cdot), k(x,\cdot)\rangle_{\mathcal{H}} \\ &\leq \sqrt{k_N(x,x)}\sqrt{K(x,x)} \qquad \forall x \in \Omega\end{aligned}$$

□

Added remark. *The subspace property does not hold for arbitrary Hilbert spaces, this tells us that a RKHS is really not the same as a normal Hilbert space!*

Start of lecture 04 (18.04.24)

Remember: Kernels of the Mercer form

$$k(x,y) = \sum_{i\in I} \lambda_i \varphi_i(x)\varphi_i(y)$$

with the summability condition

$$k(x,x) = \sum_{i\in I} \lambda_i \varphi_i^2(x) < \infty.$$

Then observe

$$\begin{aligned} |f(x)| &= \left| \sum_{i\in I} \langle f, \varphi_i\rangle_{\mathcal{H}} \phi_i(x) \right| \\ &\le \sum_{i\in I} \left| \frac{\langle f,\varphi_i\rangle_{\mathcal{H}}}{\sqrt{\lambda_i}} \right| |\varphi_i(x)|\sqrt{\lambda_i} \\ &\le \sqrt{\sum_{i\in I} \frac{\langle f,\varphi_i\rangle_{\mathcal{H}}}{\sqrt{\lambda_i}}} \sqrt{\underbrace{\sum_{i\in I} \varphi_i^2(x)\lambda_i}_{<\infty}} \end{aligned}$$

$$\mathcal{H} := \left\{ f \in \mathcal{H} : \|f\|_\lambda^2 = \sum_{i\in I} \frac{\langle f,\varphi_i\rangle_{\mathcal{H}}}{\sqrt{\lambda_i}} \right\}$$

$$\langle f, g\rangle_\lambda = \sum_{i\in I} \frac{\langle f,\varphi_i\rangle_{\mathcal{H}} \langle g,\varphi_i\rangle_{\mathcal{H}}}{\lambda_i} \qquad \forall f,g \in \mathcal{H}_\lambda \tag{3}$$

Using 3 as the kernel, we have to check if all $f_x := k(x,\cdot) \in \mathcal{H}_\lambda$.
Observe

$$\langle f_x, \varphi\rangle_{\mathcal{H}} = \lambda_i \varphi_i(x)$$

and

$$\sum_{i\in I} \frac{\langle f_x,\varphi_i\rangle_{\mathcal{H}}^2}{\lambda_i} = \sum_{i\in I} \lambda_i \varphi_i^2(x) < \infty$$

to see $f_x \in \mathcal{H}_\lambda$.

Check the reproduction equation

$$\begin{aligned} \langle f, k(x,\cdot)\rangle_\lambda &= \sum_{i\in I} \frac{\langle f,\varphi_i\rangle_{\mathcal{H}} \langle k(x,\cdot),\varphi_i\rangle_{\mathcal{H}}}{\lambda_i} \\ &= \sum_{i\in I} \frac{\langle f,\varphi_i\rangle \lambda_i \varphi_i(x)}{\lambda_i} = f(x) \qquad \forall x \in \Omega \end{aligned}$$

The kernel therefore reproduces on $\mathcal{H}_\lambda$. The proves theorem **??**.
If a Hilbert space of functions on Ω has a countable ONB $\{\varphi_i\}_{i\in I}$, each summability condition (**) leads to a reproducing mercer kernel (*) for a suitable subspace of functions with continuous point evaluations.

Corollary 1.13. *The spaces $\mathcal{H}_\lambda$ defined above are the natives spaces of the corresponding Mercer kernels.*

Example (Trigometric polynomials)**.** *Consider the space of trigometric polynomials* $\frac{1}{\sqrt{2}}, \cos(nx), \sin(nx), n \in \mathbb{N}$ *which are* ***orthonormal*** *in the inner product*

$$\langle f, g \rangle = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t)g(t)dt.$$

With $I = (0,0) \cup (\mathbb{N}, 0) \cup (0, \mathbb{N})$

$$\varphi_i(x) = \begin{cases} \frac{1}{\sqrt{2}} & i = (0,0) \\ \cos(nx) & i = (n,0), n \geq 1 \\ \sin(nx) & i = (n,0), n \geq 1 \end{cases}$$

So for $f \in \mathcal{H}$

$$f = \sum_{i \in I} \langle f, \varphi_i \rangle_{\mathcal{H}} \varphi_i.$$

All φ_i *are uniformly bounded, so the summability condition does hold when the weights are summable.*
Fixing some $m \geq 1$*, we define*

$$\lambda_i = \begin{cases} 1 & i = (0,0) \\ n^{-2m} & otherwise \end{cases}$$

We set the Mercer kernel

$$k_{2m}(x,y) \coloneqq \frac{1}{\sqrt{2}} + \sum_{n=1}^{\infty} n^{-2m} (\cos(nx)\cos(ny) + \sin(nx)\sin(ny))$$

this can also be tought of as an ***extension kernel***

This can be rewritten with the usual trigonometric rules

One can see $K''_{2m} = K_{2m-2}$*, so* $K_2 m$ *piecewise polynomial of degree* $2m$*, which is* $2m-2$ *times differentiable.*

1.2.1 Kernels for subspaces

Let us fix a nonempty set $X \subset \Omega$ and look at the closed subspace

$$\mathcal{H}_X \coloneqq \overline{\text{span}\{k(x,\cdot) | x \in X\}} \subseteq \mathcal{H}$$

Projector for $\mathcal{H}$ to the closed subspace $\mathcal{H}_0$: $\pi_0 : \mathcal{H} \to \mathcal{H}_0$ with properties

This is NOT $\{\mathcal{H}_0\}$, but a generic subspace

- $\pi_0^2 = \pi_0$
- π_0 gives unique best approximation in $\mathcal{H}_0$, $u \mapsto u_0$
- $u_0 \perp u - u_0$
- $\text{Id} - \pi_0$ projects onto the orthogonal complement $\mathcal{H}_0^{\perp} = \{u \in \mathcal{H} \mid \langle u, v \rangle_{\mathcal{H}} \forall v \in \mathcal{H}_0\}$
- $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_0^{\perp}$

Theorem 1.14. *Let* $\mathcal{H}_0$ *be a closed subspace of* $\mathcal{H}$ *with reproducing kernel* k_0 *and let* $\pi_0 : \mathcal{H} \to \mathcal{H}_0$ *be the projection onto* $\mathcal{H}_0$*.*
The subspace kernel is

$$k_0(x,\cdot) = \pi_0 k(x,\cdot)$$

for all $x \in \Omega$*. The reproducing kernel for the orthogonal complement* $\mathcal{H}_0^{\perp}$ *is* $k - k_0$*.*

Proof. $\text{Id} = \pi_0 + (\text{Id} - \pi_0) = \pi_0 + \pi_0^{\perp}$.
Thus $f(x) = (\pi_0 \circ f)(x) + (\pi_0^{\perp} \circ f)(x)$ inserted into the reproducing equation

$$\begin{aligned} f(x) &= \langle f, k(x,\cdot) \rangle_{\mathcal{H}} \\ &= \langle \pi_0 f + \pi_0^{\perp} f, \pi_0 k(x,\cdot) + \pi_0^{\perp} k(x,\cdot) \rangle_{\mathcal{H}} \\ &= \langle \pi_0 f, \pi_0 k(x,\cdot) \rangle + \langle \pi_0^{\perp} f, \pi_0^{\perp} k(x,\cdot) \rangle \end{aligned}$$

Using $f \in \mathcal{H}_0$ and $f \in \mathcal{H}_0^\perp$ eliminates on part of the sum each and the statements follow. □

Remark. *Orthogonal space decompositions correspond to additive kernel decompositions using the appropriate projections.*

Theorem 1.15. *Let $X \subseteq \Omega$ be nonempty. For the closed subspace $\mathcal{H}_X$ it holds*

$$\mathcal{H}_X^\perp = \{f \mid f \in \mathcal{H} : f(X) = \{0\}\}.$$

This is a statement we would expect for our later use case of approximation and interpolation

Proof. If $f(X) = \{0\}$, then $\langle f, v\rangle_\mathcal{H} = 0 \forall v \in \mathcal{H}_X$.

$$f(x) = \langle f, k(x, \cdot)\rangle_\mathcal{H}$$

since $f \in \mathcal{H}_X^\perp$ by the reproduction equation and conversely we set for $f \in \mathcal{H}_X^\perp$ that $f(X) = \{0\}$. □

With π_X the projector from $\mathcal{H}$ to $\mathcal{H}_X$ we denote

$$f_X \coloneqq \pi_X(f).$$

Standard results from Hilbert space theory gives us

Theorem 1.16. *Each function $f \in \mathcal{H}$ has an orthogonal decomposition*

$$f = f_X + f_{X^\perp}$$

with $f_X \in \mathcal{H}_X$ and $f_{X^\perp} \in \mathcal{H}_X^\perp$. In particular each $f \in \mathcal{H}$ has an interpolant $f_X \in \mathcal{H}_X$ recovering the values of f on X. Additionally

$$\|f - f_X\|_\mathcal{H} = \inf_{g \in \mathcal{H}_X} \|f - g\|_\mathcal{H}$$

and

$$\|f_X\|_\mathcal{H} = \inf_{\substack{g \in \mathcal{H}: \\ f(x)=g(x) \\ \forall x \in X}} \|g\|_\mathcal{H} = \inf_{v \in \mathcal{H}_{X^\perp}} \|f - v\|_\mathcal{H}$$

Corollary 1.17. *The interpolant $f_X \in \mathcal{H}_X$ to a function f on X is at the same time the best approximation to f from all functions in $\mathcal{H}_X$.*

This is just the previous theorem in words

Corollary 1.18. *The interpolant $f_X \in \mathcal{H}_X$ to a function f on X minimizes the norm under all interpolants from the full space $\mathcal{H}$.*

This property is usefull, if the norm encodes smoothness as well. Penalizing unnecessary changes of the function

Corollary 1.19. *For all sets $X \subseteq Y \subseteq \Omega$ and $f \in \mathcal{H}$ we have*

$$\|f_X\|_\mathcal{H} \leq \|f_Y\|_\mathcal{H} \leq \|f\|_\mathcal{H}$$

and

$$\|f\|_\mathcal{H} \geq \|f - f_X\|_\mathcal{H} \geq \|f - f_y\|_\mathcal{H}$$

where for completeness we define $f_\emptyset = 0, f_{\emptyset^\perp} = f$ and $\mathcal{H}_\emptyset = \{0\}$ with $\mathcal{H}_{\emptyset^\perp} = \mathcal{H}$.

Consider only $f(\cdot) = k(x, \cdot)$ for a fixed $f, x \in \Omega$.

Start of lecture 05 (23.04.24)

Definition 1.20. *The function*

$$P_X(x) \coloneqq \|k(x, \cdot) - k_X(x, \cdot)\|_\mathcal{H} \qquad x \in \Omega$$

*is called **power function** w.r.t. the set X and the kernel k.*
*A different definition goes with the **error functional** $\epsilon_{X,x} \in \mathcal{H}^*$*

$$\epsilon_{X,x} f \mapsto f(x) - (\Pi_X(f))(x).$$

The power function is then defined as $P_X(x) \coloneqq \|\epsilon_{X,x}\|_{\mathcal{H}^*}$.

Theorem 1.21. *The two definitions for the power function are equivalent. P_X has the following properties*

1. $P_X(x) = 0 \ \forall x \in X$
2. $P_\emptyset(x)^2 = k(x,x) \ \forall x \in \Omega$
3. $P_\Omega(x) = 0 \ \forall x \in \Omega$
4. $0 = P_\Omega(x) \leq P_Y(x) \leq P_X(x) \leq P_\emptyset(x)$ *for* $X \subseteq Y \subseteq \Omega$
5. $P_X(x) = \inf_{g \in \mathcal{H}_X} \|k(x,\cdot) - g\|_\mathcal{H}$
6. $P_X(x) = \sup_{f \in \mathcal{H}, \|f\|_\mathcal{H} \leq 1, f(X) = \{0\}} f(x) \ \forall x \in \Omega$
7. $\forall x \in \Omega, f \in \mathcal{H}$

$$|f(x) - f_X(x)| = |f_X^\perp(x)| \leq P_X(x)\|f_X^\perp(x)\|_\mathcal{H} = P_X(x)\|f - f_X\|_\mathcal{H} \leq P_X(x)\|f\|_\mathcal{H}$$

Added remark. *General approximation goal: Split the approximation error into an error of the space and an error of the function (similarly to SC1).*
One aim is to generalize 7. to not rely on a specific point.

Proof. Due to $\langle \epsilon_{X,x}, \epsilon_{X,x} \rangle_{\mathcal{H}^*} = \langle R(\epsilon_{X,x}), R(\epsilon_{X,x}) \rangle_\mathcal{H}$ we have to show that the Riesz representer of $\delta_x \circ \Pi_X$ is $K_X(x,\cdot)$.

$$\begin{aligned}
\langle f, R(\delta_x \circ \Pi_X) \rangle &= \delta_x \circ \Pi_X(f) = f_X(x) = \langle f_X, k(x,\cdot) \rangle_\mathcal{H} \\
&= \langle f_X, k_X(x,\cdot) + k_{X^\perp}(x,\cdot) \rangle_\mathcal{H} \\
&\overset{f_X \perp K_{X^\perp}}{=} \langle f_X, k_X(x,\cdot) \rangle_\mathcal{H} = \langle f - f_{X^\perp}, k_X(x,\cdot) \rangle_\mathcal{H} \\
&\overset{f_{X^\perp} \perp K_X}{=} \langle f, k_X(x,\cdot) \rangle_\mathcal{H}
\end{aligned}$$

Proof of 7.:

$$\begin{aligned}
f(x) - f_X(x) = f_{X^\perp}(x) &= \langle f_{X^\perp}, k(x,\cdot) \rangle_\mathcal{H} \\
&= \langle f_{X^\perp}, k(x,\cdot) - \underbrace{k_X(x,\cdot)}_{f_{X^\perp} \perp} k_X(x,\cdot) \rangle \\
&\overset{\text{C.S.}}{\leq} \cdots = \|f_{X^\perp}\| \mathcal{H} P_X(x)
\end{aligned}$$

Proof of 6.:
We see from the first inequality

$$P_X(x) \geq \sup_{\|f_{X^\perp}\|_\mathcal{H} \leq 1} |f_{X^\perp}(x)|$$

and equality must hold for the representer of $\epsilon_{X,x}$. □

Notice the connection to operator norm approaches to 6.

Remark. *Consider the subspace* $\mathcal{H}_X^* = \overline{span\{\delta_x \mid x \in X\}}$ *of the dual space of* $\mathcal{H}$. *Then* 5. *can equivalently be given as*

$$P_X(x) = \inf_{\lambda \in \mathcal{H}_X^*} \|\delta_x\|_{\mathcal{H}^\perp} \tag{4}$$

Consider the interpolation of $f(x) = k(x,\cdot) \in \mathcal{H}$.
For $x \in \Omega$ we get for the interpolant in $\mathcal{H}_X$

$$k(x_k, x) = \sum_{j=1}^{N} u_j(x) k(x_j, x_k) \qquad 1 \leq k \leq N \tag{5}$$

which has solution coefficients $u_j(x)$ as a function on Ω.

Added remark. *If the kernel matrix is invertible, u_j is either 0 or 1. See Lagrange interpolation? In our setting it is enough to know that it exists, but might not be unique.*

Theorem 1.22. *If the kernel matrix is non-singular the u_j from 4 are $\in \mathcal{H}_X$ and there is a Lagrange basis $u_j(x_k) = \delta_{jk}, 1 \leq j, k \leq N$.*
In general it still holds

$$f_X(x) = \sum_{j=1}^{N} u_j(x) f(x_j)$$

In the formula the influence of X and f are separated.

This is sometimes called quasi-interpolation

Proof. The first statement follows from 5. From the second:

$$\begin{aligned} f_X(x) &= \sum_{k=1}^{N} a_k k(x_k, x) \\ &= \sum_{k=1}^{N} a_k \sum_{j=1}^{N} u_j(x) k(x_j, x_k) \\ &= \sum_{j=1}^{N} a_j(x) \underbrace{\sum_{k=1}^{N} a_k k(x_j, x_k)}_{= f_{a,X} = f(x_j) \forall x_j \in X} = \sum_{j=1}^{N} u_j(x) f(x_j) \end{aligned}$$

□

Theorem 1.23. *The power function has the following explicit representation:*

$$P_X(x) = k(x,x) - 2\sum_{j=1}^{N} u_j(x) k(x_j, x) + \sum_{j=1}^{N}\sum_{k=1}^{N} u_j(x) u_k(x) k(x_j, x_k) = k(x,x) - k_X(x,x)$$

Proof. For $K_X \in \mathcal{H}_X$ $k_X(x,z) = \sum_{j=1}^{N} u_j(x) k(x_j, z)$

$$\begin{aligned} P_X^2(x) &= \langle k(x,\cdot) - k_X(x,\cdot), k(x,\cdot) - k_X(x,\cdot) \rangle_{\mathcal{H}} \\ &= k(x,x) - 2\langle k(x,\cdot), \sum_{j=1}^{N} u_j(x) k(x_j,\cdot) \rangle_{\mathcal{H}} + \sum_{j=1}^{N} \underbrace{\sum_{k=1}^{N}}_{a} u_j(x) \underbrace{u_k(x) k(x_j, x_k)}_{\text{with a } = k(x, x_j)} \\ &= k(x,x) - \underbrace{\sum_{j=1}^{N} u_j(x) k(x_j, x)}_{k_X(x,x)} \end{aligned}$$

□

Consider $f_X(x) = \sum_{j=1}^{N} u_j(x) f(x_j)$ the interpolant on X.
Let us also consider arbitrary estimation formulas

$$(x, f) \mapsto \sum_{j=1}^{N} v_j(x) f(x_j)$$

with no assumptions on the scalars v_j. For fixed x we get for the error functional
$f \mapsto f(x) - \sum_{j=1}^{N} v_j(x) f(x_j) = \left(\delta_x \sum_{j=1}^{N} v_j(x) \delta_{x_j}\right)(f)$.
Ad for optimal estimation for all $f \in \mathcal{H}$, we should choose v_j to minimize the following expression:

$$V_{X,v}(x) \coloneqq \|\delta_x - \sum_{j=1}^{N} v_j(x) \delta_{x_j}\|_{\mathcal{H}^*}.$$

Remember the dual form of the fifth property 4:

$$P_X(x) = \inf_{\lambda \in \mathcal{H}^*} \|\delta_x - \lambda\|_{\mathcal{H}^*}$$

we also saw that the function u_j are the solution.
We also see that the optimal error, in the worst case sense, is described to be the power function.

Theorem 1.24. *In the above sense, kernel based approximation yields the best linear estimation of unknown function values $f(x)$ from known function values $f(x_j)$ at points x_j.*

Start of lecture 06 (25.04.24)

$$k(s,t) = \operatorname{cov}(X_s, X_t)$$

The kernel comes from a covariance, where for every t in some Ω, we have a random variable with finite second moments.
Consider X_t with zero mean. In this case, what we did is called **(simple) Krigihs** connection to geo-statistics!
$V^2_{X,v}(x)$ can be understood as the variance of the prediction error.
Now define the error of some general linear predictor at x

$$\mathcal{E}_{X,V,x} \coloneqq X_x - \sum_{j=1}^{n} V_j(x) X_{x_j}$$

Statistics pov: This is an ubiased estimator

$$\begin{aligned}
\mathbb{E}(\mathcal{E}^2_{X,V,x}) &= \underbrace{\operatorname{cov}}_{=k}(X_x, X_x) - 2\sum_{j=1}^{N} V_j(x)\operatorname{cov}(X_x, X_{x_j}) + \sum_{j=1}^{N}\sum_{k=1}^{N} v_j(x)v_k(x)\operatorname{cov}(X_{x_j}, X_{x_k}) \\
&= \langle \delta_x, \delta_x\rangle_{\mathcal{H}^*} - 2\sum_{j=1}^{N} v_j \langle \delta_x, \delta_{x_j}\rangle_{\mathcal{H}^*} + \sum_{j=1}^{N}\sum_{k=1}^{N} v_j(x)v_k(x)\langle \delta_{x_j}, \delta_{x_k}\rangle_{\mathcal{H}^*} \\
&= V^2_{X,v}(x)
\end{aligned}$$

Short revision of the condition number:

$$\kappa(A) = \frac{|\lambda_{\max}(A)|}{|\lambda_{\min}(A)|}$$
$$Ax = b \frac{\Delta x}{|x|} \leq \kappa(A)\frac{|\Delta b|}{|b|}$$

Power function and stability

There is an uncertainty principle (Schabach 1995):
It is impossible to make the power function and the condition number of the kernel matrix small at the same time.
To make this precise: enrich $X = \{x_1, \dots, x_n\}$ with another point $X_0 = x$ and define $u_0(\cdot) = -1$

We can somehow fix this via regularisation, which in this case is both usefull numerically and meaningful from a statistics point of view

$$A = k(x_j, x_k)_{0 \leq j,k \leq N}$$

$$\begin{aligned}
u^\perp A u &= \sum_{j=0}^{N}\sum_{k=0}^{N} u_j(x)u_k(x)k(x_j, x_k) \\
&\overset{u_0 = -1}{=} k(x,x) - 2\sum_{j=1}^{N} u_j(x)k(x, x_j) + 2\sum_{j=1}^{N}\sum_{k=1}^{N} u_j(x)u_k(x)k(x_j, x_k) \\
&\overset{\text{thm. } 1.23}{=} P^2_X(x)
\end{aligned}$$

A has $n+1$ non-negative real eigenvalues $\lambda_0 \geq \lambda_1 \geq \dots \geq \lambda_N \geq 0$.

$$\lambda_N \|u\|_2^2 \leq u^\perp A u \leq \lambda_0 \|u\|_2^2$$

gives

$$P^2_X(x) \geq \lambda_N \left(1 + \sum_{j=1}^{N} |u_j(x)|^2\right) \geq \lambda_N$$

Elimination of the special value of the point x gives

Theorem 1.25. *The kernel matrix for N points $\{x_1, \dots, x_n\} = X$ has a smallest eigenvalue λ bounded from above by*

$$\lambda \leq \min_{1 \leq j \leq N} P^2_{X \setminus \{x_j\}}$$

This holds for every $x \in \Omega$

Back to approximation

$$|f(x) - f_X(x)| \leq |P_X(x)| \|f\|_{\mathcal{H}}$$

Assume that any directional derivative of both f and f_X is bounded by some C:

$$|f(x) - f_X(x)| \leq \underbrace{|f(x_j) - f_X(x_j)|}_{=0} + 2C\|x - x_j\|_2 \leq 2Ch_{X,\Omega}$$

if the connecting line between x and x_j is in Ω

Definition 1.26. *The **fill distance** of a set of points $X \subseteq \Omega$ for a bounded Ω is defined to be*

$$h_{X,\Omega} = \sup_{x \in \Omega} \min_{1 \leq j \leq N} \|x - x_j\|_2$$

How large are the holes in Ω such that we don't hit an $x \in X$. It describes the size of the largest data free domain

To get bounds on the optimal approximation, we can consider some functions $v_0, \dots, v_N$ instead of the optimal u_j.

$$P^2_X(x) \leq k(x,x) - 2\sum_{j=1}^{N} v_j(x)k(x_j,x) + \sum_{j=1}^{N}\sum_{k=1}^{N} v_j(x)v_k(x)k(x_j,x_k) \tag{6}$$

The simplest case uses nearest neighbor reconstruction.
Assume that for each $x \in \Omega$ we pick a $x_{nn(x)}$ and define

$$v_j(x) = \begin{cases} 1 & j = nn(x) \\ 0 & \text{else} \end{cases}$$

Then

$$P^2_X(x) \leq k(x,x) - 2k(x_{nn(x)}, x + k(x_{nn(x)}, x_{nn(x)}))$$
$$(7)\ d_k((x, x_{nn(x)}))^2 = \text{dist}(x, x_{nn(x)})^2$$

Theorem 1.27. *For k positive semi-definite the power function on non-empty sets X of interpolation points satisfies*

$$p^2_X(x) \leq \min_{x_j \in X} d_k(x, x_j)$$

with d_k as in (7).

Assume that we can prove $P_X(x) \leq CE(x,h)$ for all data sets X with fill distance h.
This implies (by theorem 1.21)

$$|f(x) - \sum_{j=1}^{N} u_j(x)f(x_j)| \leq CE(x,h)\|f\|_{\mathcal{H}}$$

We know introduce the error operator

$$E^y_x(f(y)) \coloneqq f(x) - \sum_{j=1}^{N} v_j(x)f(x_j)$$

This simplifies the notation, once one understands what is happening :)

to set

$$P^2_X(x) \leq (6) = k(x,x) + \sum_{j=1}^{N} v_j(x)\left(\sum_{k=1}^{N} v_k(x)k(x_j,x_k) - k(x_j,x)\right)$$
$$= E^z_x(k(z,x)) - \sum_{j=1}^{N} v_j(x)E^z_x(k(z,x_j))$$
$$= E^y_x E^z_x(k(z,y))$$

We are after a bound such as

$$|E_x^y(f(y))| = \left| f(x) - \sum_{j=1}^{N} v_j(x) f(x_j) \right| \leq \mathcal{E}_{X,k}(h) \|Lf\|$$

We then bound the power function by

$$P_X^2(x)\, |E_x^y E_x^z k(z,y)| \leq \mathcal{E}_{x,k}(h) \|L^y E_x^z k(z,y)\| \leq \mathcal{E}_{X,k}^2 \|L^y\| \|L^z k(y,z)\|$$

assume the final expression makes sense.
First, univariate case, $\Omega = [a,b]$, $X = \{x_1, \ldots, x_n\} \subset \Omega$. For a given $x \in \Omega$

Start of lecture 07 (30.04.24)

$$X_x = \{x_j \in X \mid j \in N(x) \subseteq \{1, \ldots, N\}\}$$

$f \in C^k$, Taylor polynomial at x_0

$$p(x) = \sum_{j=0}^{k-1} \frac{f^{(j)}(x_0)}{j!} (x - x_0)^j$$

for $|x - x_0| \leq h$ we have the local approximation error

$$|f(x) - p(x)| = \frac{|f^{(k)}|}{n!} |x - x_0|^k \leq C(f) h^k$$

This approximation error holds for approximation which recovers polynomials locally!

From formula for interpolation in Newton form

$$f(x) - p_X(x) = [x, X_x] f \prod_{x_j \in X_x} (x - x_j) \forall x \in [a,b]$$
$$\leq \frac{\|f^{(k)}\|_{\infty,[a,b]}}{k!} \underbrace{\prod_{x_j \in X_x} (x - x_j)}_{\leq C h^k}$$

We can now use this to bound

If we are careful, we can controll the constant C above!

$$p_X^2(x) \leq (Ch^k)^2 \sup_{a \leq z \leq b} \sup_{a \leq y \leq b} \left| \frac{\partial^k}{\partial z^k} \frac{\partial^k}{\partial y^k} k(a,b) \right|$$

Theorem 1.28. *Assume a psd kernel k on $[a,b]$ that is k times differentiable. Then for every point set $X \subset [a,b]$ of at least k points with fill distance at most h the power function can be bounded*

$$P_X(x) \leq C_k h^k \tag{7}$$

with C_k depending on k and X.

Definition 1.29. *A compact domain $\Omega \subset \mathbb{R}^d$ allows* ***uniformly stable local polynomial reproduction*** *of order $l \geq 1$, if there are positive constants c_1, c_2, h_0, s.t. for all finite sets of points $X := \{x_1, \ldots, x_n\}$ with fill distance $h_{X,\Omega} \leq h_0$ there are scalar functions $u_1(x), \ldots, x_N(x)$ s.t.*

1. $$\sum_{j=1}^{N} u_j(x) p(x_j) = p(x)$$
   for all polynomials $p \in \mathcal{P}_l^d$ and $x \in \Omega$.
2. $\sum_{j=1}^{N} |u_j(x)| \leq c_1$
3. $u_j(x) = 0$ *if* $\|x - x_j\|_2 > C_s h_{X,\Omega}$.

Added remark. *We will only handle positive definite kernels, the results generalizes for psd kernels with additional conditions on the kernel.*

We know focus on positive definite kernels.

Theorem 1.30. *Let $\Omega \subset \mathbb{R}^d$ and let $k : \Omega \to \Omega$ be a p.d. kernel. Let X be a set of N distinct points of Ω and define the quadratic form $\Omega : \mathbb{R}^n \to \mathbb{R}$ for any $x \in \Omega$ (see 1.23)*

$$Q(u) = k(x,x) - 2\sum_{j=1}^{N} a_j(x,x_j) + \sum_{j=1}^{N}\sum_{k=1}^{N} u_j u_k k(x_k,x_j)$$

The min of $Q(u)$ is given for the vector from 2.3 denoted as u^* with $u_j^*(x_k) = \delta_{jk}$ and we have

$$Q(u^*(x)) \leq Q(u)$$

Proof. With $b = [k(x,\cdot),\dots,k(x_k,\cdot)]^\perp$ and $A_{i,j} = k(x_i,x_j)$, $i,j = 1,\dots,N$ we have

$$Q(u) = k(x,x) - 2b^\perp(x)u + u^\perp Au.$$

The min is the solution of $Au = b$

Remark. *in the positive definite setup only!, which is fullfilled by $u = u^*(x)$.* □

Theorem 1.31. *Assume $\Omega \subseteq \mathbb{R}^d$ bounded and satisfies an interior cone condition. Suppose $k \in C^{2k}(\Omega \times \Omega)$ is a symmetric positive definite kernel with native space $\mathcal{H}$. Let f_X be the interpolant to $f \in \mathcal{H}$ on the set $X = \{x_1,\dots,x_n\}$. Then there are positive constants h_0, C (independent of x, f, k) s.t.*

$$|f(x) - f_X(x)| \leq C h_{X,\Omega}^k \sqrt{C_k(x)} \|f\|_{\mathcal{H}}$$

provided $h_{X,\Omega} \leq C h_0$. Here

$$C_k(x) = \max_{|\beta|=2k} \sup_{x,y \in \Omega \cap B(x, C_2 h_{X,\Omega})} \left| D_2^\beta (k(x,y)) \right|$$

First some further notation:
For $\beta = (\beta_1,\dots,\beta_d) \in \mathbb{N}_0^d$ we define

$$D^\beta = \frac{\partial^{|\beta|}}{(\partial x_1)^{\beta_1} \cdot \dots \cdot (\partial x_d)^{\beta_d}}$$

with D_2^β we indicate that D^β is applied to $k(x,\cdot)$. Multivariate Taylor expansion of $k(x,\cdot)$ centered at x:

$$k(x,y) = \underbrace{\sum_{|\beta|<2l} \frac{D_2^\beta k(x,x)}{\beta!}(y-x)^\beta}_{\sum_\beta T(x,\beta)} + R(x,y)$$

$$R(x,y) = \sum_{|\beta|=2l} \frac{D_2^\beta k(x,\xi_{x,y})}{\beta}(y-x)^\beta$$

where $\xi_{x,y}$ lines on the line connecting x, y.

Proof. Theorem 1.21 $|f(x) - f_X(x)| \leq P_X(x)\|f\|_{\mathcal{H}}$. We know $P_X^2(x) = Q(u^*(x))$. Given the interior cone condition, we can obtain a $u(x)$ that has polynomial precision of degree $l \geq 2k-1$. For those u we see

$$P_X^2(x) \leq Q(u) = k(x,x) - 2\sum_{k=1}^{N} u_k(x,x_k) + \sum_{j=1}^{N}\sum_{k=1}^{N} u_j u_k k(x_j,x_k)$$

Apply Taylor expansion centered at x to $K(x,\cdot)$ and centered at x_j to $k(x_j,\cdot)$

$$Q(u) = k(x,x) - 2\sum_{k=1}^{N} u_K \left[\sum T(x,\beta)(x_k - x)^\beta + R(x,x_k)\right] + \sum_{j=1}^{N}\sum_{k=1}^{N} u_j u_k \left[\sum T(x_j,\beta)(x_k - x_j)^\beta R(x_j,x_k)\right]$$

We identify $p(z) = (z-x)^\beta$, so that $p(x) = 0$ unless $\beta = 0$.
With the polynomial reproduction of u, this simplifies to

$$Q(u) = k(x,x) - \underbrace{2k(x,x)}_{\beta=0} - 2\sum_{k=1}^{N} u_k R(x,x_k) + \sum_{j=1}^{N} u_j \sum T(x_j,\beta)(x - x_j)^\beta + \sum_{j=1}^{N}\sum_{k=1}^{N} u_j u_k R(x_j,x_k)$$

Look at Taylor expansion

$$\sum T(x_j,\beta)(x - x_j)^\beta = k(x_j,x) - R(x_j,x)$$

This gives

$$Q(u) = k(x,x) - \sum_k u_k \left[2R(x,x_k) - \sum_{j=1}^{N} u_j R(x_j,x_k)\right] + \sum_{j=1}^{N} u_j \left[k(x_j,x) - R(x_j,x)\right]$$

Once more Taylor: $k(x_j,x) = k(x,x_j) = \sum_\beta T(x,\beta)(x_x - x)^\beta + R(x,x_j)$

$$= 0 - \sum_k u_k \left[R(x,x_k) - \sum_{j=1}^{N} u_j R(x_j,x_k) + R(x_k,x)\right]$$

The polynomial reproduction gives uniform stability

$$\sum_k |u_k| \le C_1$$

For $u_j \neq 0$ (with 3.) we have $\|x - x_j\|_2 \le C_2 h_{X,\Omega}$ and it holds $\|x_j - x_k\| \le 2C_2 h_{X,\Omega}$. Thereby all three can be bounded by an expression such as $C h_{X,\Omega}^{2k} C_k(x)$.
The interior cone condition shows that the ball remains inside, so that $C_k(x)$ is well defined.
Combining these bounds and taking the square root gives the bound for the power function. □

Other interesting functionals:
Derivatives: $\lambda(f) = \frac{\partial f}{\partial x_j}(x)$
Integration: $\lambda(f) = \int_\Omega f(y)dy$
Consider $\Lambda \subseteq \mathcal{H}^*$ that generalizes the role of the point set X and the associated δ_{x_i}.

Start of lecture 08 (2025-04-10). This is what we will focus on for now. This yields quasi monte carlo integration

$$\{(x_i, \lambda_i f)\}_{i=1}^N$$

more general data instead of $\{(x_i, f(x_i))\}$.
Dirichlet boundary value problem :

$$\begin{aligned} Lu &= f \quad \text{on } \Omega \subset \mathbb{R}^d \\ u &= g \quad \text{on } \partial\Omega \end{aligned} \tag{8}$$

with L a linear differential operator.
Collocation is a general approach that discretizes this by
The exact solution u^* of 8 solves **??**.
Consider $U \subseteq \mathcal{H}$ of dimension at least N. Let $u \in U$.
Assume $\lambda_i \in \mathcal{H}^*$ of the form $\lambda_i = \delta_{x_i} \circ D^{\alpha(i)}$. Further assume that $\alpha(i) \neq \alpha(k)$ if $x_i = x_k$.
Then the λ_i are linearly independent on the native space of a p.d. kernel(Compare: Wendland).
We can proceed via **Hermite interpolation**. We assume $\{(x_i, \lambda_i f)\}_{i=1}^N, x_j \in \Omega, \lambda_j \in \Lambda$ with $\Lambda = \{\lambda_1, \ldots, \lambda_n\}$ linearly independent set of continuous linear functionals.

$$u(x) = \sum_{j=1}^{N} a_j \lambda_j^{(j)} k(x_j, x) \quad x \in \mathbb{R}^d$$

that satisfies

$$\lambda_j u = \lambda_j f \quad j = 1, \dots, N \quad f \in \mathcal{H}$$

$\lambda_i^{(1)}$ indicates that the functional acts on the first argument of k.
The LES has entries $A_{jk} \lambda_j^{(2)} \lambda_k^{(1)} k(x_k, x_j)$ for $j, k = 1, \dots, N$.

Example. *Denote the centers of radial basis functions (RBFs) by ξ_j and denote the data location $\underline{x_j}$. Given*

$$\{(\underline{x_j}, f(\underline{x_j}))\}_{i=1}^{p}$$

and

$$\{(\underline{x_j}, \frac{\partial f}{\partial x})(\underline{x_j})_{j=p+1}^{N}\}$$

Thus

$$\lambda_j = \begin{cases} \delta_{\underline{x_j}} & j = 1, \dots, p \\ \delta_{\underline{x_j}} \frac{\partial}{\partial x} & j = p+1, \dots, N \end{cases}$$

with $k(\underline{x_j}, \underline{x_k}) = \varphi(\|\underline{x_j} - \underline{x_k}\|)$

$$\begin{aligned} u(\underline{x}) = \sum_{j=1}^{N} a_j k(\cdot, \underline{x}) \quad &= \textstyle\sum_{j=1}^{p} a_j k(\cdot, \underline{x}) + \sum_{j=p+1}^{N} a_j \frac{\partial}{\partial \xi_1} k(\xi, \underline{x}) \\ &= \textstyle\sum_{j=1}^{N} a_j k(\xi_j, \underline{x}) - \sum_{j=p+1}^{N} a_j \frac{\partial}{\partial x} k(\xi_j, \underline{x}) \end{aligned}$$

since system matrix after ... u into $\lambda_j u = \lambda_j f$

$$\begin{bmatrix} K & K_\xi \\ K_x & K_{xx} \end{bmatrix}$$

with $K_{jk} = K(\xi_k, x_j) = \varphi(\|\xi_k - x_j\|)$ and

$$\begin{aligned} K_{\xi,jk} &= \frac{\partial \varphi}{\partial \xi} \varphi(\|\xi_k - x_j\|) = -\frac{\partial \varphi}{\partial x}(\|\xi_k - x_j\|) \\ K_{x,jk} &= \frac{\partial \varphi}{\partial x}(\|\xi_k, x_j\|) \\ K_{xx,jk} &= \frac{\partial^2 \varphi}{\partial x^2}(\|\xi_k, x_j) \end{aligned}$$

$\underline{x_j}$ is the multiindex, x is the first entry: $\underline{x_j} = (x, y)$

CAREFUL: In this calculation a lot of stuff (everything with a non-constant index?) should have an underline? He added them inconsistently and often corrected himself, so I couldn't keep up.

Added remark. *We can do everything we did, but replacing point evaluations with point evaluations of (weak) derivatives to get a similar theory weak derivatives, without relying on point evaluations.*

To measure errors we use generalized power functions

$$P_\Lambda(\mu) = \|\mu_\mu \circ \Pi_\Lambda\|_{\mathcal{H}^*}$$

where we use $\mu \in \mathcal{H}^*$ to measure the error instead of point evaluation functionals

$$\mu(f - f_\lambda) = (\mu - \mu \circ \Pi_\Lambda) f.$$

$$\begin{aligned} Lu &= f \quad \Omega \subseteq \mathbb{R}^d \\ u &= g \quad \gamma = \partial\Omega \end{aligned}$$

with kernel based collocation method.
We use

$$u(x) = \underbrace{\sum_{j=1}^{p} a_j k(x_j, x)}_{\text{boundary } B} + \underbrace{\sum_{j=p+1}^{N} a_j L^{(1)} k(x_j, x)}_{\text{interior } I} \tag{9}$$

$X = B \cup I$.
We get a block matrix

$$A = \begin{bmatrix} K & L^{(1)}K \\ L^{(2)}K & L^{(2)}L^{(1)}K \end{bmatrix}$$

where $Au = \begin{bmatrix} g \\ f \end{bmatrix}$.
with

$$\begin{aligned} K_{j,k} &= k(x_j, x_k) && x_j, x_k \in B \\ L^{(1)}K_{j,k} &= L^{(1)}K(\tilde{x}_k, x_j) && x_j \in B \tilde{x}_k \in I \\ L^{(2)}K_{j,k} &= L^{(1)}K(x_k, \tilde{x}_j) && x_k \in B \tilde{x}_j \in I \\ L^{(2)}L^{(1)}K_{j,k} &= L^{(2)}L^{(1)}K(\tilde{x}_k, \tilde{x}_j) && \tilde{x}_j, \tilde{x}_k \in U \end{aligned}$$

Same structure as for Hermite interpolation: Non-singular if $\delta_{x_i} K, LK$ are linearly independent holds for suitable K.

Theorem 1.32. *Let $\Omega \subseteq \mathbb{R}^d$ be a polygonal and open domain. Let L be a second order elliptic differential operator with coefficients ch $C^{2(k-2)}(\bar{\Omega})$ that either vanishes on $\partial\Omega$ or have no zero here.*
Suppose that $k \in C^{2k}(\mathbb{R}^d \times \mathbb{R}^d)$ is a positive definite kernel. Assume that $Lu = f$ in the system 8 has a unique solution $u \in \mathcal{N}_k(\Omega)$ for some $f \in C(\Omega, g \in C(\Gamma))$. Let $\hat{u}$ be the approximation 10. Then

$$\|u - \hat{u}\|_{L_\infty(\Omega)} \leq C h_{I,\Omega}^{k-2} \|u\|_{\mathcal{N}_k(\Omega)}$$

and

$$\|u - \hat{u}\|_{L_\infty(\partial\Omega)} \leq C h_{B,\partial\Omega}^{k} \|u\|_{\mathcal{N}_k}$$

Sketch of the proof. For interior essentially as before for $L(u) - L\hat{u}$ and LLk is p.d. for p.d. k. □

Start of lecture 09 (07.05.24)

1.3 Kernel Methods for prediction

Added remark. *Statistics: finding structure in the data, while ML tries to use the same math to make predictions*

Start of lecture 10 (14.05.24)

Definition 1.33. *Let Ω, Σ be a measurable space and $Y \subseteq \mathbb{R}$ be a closed subset. Denote by $(x, y, f(x)) \in \Omega \times Y \times \mathbb{R}$ the triplet consisting of **attributes (or features)** x, an **observation** y and a **prediction** y.*
*A function $l : \Omega \times Y \times \mathbb{R} \to [0\infty)$ is called a **loss function** if it is measurable and $l(x, y, y) = 0$ holds for all $x \in \Omega, y \in Y$.*

Example.

- *l_2 loss, which relates to the mean*
- *l_1 loss, which relates to the median*
- $l_H = \begin{cases} \frac{1}{2}\xi^2 & |\xi| \leq \sigma \\ \sigma|\xi| - \frac{1}{2}\sigma^2 & \text{otherwise} \end{cases}$ *hubert loss*

- $l_\epsilon(\xi) = \max(|\xi| - \epsilon, 0) =: |\xi|_\epsilon$ *ϵ-sensitive loss*

Weighting loss functions might be useful to emphasize important data points! For Classification:

- $l(x, y, f(x)) = \begin{cases} 0 & y = f(x) \\ 1 & otherwise \end{cases}$
- $l(x, y, f(x)) = \begin{cases} 0 & y = sgn(f(x)) \\ 1 & otherwise \end{cases}$
- $l(x, y, f(x)) = l_1(1 + \exp(-yf(x)))$ *logistic loss, relates to probability*
- *soft margin / hinge loss* $\max(1 - yf(x), 0)$*, important for SVMs*

much of the past research efforts where focused on SVMs

Added remark. *l_1, l_2 losses penalize overestimation in classification problems, therefore the other losses might be a better idea.*
Both hinge loss and logistic loss functions give a way to rank the data.

Definition 1.34. *Let $l : \Omega \times Y \times \mathbb{R} \to [0, \infty)$ be a loss function and $\mathbb{P}$ be a probability measure on $\Omega \times Y$. Then, for a measurable function $f : \Omega \to \mathbb{R}$, the **expected l-risk** is defined by*

$$R_{l,p}(f) := \int_{\Omega \times Y} l(x, y, f(x)) d\mathbb{P}(x, y) = \int_\Omega \int_Y l(x, y, f(x)) d\mathbb{P}(y|x) d\mathbb{P}_\Omega(x).$$

For a given data set $D := \{x_j, y_j\}_{j=1}^N$ with $x_j \in \Omega, y_j \in Y$ we can define the empirical measure

$$P_{\text{imp}}(x, y) = \frac{1}{N} \delta_{x_j, y_j}$$

Definition 1.35. *The **empirical l-risk** of a function $f_\Omega \to \mathbb{R}$ is defined as*

$$R_{l,emp}(f) = \int_{\Omega \times Y} l(x, y, f(x)) dP_{imp}(x, y) = \frac{1}{N} \sum_{j=1}^N l(x_j, y_j, f(x_j))$$

Added remark. *Regularization via penalty terms or by enforcing some sparsity condition on the α_j.*

We will assume that $R_{l,\text{emp}}(f)$ is continuous on f.

Operator inversion lemma

$$R_{l,\text{reg}}(f) = R_{l,\text{emp}}(f) + \lambda s(f)$$

Here, the smoothness or sparsity is enforced by the regularization term s.
Often s is convex. The regularization parameter λ balances the empirical error and the regularization.

Theorem 1.36 (Representer theorem)**.** *Let $s : [0, \infty) \to \mathbb{R}$ be a strictly monotone increasing function, Ω be a set, $\mathcal{H}$ a RKHS over Ω and let $l : \Omega \times Y \times \mathbb{R}$ he a continuous loss function. Then, for given data $D = \{(x_j, y_j)\}_{j=1}^N, x_j \in \Omega, y_j \in Y$ and $\lambda > 0$, each minimizer $f \in \mathcal{H}$ of the regularized empirical risk*

$$R_{l,reg}(f) = \frac{1}{N} \sum_{j=1}^N l(x_k, y_j, f(x_j)) + \lambda s(\|f\|_{\mathcal{H}})$$

admits a representation $f(x) = \sum_{j=1}^N \alpha_j k(x_j, x)$, that is $f \in \mathcal{H}_X, X = \{x_1, \ldots, x_N\}$.

Proof. w.l.o.g. we assume $s(\|f\|_{\mathcal{H}}) = \overline{s}(\|f\|_{\mathcal{H}})$.
We decompose any $f \in \mathcal{H}$ into $f_X \in \mathcal{H}_X$ and $f_{X^\perp} \in \mathcal{H}_{X^\perp}$ (Theorem 1.16)

$$f = f_X + f_{X^\perp} = \sum_{j=1}^N \alpha_j k(x_j, x) + f(x)_{X^\perp}$$

We know

$$\langle f_{X^\perp}, k(x_k, \cdot)\rangle_{\mathcal{H}} = 0$$

with the reproduction equation we write

$$f(x_i) = \langle f, k(x_i, \cdot)\rangle_{\mathcal{H}} = \sum_{j=1}^{N} \alpha_j k(x_i, x_j) + \langle f_{X^\perp}, k(x_i)\rangle_{\mathcal{H}} = \sum_{j=1}^{N} \alpha_j k(x_i, x_j)$$

The loss term part does not depend on $f_{X^\perp}$. Further, for all $f_{X^\perp}$ it holds

$$s(\|f\|_{\mathcal{H}}) = \overline{s}(\|f\|_{\mathcal{H}}^2 + \|f_{X^\perp}\|^2) \geq \overline{s}(\|f_X\|_c H^2)$$

Therefore for any fixed $\alpha \in \mathbb{R}^N$ the objective is minimal if $f_{X^\perp} = 0$. This has to hold for any minimizer f.

□

Remark. *$f + q$, $f \in \mathcal{H}$, $q \in span\{\varphi_p\}$ For this setup a corresponding representer theorem does hold.*

Remark. *If both loss function and s are convex, one has a single minimum.*

Consider regularized least squares regression,

$$R_{l_2,\text{reg}}(f) = \frac{1}{N}\sum_{j=1}^{N}(f(x_j) - y_j)^2 + \frac{\lambda}{2}\|f\|_{\mathcal{H}}^2$$

where $f(x) = \sum_{j=1}^{N} \alpha_j k(x_j, x)$.

$$\frac{1}{N}\sum_{j=1}^{N}\left(\sum_{k=1}^{N}\alpha_k k(x_k, x_j) - y_j\right)^2 + \frac{\lambda}{2}\sum_{j,k=1}^{N}\alpha_j\alpha_k k(x_j, x_k)$$

derivation w.r.t. α_k yields:

$$\frac{2}{N}\sum_{j=1}^{N}\left(\sum_{k=1}^{N}\alpha_k k(x_k, x_j) - y_j\right)k(x_k, x_j) + \frac{\lambda}{2}\sum_{j=1}^{N}\alpha_j(x_j, x_k)$$

All together for all a_k this holds and gives

$$\begin{aligned} 0 &= \frac{2}{N}K(K\alpha - Y) + \frac{\lambda}{2}K\alpha \\ \implies & K(K + \lambda N I)\alpha = KY \\ \implies & (K + \lambda N I)\alpha = Y \end{aligned}$$

In $L^2(\Omega)$ we have $\langle f, g\rangle = \int_\Omega fg dx$. We aim to write $\langle f, g\rangle_{\mathcal{H}} = \langle Sf, Sg\rangle_{L^2(\Omega)} = \int_\Omega Sf(x) \cdot Sg(x) dx$, where S is called a **regularization operator**.

Start of lecture 11 (16.05.24)

Definition 1.37. *A **regularization operator** S is defined as a linear map from the space of functions*

$$\{f \mid f : \Omega \to \mathbb{R}\}$$

into a space D equipped with a scalar product. The regularization term $s(f)$ takes the form

$$s(f) \coloneqq \langle S(f), S(f)\rangle_D.$$

sometimes we multiply $\frac{1}{2}$ to s

Remark. *Since we can always define $\tilde{S} = (S^*S)^{\frac{1}{2}}$ and*

$$\langle f, S^*Sf\rangle_D = \langle Sf, Sf\rangle_D$$

we can assume S is a positive semidefinite (regularization) operator.

Definition 1.38. *Let $k : \Omega \times \Omega \to \mathbb{R}$ be continuous, Ω be a compact domain, ν be a Borel measure and $L_2^\nu(\Omega)$ be the Hilbert space of square integrable functions on Ω.*
*We define the **integral operator** $T_k : L_2^\nu(\Omega) \to L_2^\nu(\Omega)$ by*

$$T_k(f)(\cdot) = \int_\Omega k(x, \cdot) f(x) d\nu$$

and we call k the kernel of T_k.

Mercer kernels

$$K(x, y) = \sum_{i=1}^{\infty} \lambda_j \phi_j(x) \phi_j(y)$$

with eigenvalues λ_j and eigenfunctions ϕ_j w.r.t. the eigenproblem

Fredhom integration operator of the second kind

$$\langle k(x, \cdot), \phi \rangle_\sigma = \int_\Omega k(x, y) \phi(x) \sigma(x) dx = \lambda \phi(y) \iff (T_k \phi)(y) = \lambda \phi(y)$$

Definition 1.39. *Given a linear ... or partial differential operator $\mathcal{L}$ on $\Omega \subseteq \mathbb{R}^d$, the **Green's kernel** g of $\mathcal{L}$ is defined as the solution of*

$$\mathcal{L}(g)(x, z) = \delta(x - z)$$

$\int f(z) \delta(x - z) dx = f(x)$.

The Green kernel is not uniquely defined this way, so one adds homogenous boundary conditions e.g. $g(x, z) = 0$ for $x \in \partial\Omega$, $\lim_{\|x\| \to \infty} g(x, z) = 0$.
Solutions of $\mathcal{L}u = f$ with appropriate boundary conditions can now be given as

$$u(x) = \int_\Omega g(x, z) f(z) dz$$

Check

$$\begin{aligned} \mathcal{L}u(x) &= \mathcal{L} \int_\Omega g(x, z) f(z) dz \\ &= \int_\Omega \mathcal{L} g(x, z) f(z) dz \\ &= \int_\Omega \delta(x - z) f(z) dz = f(x) \end{aligned}$$

We can ...

$$Gf(x) = \int_\Omega g(x, z) f(z) dz$$

as the "inverse" of the differential operator $\mathcal{L}$, i.e.

$$\mathcal{L}u = f \iff u = Gf$$

Example (Brownian Bridge kernel)**.** *$\Omega = [0, 1]$, consider bvp (boundary value problem)*

$$-u''(x) = f(x), u(0) = 0 = u(1)$$

The corresponding Green's kernel is

$$g(x, z) = \min(x, z) - xz = \begin{cases} x(1 - z) & x \leq z \\ z(1 - x) & x \geq z \end{cases}$$

We an observe that for g it must hold

$$\mathcal{L} g(x, z) = 0$$

for $x \neq z$, z fixed.

- $g(0,z) = g(1,z) = 0$
- *g is continuous along the diagonal $x = z$*
- *for fixed $z \in (0,1)$ one observes for $\frac{dg}{dx}$ a jump disc. at $x = z$ of the form*

$$\lim_{x \to z^-} \frac{dg}{dx}(x,z) = 1 + \lim_{x \to z^+} \frac{dg}{dx}(x,z)$$

There is a further connection to the Brownian bridge of stochastic analysis? Not just the end points

Remark. *Whenever $\mathcal{L}$ is a self adjoint differential operator, the corresponding Green's kernel is symmetric and the integral operator G is self adjoint.*

Theorem 1.40. *For every RKHS $\mathcal{H}$ with reproducing kernel k there exists a corresponding regularization operator $S : \mathcal{H} \to D$ s.t. for all $f \in \mathcal{H}$*

$$f(x) = \langle Sk(x,\cdot), Sf(\cdot)\rangle_D \tag{10}$$

In particular

$$\langle Sk(x,\cdot), Sk(y,\cdot)\rangle_D = k(x,y)$$

likewise, for every regularization operator $S : \mathcal{F} \to D$, where $\mathcal{F}$ is some function space equipped with a scalar product and with corresponding Green's kernel f on S^*S, there exists a corresponding RKHS $\mathcal{H}$ with reproducing kernel K, s.t. both equations are fulfilled.

The second statement is much more interesting, the first follows from $S = Id$

Proof. First direction: $S = \mathrm{Id}, D = \mathcal{H}$.
Second direction:

$$f(x) = \langle f, \delta(x-z)\rangle_{\mathcal{F}} = \langle f, \mathcal{L}g_x\rangle_{\mathcal{F}} = \langle f, S^*Sg_x\rangle_{\mathcal{F}} = \langle Sf, Sg_x\rangle_D$$

for all $f \in S^*S\mathcal{F}$, where g_x is the Green's kernel for S^*S and natural boundary conditions.
Further we have with $f = g_z$

$$g_z(x) = \langle Sg_x, Sg_z\rangle = \langle Sg_z, Sg_x\rangle = g_x(z)$$

In this sense g is symmetric and we write

$$k(x,z) = g_z(x).$$

We observe that $x \to Sg_x$ is actually a feature map, i.e. $\langle Sg_x, Sg_z\rangle_D$. Since kernels arising from feature maps result in Gram matrices for the kernel matrix we set that K is a p.s.d..
It can be seen that the corresponding RKHS is the closure of

$$\{f \in S^*S\mathcal{F} \mid \|Sf\|_D^2 < \infty\}$$

□

To simplify, we consider the full space kernel, i.e. without boundary / decay conditions. For $g_z(x) = k(x,z)$, g for the differential operator $\mathcal{L}$, we observe

$$\begin{aligned} & \mathcal{L}\int_\Omega k(x,z)\sigma(x)dx = \mathcal{L}\lambda\lambda\phi(z) \\ \iff & \underbrace{\int_\Omega \delta(x-z)\phi(x)\sigma(x)dx}_{\phi(z)\sigma(z)} = \lambda\mathcal{L}\phi(z) \\ & \implies \ldots \implies L\phi(z) = \frac{1}{\lambda}\phi(z)\sigma(z) \end{aligned}$$

For simplicity we assume that $\mathcal{L}$ has no Eigenvalue 0.

Example. *We have* $\int_\Omega k(x,z)\phi(x)\sigma(x)dx = \lambda\phi(z)$ *with* $\sigma = 1, k(x,z) = \min(x,z) - xz$ *on* $\Omega = [0,1]$.
This gives

$$\int_0^z x\phi(x)dx + \int_z^1 z\phi(x)dx - \int_0^1 xz\phi(x)dx = \lambda\phi(z)$$

Now apply $\mathcal{L} = -\frac{d^2}{dz^2}$ *to the equation:*

$$\frac{d}{dz}\left(z\varphi(z) - \int_1^z \phi(x)dx - z\phi(z) - \int_0^1 x\phi(x)dx\right) = \lambda\phi''(z)$$
$$\iff \frac{1}{\lambda}\phi(z) = \phi''(z)$$

Theorem 1.41. *Given a regularization operator* S *with an expansion of* S^*S *into a discrete normalized eigendecomposition with eigenvalues and eigenfunctions* γ_i, ϕ_i*, we define a kernel with*

$$k(x,y) = \sum_{i,\gamma_i\neq 0} \frac{d_i}{\gamma_i}\phi_i(x)\phi_i(z)$$

where $d \in \{0,1\}$ *for all* i *and* $\sum_{i=1}^\infty \frac{d_i}{\gamma_i}$ *is ... Then* k *satisfies theorem 1.40*

$$\langle Sk(x,\cdot), Sk(z,\cdot)\rangle_D = k(x,z) = \langle k(x,\cdot), k(z,\cdot)\rangle_{\mathcal{H}}$$

where the RKHS is given by span$\{\phi_i | d_i = 1\}$

Proof.

$$\begin{aligned}\langle Sk(x,\cdot), Sk(z,\cdot)\rangle &= \langle k(x,\cdot), S^*Sk(z,\cdot)\rangle \\ &= \langle \sum_i \frac{d_i}{\gamma_i}\phi_i(x)\phi_j(\cdot), S^*S\sum_i \frac{d_i}{\gamma_i}\phi_i(x)\phi_j(\cdot)\rangle \\ &= \sum_{j,k}\frac{d_j}{\gamma_j}\frac{d_k}{\gamma_k}\phi_j(x)\phi_k(z)\langle\phi_j(\cdot), \underbrace{S^*S\phi_k(\cdot)}_{\gamma_k\phi_k}\rangle \\ &\overset{\text{ONB}}{=} \sum_j \frac{d_j}{\gamma_j^2}\gamma_j\phi_j(x)\phi_j(z) = k(x,z)\end{aligned}$$

From the construction of k follows the statement of the span. □

Start of lecture 12 (28.05.24)

1.4 Model selection

To estimate the predictive performance of a learned model, we use train- and test/ validation data. Where D_t, D_V are the training and the validation data sets, respectively. The **empirical risk** on D_V is used to measure the generalization performance.
In case of hyperparameters, a simple strategy is to use a selection of hyperparameters, train models, and pick the hyperparameters with the best empirical risk.

80/20, 70/30 are common splits, this does depend on the size of the dataset! Might not be the best idea in practice, where training may take weaks! Notice how the run time scales exponetially in the number of hyperparameters

Added remark. *For time series data a random split might be bad (if there is a drift), therefore we might prefer taking years up to year x!*

Added remark. *If we use hyperparameter search, we also have to split the data into 3 parts. One for training, 1 for hyperparameter search and one to estimate the predictive power.*

If the number of data is small, the measured performance on the validation data can have a large uncertainty. A strategy to use is k-fold cross validation.
We use k disjoint equally sized subsets, use each one once for D_V and the $k-1$ other ones as training data D_t. The average performance over the k runs is then the performance measure.

Added remark. *In the deep learning setting run the same training with different seeds, then take the average.*

For $k = N$ is known as **leave-one-out** cross validation.

Definition 1.42. *There is a exact definition in the script (this was not done in the lecture).*

Definition 1.43. *A **Gaussian process** is a collection of random variables, any finite number of which have a joint Gaussian distribution.*
Mean $m(x) = \mathbb{E}(f(X))$ *and covariance* $k(x,z) = \mathbb{E}((f(x) - m(x))(f(z) - m(z)))$

$$f(x) = GP(m(x), k(x,z))$$

Key example: Gaussian kernel:

$$\operatorname{cov}(f(x), f(z)) = k(x,z) = \exp(-\frac{1}{2\sigma^2}\|x - z\|^2)$$

Added remark. *We can then sample from this space of functions! The better fitted the space is to our data, the better our predictions.*

Choose $X_* \coloneqq \{x_1, \dots, x_N\}$ and generate a random process with a covariance matrix

$$f_* = \mathcal{N}(0, k(X_*, X_*))$$

Consider noisy data with additive gaussian noise ϵ, with variance σ_N^2;

$$y = f(x) + \epsilon$$

The prior on the noisy observations becomes

$$\operatorname{cov}(y_p, y_q) = k(x_p, x_q) + \sigma_N^2 \delta_{pq}.$$

or

$$\operatorname{cov}(Y) = k(X,X) + \sigma_N^2 I$$

Joint distribution of observed target and f at test locations

$$\begin{bmatrix} y \\ f_* \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} k(x,x) + \sigma_N^2 I & k(x, x_*) \\ k(x_*, x) & k(x_*, x_*) \end{bmatrix}\right)$$

We need to restrict this joint distribution to contain only those functions that "agree" with the observed data.

$$f_* \mid X, Y, x_* \sim \mathcal{N}\left(k(x_*, X)[k(X,X) + \sigma_N^2 I]^{-1} Y, k(x_*, x_*) - k(x_*, X)[k(X,X) + \sigma_N^2 I]^{-1} k(X, x_*)\right)$$

Boil down to one evaluation x_l we have

$$f(x_l) = k(X, x_l)^\intercal (k(X,X) + \sigma_n^2 I)^{-1} Y = \sum_{i=1}^{N} \alpha_i k(x_i, x_l)$$

$$V(f) = k(x_l, x_l) - k(X, x_l)^\intercal [k(X,X) + \sigma_N^2 I]^{-1} k(X, x_l)$$

Added remark. *What is a length scale? Variance in data points?*

Consider the marginal likelihood or evidence

$$p(Y \mid X) = \int \underbrace{p(Y \mid f, X)}_{\text{likelihood}} \underbrace{p(f \mid X)}_{prior} df$$

One can obtain for the log marginal likelihood

$$\log(p(Y \mid X)) = -\frac{1}{2} Y^\intercal (K + \sigma_N^2)^{-1} Y \frac{1}{2} \log(K + \sigma_N^2 I) - \frac{N}{2} \log(2\pi)$$

θ hyperparameters of K:

$$\log(p(Y \mid X, \theta)) = -\frac{1}{2}\underbrace{Y^\intercal (K_\theta + \sigma_N^2)^{-1} Y}_{\text{data fit}} \underbrace{\frac{1}{2}\log(K_\theta + \sigma_N^2 I)}_{\text{complexity penalty}} - \underbrace{\frac{N}{2}\log(2\pi)}_{\text{Normalization parameter}}$$

One aims to optimize the evidence of the data, in this Bayesian optimization one can also include the hyperparameters.

Added remark. *Bayesian optimization. Optimize which data point would minimize unexplained variance?*

$k(x,y) = \sum_{i=1}^{\infty} \gamma_i \phi_i(x)\phi_i(y)$ a mercel kernel. For $f \in \mathcal{H}_K$

$$f(x) = \sum_{i=1}^{\infty} c_i \phi_i(x)$$

$$\langle f, f\rangle_{\mathcal{H}_K} = \langle Sf, Sf\rangle_{L^2} = \langle f, Sf\rangle_{L^2} = \sum_{i=1}^{\infty} \frac{c_i^2}{\gamma_i} < \infty$$

The rough terms ϕ_i have smaller prior variance and are therefore more strongly penalized by the regularization.

Start of lecture 13 (04.06.24)

Added remark.

- *Motivation: Finding a classifier, specifically by separating data by a hyperplane!*
- *Idea for SVMs: find a separating hyperplane while maximizing the margin between the hyperplane and the data points.*
- *Outliers or not linearly separable data is a problem!*
- *For SVMs slack variables can be a good idea to counteract some of those problems (where C is another regularization parameter)*
- *We can also use feature maps to embed our data into a higher dimensional space, where it might be linearly separable*
- *Not a unique way to choose such a feature map*
- *Sadly the number of support vectors in linear in the number of data points*

$$\begin{aligned} \xi_i &\geq 1 - y_i(\langle w_i, \Phi(x_i)\rangle + b),\ \xi_i \geq 0 \\ \xi_i &\geq \max(0, y_i(\langle w_i, \Phi(x_i)\rangle + b)) \\ &= l_h(y_i, \langle w_i, \Phi(x_i)\rangle + b) \end{aligned}$$

It is therefore related to the hinge loss!
(w,b):

$$f_{(w,b)}(x) = \langle w, \Phi(x)\rangle + b$$

$$\min_{(w,b)} \underbrace{\langle w, w\rangle}_{\|f\|_{\mathcal{H}}} + C\sum_{i=1}^{N} l_h(y_i, \langle w_i, \Phi(x_i)\rangle + b)$$

This gives the RKHS view on SVMs.
This, once more, motivates

$$k(x,y) = \langle \Phi(x), \Phi(y)\rangle$$

$$\begin{aligned}\|\Phi(x)-\Phi(y)\|^2 &= \langle\Phi(x),\Phi(x)\rangle - 2\langle\Phi(x),\Phi(y)\rangle + \langle\Phi(y),\Phi(y)\rangle\\ &= k(x,x) - 2k(x,y) + k(y,y)\end{aligned}$$

Shifting data: $x \mapsto x - t$, $\|x-y\|^2$ is invariant under the shift, but $\langle x, y\rangle$ is not!

There was a mistake here in the lecture!

$$\begin{aligned}\langle x-t, y-t\rangle &= \langle x,y\rangle - \langle x,t\rangle - \langle t,y\rangle + \langle t,t\rangle\\ &= \frac{1}{2}\left(\langle x,x\rangle - 2\langle x,t\rangle + \langle t,t\rangle + \langle y,y\rangle - 2\langle y,t\rangle + \langle t,t\rangle + 2\langle x,y\rangle - \langle x,x\rangle - \langle y,y\rangle\right)\\ &= \frac{1}{2}\left(\|x-t\|^2 + \|y-t\|^2 - \|x-y\|^2\right)\\ &\sim \tilde{k}(x,y)\end{aligned}$$

This $\tilde{k}(x,y) = \langle x-t, y-t\rangle$ is still psd.

$$\sum_{j,k} a_j a_k \langle x_j - t, x_k - t\rangle = \|\sum_j c_j(x_k - t)\|^2$$

So, for any choice of $t \in \mathbb{R}$ we get a similarity measure $\tilde{K}(x,y)$ associated with the dissimilarity measure $\|x-y\|$
Now replace $\langle\cdot,\cdot\rangle$ by k.

Lemma 1.44. *Let $t \in \Omega$ and K be a symmetric kernel on $\Omega\times\Omega$. Then $\tilde{k}(x,y) = \frac{1}{2}(k(x,y) - k(x,t) - k(t,y) + k(t,t))$ is positive semidefinite if and only if K is cond. psd. of order 1.*
If $k(t,t) \le 0$, then

$$\hat{K}(x,y) \coloneqq \frac{1}{2}(k(x,y) - k(x,t) - k(t,y))$$

is psd iff K is cpsd. of order 1.

Proof. 1. $\tilde{k}$ psd $\implies$ K cpsd:
Let $a \in \mathbb{R}^n$ s.t. $\sum a_i = 0$ and let $(x_i)_{i=1}^N$, then

$$0 \le \sum_{i,j=1}^N a_i a_j \tilde{k}(x_i,x_j) = \sum_{i,j}\sum_{i,j=1}^N a_i a_j k(x_i,x_j)$$

Since

$$\sum_j a_j \underbrace{\sum_i a_i k(x_i,t)}_{=c} = 0$$

2. K cpsd. $\implies$ $\tilde{k}$ psd.:
Let $a \in \mathbb{R}^n$, $(x_i)_{i=1}^N$, let $x_0 = t, a_0 = -\sum_{i=1}^N a_i$. Then

$$0 \le \sum_{i,j=1}^N a_i a_j k(x_i,x_j) = \sum_{i,j=1}^N a_i a_j \tilde{k}(x_i,x_j)$$

Thus $\tilde{k}$ is psd. □

If we take negative square distance, here $\sum_i a_i = 0$ implies

$$-\sum_{i,j} a_j a_k \|x_j - x_i\|^2 = -\sum_j a_j \sum_k \|x_k\|^2 - \sum_k a_k \sum_j \|x_j\|^2 + -\sum_j a_j \sum_k \langle x_j, x_k\rangle$$

so $-\|x-y\|$ is cpsd.
Therefore kernels that are cspd. of order 1 are sometimes called negative definite kernels for $-K$.
From Mercers theorem we have that $\tilde{k}$ (psd) has a feature map $\phi : \Omega \to \mathcal{F}$, $\tilde{k}(x,y) = \langle\Phi(x),\Phi(y)\rangle$.
Therefore $\|\Phi(x)-\Phi(y)\|^2 = \tilde{k}(x,x) + \tilde{(k)}(y,y) - 2\tilde{(k)}(x,y)$. For fixed $t \in \mathbb{R}$ we use the definition of $\tilde{k}$.

$t \in \mathcal{F}$ prob. ???

$$\begin{aligned}\|\Phi(x)-\Phi(y)\|^2 &= \frac{1}{2}(k(x,x)-k(x,t)-k(t,x)+k(t,t)+k(y,y)-k(y,t)-k(t,y)+k(t,t)-2(k(x,y)-k(x,t)-k(t,y)+k(t,t)))\\ &= -k(x,y)+\frac{1}{2}(k(x,x)+k(y,y))\end{aligned}$$

This shows

Theorem 1.45. *Let k be a cspd kernel of order 1 on Ω. Then there exists a Hilbert space $\mathcal{F}$ and a mapping $\Phi:\Omega\to\mathcal{F}$ s.t.*

$$-k(x,y)+\frac{1}{2}(k(x,x)+k(y,y))=\|\Phi(x)-\Phi(y)\|_{\mathcal{F}}^2$$

If $k(x,x)=0$ for all $x\in\Omega$, we have

$$k(x,y)=-\|\Phi(x)-\Phi(y)\|_{\mathcal{F}}^2$$

and $\sqrt{-k(x,y)}$ is a semi-metric and a metric if $k(x,y)\neq 0$ for $x\neq y$.

Start of lecture 14 (06.06.24)

Consider the

$$F[f](\omega)=\frac{1}{(2\pi)^{-d/2}}\int_{\mathbb{R}^d} f(x)\exp(-i\langle x,\omega\rangle)dx$$

and the **inverse Fourier transform**

$$F^{-1}[f](x)=\frac{1}{(2\pi)^{-d/2}}\int_{\mathbb{R}^d} f(\omega)\exp(i\langle i,\omega\rangle)$$

where

$$f(x)=F^{-1}[F[f]](x)$$

Consider the regularization operator ...

Consider S, where S^* is diagonalizable on th Fourier basis.
Denote $v(\omega)$ a nonnegative, symmetric function on $\mathbb{R}^d$:

$$v(\omega)=v(-\omega)\geq 0$$

further assume $v(\omega)\to 0$ for $\|\omega\|\to\infty$ and denote by Ω the support of v.

$$\langle Sf,Sg\rangle_D=(2\pi)^{\frac{d}{2}}\int_\Omega \frac{\overline{F[f](\omega)}F[g](\omega)}{v(\omega)}d\omega$$

Small values of $v(\omega)$ correspond to strong damping of the corresponding frequencies. This is desirable for large ω, i.e. high frequency components that correspond to rapid changes in f.
Now look at $g(x,z)=(2\pi)^{d/2}\int_\Omega e^{i\omega(x-z)}v(\omega)d\omega$. Let f have the support of its Fourier transform contained in Ω. We see

$$\begin{aligned}\langle Sg(x,\cdot),Sf\rangle &= (2\pi)^{d/2}\int_\Omega \frac{\overline{F[g(x,\cdot)](\omega)}F[f](\omega)}{v(\omega)}d\omega\\ &= (2\pi)^{-d/2}\int_\Omega \frac{\overline{v(\omega)}\exp(i\langle x,\omega\rangle)F[f](\omega)}{v(\omega)}d\omega\\ &= (2\pi)^{-d/2}\int_\Omega \exp(i\langle x,\omega\rangle)F[f](\omega)d\omega=f(x)\end{aligned}$$

According to theorem 1.40 g is the kernel corresponding to S.
This is a special case of

Theorem (Bocher's theorem)**.** *For given $\kappa:\mathbb{R}^d\to\mathbb{C}$ the expression*

$$k(x,y)=\kappa(x-y)$$

defines a kernel if and only if there exists a unique finite Borel measure μ on $\mathbb{R}^d$ s.t.

$$\kappa(x)=\int_{\mathbb{R}^d}\underbrace{\exp(i\langle x,y\rangle)}_{\cos(\langle x,y\rangle)\text{ for the real case}}d\mu(y)$$

Added remark. *random kitchen sink paper ... 20007*

Chapter 2: Dimensionality reduction

Added remark. *Idea: High dimensional data $Y \to$ find low dimensional data X which represents Y to a good degree.*
For example: Represent vectors w.r.t. to a subset of the basis!

Set Y of $y_i \in \mathbb{R}^d$, $i = 1, \dots, N$ goal is to find

We are now in the unsupervised setting

$$x_i \in \mathbb{R}^p, p \ll d$$

d is called the **extrinsic** dimension, while p is the **intrinsic** dimension.

2.1 Linear dimensionality reduction

$\{y_i\}_{i=1}^N$ are samples of a random variable $Y(\omega) \in \mathbb{R}^d$. We assume Y stems from p unknown latent variables $X(\omega) \in \mathbb{R}^p$ by a linear transformation W.

He writes $Y \in \mathbb{R}^d$, which seems to be the wrong space for a random variable ...

$$Y = WX$$

which can be read as a statement about vectors (a single realization of the random variable) or in terms of matrices (the sampled realizations as a whole)-
We assume that Y, X are mean centered, i.e. $\mathbb{E}(Y) = 0$. We further assume W to be an axis change, i.e. the columns w_i of W are orthogonal to each other and unit norm:

$$W^\intercal W = I_p$$

We write the data in matrix form

with slightly abusive notation, as the matrix Y consists of N samples of the random variable Y

$$Y = \begin{bmatrix} | & & | \\ y_1 & \dots & y_N \\ | & & | \end{bmatrix}$$

For any W, consider the pseudo inverse

$$W^\dagger = (W^\intercal W)^{-1} W^\intercal = W^\intercal$$

and therefore

$$X_i = W^T y_i.$$

We aim for a good reconstruction of Y by X:

$$\begin{aligned} &\mathbb{E}(\|y - W(W^T y)\|_2^2) \\ &= \mathbb{E}(y^\intercal y - 2y^\intercal W W^\intercal y + y^\intercal W W^\intercal W W^\intercal y) \\ &= \mathbb{E}(y^\intercal y - y^\intercal W W^\intercal y) \end{aligned}$$

where

$$\begin{aligned}\mathbb{E}(Y^\intercal WW^\intercal \underbrace{Y}_{\in\Omega\times\mathbb{R}^d}) &\approx \frac{1}{N}\sum_{i=1}^{N} y_i^\intercal WW^\intercal y_i \\ &= \frac{1}{N}\mathrm{tr}(Y^\intercal WW^\intercal \underbrace{Y}_{\in\mathbb{R}^{d\times N}}) \\ &= \frac{1}{N}\mathrm{tr}(W^\intercal YY^\intercal W)\end{aligned}$$

Adding the constraint, we set the lagrangian

$$\mathcal{L} = \mathrm{tr}(W^\intercal YY^\intercal W) + \mathrm{tr}((I_p - W^\intercal W)\Lambda)$$

where $\Lambda = \Lambda^T \in \mathbb{R}^{p\times p}$.
Conditions for an extrema:

$$(\star) : YY^\intercal W = W\Lambda \implies \Lambda = W^\intercal YY^\intercal W$$

The objective reduces to $\mathrm{tr}(\Lambda)$. We can rotate W and have the same **reconstruction error**, i.e. we can use $W' = WR$ giving $\Lambda' = R\Lambda R^T$ for some rotation matrix R. $\implies$ $\Lambda = \Lambda^T$ is diagonalizable with orthogonal matrices, so we choose R s.t. Λ' is diagonal, w.l.o.g. Λ is diagonal. From $(\star)$ follows that the columns of W must be eigenvectors of $YY^\intercal$ with corresponding eigenvalues as the diagonal of Λ. Since we maximize $\mathrm{tr}(\Lambda)$, we take the p largest eigenvalues of $YY^\intercal$ and the corresponding eigenvectors.
SVD of Y: $U\Sigma V^\intercal$, we take the first p columns of U for W, i.e. $W = UI_{d\times p}$. Furthermore, as U is orthogonal,

$$X = W^\intercal Y = W^\intercal U\Sigma V^\intercal = I_{p\times d}\Sigma V^\intercal.$$

Using $\Lambda = W^\intercal U\Sigma^2 UW$, we get

$$\mathrm{tr}(\Sigma^2) - \mathrm{tr}(I_{p\times d}\Sigma^2) = \sum_{i=p+1}^{d}\sigma_i^2 = \sum_{i=p+1}^{d}\lambda_i$$

Theorem 2.1. *Let $Y = [y_1, \dots, y_N] \in \mathbb{R}^{d\times N}$ be a matrix of zero mean data points. Denote the SVD of Y by $Y = U\Sigma V^\intercal$. Then for given $p < d$, the minimizer W for*

$$\min_{\substack{W\\ W^\intercal W = I_p}} \sum_{i=1}^{N} \|y_i - WW^\intercal y_i\|_2^2$$

*is given using $W = [u_1, \dots, u_p]$. The lower dimensional embedding is given by $X = I_{p\times d}\Sigma V^\intercal = I_{p\times d}U^\intercal Y$ and the **reconstruction error** is*

$$\sum_{i=p+1}^{N}\sigma_i^2$$

To get compactness: Take a**ball of functions: $\|f\| <= r$** and use Arzelà-Ascoli.

Start of lecture 15 (11.06.24)

2.1.1 Alternative derivations of PCA

- Projection: We aim for $y = \sum_{i=1}^{p} x_i w_i$ with $y_i, w_i \in \mathbb{R}^d, w_i^\intercal, w_j = \delta_{ij}$. Then $x_i = \langle y_i, w_i\rangle$.
- Approximation with rank constraints:

  $$\min_A \|Y - A\|_F^2$$

  s.t. rank $A = p$
- From the statistical perspective:

Definition 2.2. *Given a zero mean multivariate random variable $Y \in \Omega \times \mathbb{R}^d$. The p **principle components** of Y are defined as the p uncorrelated linear components of Y:*

$$x_i = w_i^\intercal y \in \mathbb{R},\ w_i \in \mathbb{R}^d,\ i = 1, \dots, p$$

s.t. the variance of x_i maximized subject to $w_i^\intercal w_i = 1$ and $Var(x_1) \geq Var(x_2) \geq \cdots \geq Var(x_p)$

Theorem 2.3. *Assume that the rank of the covariance matrix $\mathbb{E}(YY^\intercal)$ is larger than p. Then the first p principle components of a zero mean, multivariate random variable Y, denoted by $x_i, i = 1, \dots, p$ are given by*

$$x_i = w_i^\intercal Y$$

where $\{w_i\}_{i=1}^p$ are the p orthonormal eigenvectors of $\mathbb{E}(YY^\intercal)$ associated its p largest eigenvalues $\{\lambda_i\}_{i=1}^p$. Moreover $\lambda_i = Var(X_i)$.

In the exercise we show that the greedy approach works in this specific setting?

Added remark. *Y, which has N columns and d rows ...*

Added remark. *In general we might want to work with tensors (for example if we have a time dependent structure). This is possible, but can be generalized in multiple, non-equivalent, ways. The sum of vectors representation is not so nice, there are counter examples ...*

We aim for embeddings that approximately preserve distances.

Here, we always talk about euclidean distances!

$$d^d(y_1, y_2) \approx d^p(x_1, x_2)$$

Definition 2.4. *A $N \times N$ symmetric matrix D is called **Euclidean distance matrix (EDM)**, if there exists an integer $d > 0$ and a vector set $Y = \{y_1, \dots, y_N\}, y_i \in \mathbb{R}^d$, s.t. $D_{i,j} = d_E^2(y_i, y_j)$, where d_E is the euclidean distance. The vector set Y is called the **configuration** of D. We write $D \in EDM$.*

Careful! Some authors use the euclidean distance matrix with a square, and some without the square!

Definition 2.5. *A $N \times N$ symmetric matrix D with non-negative entries $d_{i,j}$ is called **distance matrix**, if $d_{ii} = 0$ for all i and*

$$\sqrt{d_{ij}} \leq \sqrt{d_{ik}} + \sqrt{d_{kj}}$$

for all i, j, k. We write $D \in DM$.

Obviously EDM $\subset$ DM.

$$(\star)\ d_E^2(y_i, y_j) = \underbrace{\langle y_i, y_i \rangle}_{G_{ii}} - 2\underbrace{\langle y_i, y_j \rangle}_{G_{ij}} + \underbrace{\langle y_j, y_j \rangle}_{G_{jj}}$$

where $G_{ij} = \langle y_i, y_j \rangle = (Y^\intercal Y)_{ij}$.
As for PCA, we aim for mean centered data, where we use the centering matrix

$$H = I - \frac{1}{N} 1_N,$$

where $1_W = 1_N \cdot 1_N^\intercal$ is the matrix of all ones, where 1_N is the vector of all ones. with

$$Y^c = Y - (\frac{1}{N} Y 1_N) 1_N^\intercal = YH.$$

We set the centered data. The centered Gram matrix

$$G^c = (Y^c)^\intercal Y^c = H^\intercal Y^\intercal Y H = H^\intercal G H$$

Theorem 2.6. *For the Euclidean distance matrix D and the centered Gram matrix $G1c$ of a data set Y, it holds*

$$G^c = -\frac{1}{2} HDH$$

Proof. Straight forward calculation from $(\star)$. □

Lemma 2.7. *Assume that the matrix $D \in EDM$ and let $G^c = -\frac{1}{2}HDH$. If the rank of G^c is r, then there is a centered r dimensional configuration $Y = \{y_1, \dots, y_N\} \in \mathbb{R}^r$, s.t. $d_E(y_i, y_j) = d_{ij}$.*

Proof. Since $D \in$ EDM, there exists a set $Z = \{z_1, \dots, z_n\} \in \mathbb{R}^d$, s.t. $d_{ij} = d_E(z_i, z_j)$, G^c is the Gram matrix of Z and therefore psd. The rank is r, so we have $G^c = Y^\intercal Y$ with a centered data matrix (via EDM). The centered data satisfies $d_{i,j} = d_E(y_i, y_j)$. We call r the **intrinsic configuration dimension** and Y is the **exact configuration** of D. □

2.1.2 (classical) multidimensional scaling (MDS)

Instead of exact configuration of dimension r, we seek a lower dimensional configuration $Y \subset \mathbb{R}^p$, $p < r$;

$$X = \underset{X \subset \mathbb{R}^{p \times N}}{\operatorname{argmin}} \sum_{i,j}^{N} |d_{ij}^2 - d_E^2(x_i, x_j)| \quad (\star\star)$$

s.t. $X = T(Y)$, with T an orthogonal projection from $\mathbb{R}^r$ to a p-dimensional space $S_p \subset \mathbb{R}^r$ and Y is an exact configuration.

Lemma 2.8. *Let $Z \subset \mathbb{R}^r$ be a given data set with $D_Z = [d_E^2(z_i, z_j)]_{i,j=1}^N$ and let $G_Z^c = -\frac{1}{2}HD_ZH$. Then*

$$tr(G_Z^2) = \frac{1}{2N} \sum_{i,j=1}^{N} d_E^2(z_i, z_j)$$

Proof. Write out G_Z^2, look at diagonal, straight forward calculation. □

Lemma 2.9. *Let D_Z as before. $ZH =: \tilde{Z} = [\tilde{z}_1, \dots, \tilde{z}_n]$. Then $\|\hat{Z}\|_F = \frac{1}{\sqrt{2N}}\|D_Z\|_F$.*

Proof. With $\|D_Z\|_F^2 = \sum d_E^2(z_i, z_j)$ and $\|\hat{Z}\|_F^2 = \operatorname{tr}(\hat{Z}^\intercal \hat{Z}) = \operatorname{tr}(\hat{G}_z^2)$. The result follows from lemma 2.8. □

Theorem 2.10. *Let $Y \subset \mathbb{R}^r$ be an exact configuration of $D \in EDM$. The SVD of Y is given by $U\Sigma V^\intercal$. For a given $p \le r$, let $U_p = [u_1, \dots, u_p]$. Then*

$$X = U_p^\intercal Y$$

is a solution of the MDS minimization problem $(\star\star)$ with an error of

$$2N \sum_{i=p+1}^{r} \sigma_i^2.$$

Proof. Let S_p be a p-dim subspace of $\mathbb{R}^r$. Let B be a $r \times p$ orthogonal matrix, whose columns form an orthonormal basis of S_p. We have $T(y) = BB^\intercal y$ and observe

$$d_E(B^\intercal y_i B^\intercal y_j) = \|B^\intercal(y_i - y_j)\| T(y_i - y_j) = d_E(Ty_i, Ty_j).$$

Wih $\|y_i - y_j\| \ge \|T(y_i - y_j)\|$. We get for the objective function

$$\begin{aligned}\sum_{i,j=1}^{N} d_E^2(y_i, y_j) - d_E^2(B^\intercal y_i, B^\intercal y_j) &= \sum_{i,j=1}^{N} \langle y_i - y_j, y_i - y_j\rangle - \langle B^\intercal(y_i - y_j), B^\intercal(y_i - y_j)\rangle \\ &\overset{\langle B^\intercal y, B^\intercal y\rangle = \langle B^\intercal B y, B^\intercal y\rangle}{=} \dots - 2\langle BB^\intercal(y_i - y_j), (y_i - y_j)\rangle + \langle BB^\intercal(y_i - y_j), (y_i - y_j)\rangle \\ &= \sum_{i,j=1}^{N} |(I - BB^\intercal)(y_i - y_j)|^2 = \|D_Z\|_F^2\end{aligned}$$

wih $Z = (I - BB^\intercal)Y$. Using Lemma 2.9, we get $\|D_Z\|_F^2 = 2N\|ZH\|_F^2 = 2N\|Z\|_F^2$, since Y is centered Z is also centered. Therefore we have to solve

$$\underset{\substack{B \in \mathbb{R}^{r \times p} \\ B^\intercal B = I_p}}{\operatorname{argmin}} \|Y - BB^\intercal Y\|_F.$$

Again we use Schmidt-Eckart-Yanns for the SVD. THe matrix $U_p\Sigma_p V_p^\intercal$??? So getting $B = U_p$ gives

$$U_p U_p^\intercal U \Sigma V^\intercal = U_p \Sigma_p V_p^\intercal$$

and $X = U_p^\intercal Y$. The error estimate follows from ??? SVD and Lemma 2.9. □

It is important to understand the flip: You can choose the minimum of the number of dimensions and the number of data points.

Start of lecture 16 (13.06.24)

Recap:
$G^c = Y^\intercal Y = (W^\intercal X | WX) = X^\intercal W^\intercal W X = X^\intercal X$
EVD of G^c:

EVD= Eigen value decomposition

$$\begin{aligned} G^c = V\Lambda V^\intercal &= (V\Lambda^{\frac{1}{2}})(\Lambda^{\frac{1}{2}} V^\intercal) \\ &= (\Lambda^{\frac{1}{2}} V^\intercal)^\intercal (\Lambda^{\frac{1}{2}} V^\intercal) \end{aligned}$$

Taking the top p eigenvalues gives

$$X_{\text{MDS}} = I_{p\times N} \Lambda^{\frac{1}{2}} V^\intercal$$

Also $Y = U\Sigma V^\intercal$ for PCA:

$$\begin{aligned} X_{\text{PCA}} &= I_{p\times d} U^\intercal Y = I_{p\times d} \Sigma V^\intercal \\ &= I_{p\times d} (\Sigma^\intercal \Sigma)^{\frac{1}{2}} V^\intercal = I_{p\times d} \Lambda^{\frac{1}{2}} V^\intercal \end{aligned}$$

We can use the following approaches:

- SVD of Y: $(d \times N)$: Reconstruct Y
- EVD of $YY^\intercal$ $(d \times d)$: maximal variance
- EVD of $Y^\intercal Y$ $(N \times N)$: preserving similarity

The SVD is most commenly used and ist most stable. If you have extreme differences in d and N, it might be worth to use on of the other two approaches

Algorithm 1 MDS

Input: EDM D, P
Output: embedding X in p dimensions

$G = -\frac{1}{2} HDH$
$[V_p, \Lambda_p] = \text{EVD}(G, p)$
Return $\Lambda_p^{\frac{1}{2}} V^\intercal$

Added remark. *There are multiple generalizations!*

2.1.3 Strange effects in high dimensions

Angles

First we look at angles between vectors. In 2d the angle between the diagonal and an axis is $\frac{\pi}{4}$. In general:

$$\varphi = \arccos \frac{\langle x, y \rangle}{\|x\| \|y\|}$$

Then $\alpha = \frac{1}{\sqrt{d}}$.

Volume

The volume of the hypersphere in d dimensions:

$$\frac{r^d \pi^{\frac{d}{2}}}{\Gamma(1 + \frac{d}{2})}$$

The Volume of the hypercube is $(2r)^d$.
Therefore in higher dimensions the sizes of a unit hypersphere and its bounding hypercube are not close, their ratio goes to 0!

Concentration of measure

If we increase the radius of the sphere by just some small ϵ, we can see that most of the mass lies in the outer shell of hyperspheres!

$$\frac{V_r}{V_{r(1-\epsilon)}} = \frac{1}{(1-\epsilon)^d}$$

Curse of dimensionality

The higher the dimension, the more points I need to approximate functions of the same complexity as the dimension increases. This scaling is exponential! Therefore we need lots of data to recover functions in higher dimensions.

If we do datascience in higher dimensions, we always implicitly assume that there is more structure, otherwise most problems would not be feasable

ANOVA decomposition

However the dimensions might be highly correlated! We can than use the ANOVA decomposition:

$$f(x) = \sum_{\tilde{d}_i=1,\dots,D} f_{\tilde{d}_i}(x_{\tilde{1}}, \dots, x_{\tilde{p}})$$

2.1.4 Properties in dimensionality reduction approaches

1. Estimate the intrinsic dimensionality
2. What kind of properties of the original data does one (implicitly or explicitly) assume to hold and to approximately preserve
3. One often aims for latent variable separation (statistical independence, orthogonality)[1]

For PCA/MDS, we can consider the rank of the matrix as the intrinsic dimensionality. We can use criteria such as

$$\frac{\sum_{i=1}^{p} \lambda_i}{\sum_{i=1}^{d} \lambda_i} \geq 0.95$$

This assumes no noise, otherwise we can be reasonably sure that the intrinsic dimensionality is smaller than the rank

or

$$\lambda_{p+1} \leq 0.01 \sum_{i=1}^{d} \lambda_i$$

Another procedure: The L-curve: Linearly approximate the eigenvalues as a function of the index from both the left and the right and take the intersection as the cutoff point.
In the latter approaches we assume a fast decline in eigenvalues.

2.2 nonlinear dimensionality reduction

We use manifolds instead of linear subspaces. Ideally we use geodesic distances $d_M(x, y)$ and preserve d_M in the embedding. But both M and d_M are unknown, only $D \subset M$ is given.
Approach: Build an undirected neighborhood graph $[Y, E]$ and use the graph distances d_G instead of d_M and aim to preserve it.

Definition 2.11. *Given a graph $[Y, E]$ for a data set $Y \subset \mathbb{R}^d$, s.t. $(y_i, y_j) \in E$ if and only if y_i, y_j are adjacent[a]. We define the **graph distance** d_G between two points $y_i, y_j \in Y$ by*

1. *If $(y_i, y_j) \in E$ then $d_G(y_i, y_j) = d_E(y_i, y_j)$*
2. *If $(y_i, y_j) \notin E$ then let $\Gamma\{\gamma \mid \gamma = (\gamma_0, \dots, \gamma_s), \gamma_i \in Y, \gamma_0 = y_i, \gamma_s = y_j\}$ and define*

$$d_G(y_i, y_j) = \min_{\gamma \in \Gamma} \sum_{i=0,\dots,s-1} d_E(\gamma_i, \gamma_{i+1})$$

[a] in some geometric senes

[1] this is also useful for interpretability!

We assume $Y \subset M \subset \mathbb{R}^d$ and that an isometric mapping

isometric means distance preserving

$$f : M \to \mathbb{R}^p$$

exists $f(y) = x$ for $y \in M$ and

$$d_E(f(y_i), f(y_j)) = d_M(y_i, y_j)$$

for all $y_i, y_j \in M$.
Assume Y is sampled densely enough from M, we expect that

$$d_G(y_i, y_j) \approx d_M(y_i, y_j).$$

$D_G = [d_G^2(y_i, y_j)]_{i,j=1}^N$, we aim for $D \in \text{EDM}$, with a configuration $X \in \mathbb{R}^p$ s.t.
$D_G \approx D = [d_E^2(x_i, x_j)]_{i,j=1}^N$.

Algorithm 2 Isomap

Input: Dataset Y, p
Output: data set embedding X in p dimensions

Build a neighborhood graph $[Y, E]$
$D_{ij} = [d_E^2(x_i, x_j)]$ using Dijkstra's algorithm
$G = -\frac{1}{2} HDH$
$[V_p, \Lambda_p] = \text{EVD}(G, p)$
Return $\Lambda_p^{\frac{1}{2}} V^\intercal$

Assume $D_G \in \text{EDM}$ we can invoke the MDS theorem 2.10. We get

$$\sum_{,j=1}^{N} |d_G^2(y_i, y_j) - d_E^2(x_i, x_j) \leq 2N \sum_{l=p+1}^{N} \lambda_l.$$

For the analysis we will use r-ball graphs:
$(y_i, y_j) \in E \iff \|y_i - y_j\|_E \leq r$.
Furthermore we use the Hausdorff distance between Y and M

$$\epsilon = H(M \mid Y) = \sup_{y \in M} \min_{y_i \in Y} \|y - y_i\|$$

Theorem 2.12. *Consider $M \subset \mathbb{R}^d$ compact and a sample $Y = \{y_1, \ldots, y_N\} \subset M$ and let $\epsilon = H(M \mid Y)$. For $r > 0$ form the corresponding r-ball graph. When $\epsilon \leq \frac{r}{4}$, we have for any $x, z \in Y$*

$$d_G(x, z) \leq \left(1 + \frac{4\epsilon}{r}\right) d_M(x, z)$$

In practice we often choose k-nearest neighbors instead of r-ball neighborhoods!

Start of lecture 17 (18.06.24)

Added remark. *CMDS is the same as MDS in our lecture. This is relevant for the sheets.*

Proof. For $d_E(x, z) \leq r$ we have that $(x, z) \in E$ in the r-ball graph and so

$$d_G(x, z) = d_E(x, z) \leq d_M(x, z).$$

Now consider $d_E(x, z) > r$ and let $a = d_M(x, z)$ and let $\gamma : [0, a] \to M$ be parametrized by arc length s.t. $\gamma(0) = x = y_{i_0}$ and $\gamma(a) = z = y_{i_s}$. Let $\hat{y}_{i_j} = \gamma\left(\frac{ja}{s}\right)$ for $j = 0, \ldots, s$ where $s = \lceil 2a/r \rceil \geq 2$, where $\hat{y}_0 = a, \hat{y}_s = z$. Let $y_j = \text{argmin}_{y \in Y} d_E(y, \hat{y}_j)$. Clearly $\max_s d_E(y_{i,j} \hat{y}_j) \leq \epsilon$ for any $j = 0, \ldots, s-1$.

$$\begin{aligned} d_E(y_{i_j}, y_{i_{j+1}}) &\leq d_E(y_{i_j}, \hat{y}_j) + d_E(\hat{y}_j, \hat{y}_{j+1}) + d_E(\hat{y}_{j+1}, y_{i_{j+1}}) \\ &\leq \epsilon + d_M(\hat{y}_j, \hat{y}_{j+1}) + \epsilon \\ &= a/s + 2\epsilon \leq r/2 + 2\epsilon < r \end{aligned}$$

Therefore $(y_{i_0}, \dots, y_{i_s})$ forms a path in the r-ball graph.

This might not be the shortest path in the graph

$$\begin{aligned} d_G(x,z) &\leq \sum_{i=j}^{s-1} d_E(y_j, y_{j+1}) \\ &\leq d_M(\underbrace{\hat{y}_0}_{=x}, \hat{y}_1) + \epsilon + \sum_{j=1}^{s-2} d_M(\hat{y}_j, \hat{y}_{j+1}) + 2\epsilon + d_M(\hat{y}_{s-1}, \underbrace{\hat{y}_s}_{=z}) + \epsilon \\ &= d_M(x,z) + 2(s-1)\epsilon \\ &\leq \left(1 + \frac{4\epsilon}{r}\right) d_M(x,z) \end{aligned}$$

we use that $s - 1 \leq \frac{2a}{r}$ with $a = d_M(x,z)$. □

Added remark. *Here we use that the subset of a shortest path is still a shortest path for the specific start and end points.*

Lemma 2.13. *Let $\gamma : [0,a] \to \mathbb{R}^d$ be a unit speed curve with curvature bounded by κ. Then $d_E(\gamma(s), \gamma(t)) \geq \frac{2}{\kappa} \sin\left(\frac{\kappa|t-s|}{2}\right)$*

Proof of a weaker statement. Let c denote the unit-speed parametrization of a circle of radius $\frac{1}{\kappa}$. From Darbins (1957) we obtain $|t-s| \leq \frac{\pi}{\kappa}$:

$$\langle \gamma(s), \gamma(t) \rangle \geq \langle c(s), c(a) \rangle$$

This leads to

$$\begin{aligned} \|\gamma(t) - \gamma(s)\| \|\dot{\gamma}(s) \overset{\text{C.S.}}{\geq} \langle \dot{\gamma}(s), \gamma(t) - \gamma(s) \rangle &= \int_s^t \langle \dot{\gamma}(s), \gamma(u) \rangle du \\ &\geq \int_s^t \langle c(s), c(u) \rangle du \\ &= \langle c(s), c(t) - c(s) \rangle \\ &= \frac{1}{\kappa} \sin(\kappa \cdot (|t-s|)) \end{aligned}$$

when $0 \leq t- \leq \frac{\pi}{\kappa}$.
We now assume $M \subset \mathbb{R}^d$ is compact and connected C^2-manifold with empty or C^2-boundary. In particular, shortest path on M have curvature bounded by some κ. □

Lemma 2.14. *Suppose $M \subset \mathbb{R}^d$ has the above properties. Then for any $x, z \in M$ s.t. $d_M(x,z) \leq \frac{\pi}{\kappa}$*

1. *$d_M(x,z) \max\left(\frac{2}{\pi}, 1 - \frac{\kappa^2}{24} d_M(x,z)^2\right) \leq d_E(x,z) \leq d_M(x,z)$. Moreover there is $\tau > 0$ depending on M s.t. for all $x, z \in M$ with $d_E(x,z) \leq \tau$ it holds*
2. *$d_E(x,z) \leq d_M(x,z) \leq d_E(x,z) \min\left(\frac{\pi}{2} + C_0 \kappa^2 d_E(x,z)^2\right)$ where c_0 is a constant that can be taken to be $c_0 = \frac{\pi^2}{50}$.*

Proof. For 1.:
Take $x, z \in M$ and let $a = d_M(x,z) \leq \frac{\pi}{\kappa}$. Let $\gamma : [0,a] \to M$ be a unit-speed shortest path on M s.t. $\gamma(0) = x, \gamma(a) = z$. By assumption γ has curvature bounded by κ. Applying lemma 2.13 gives

$$d_E(x,z) = d_E(\gamma(0), \gamma(a)) \geq \frac{2}{\kappa} \sin\left(\kappa \frac{a}{2}\right) \geq \max\left(a - \frac{\kappa^2}{24} a^3, \frac{2}{\pi} a\right)$$

and $\sin(t) \geq t - \frac{t^3}{6}, \sin(t) \geq \frac{2t}{\pi} \forall t \leq \frac{\pi}{2}$.

For 2.: by 1. $d_M(x,z) \leq \frac{\pi}{\kappa}$, then $d_M(x,z) \leq \frac{\pi}{2} d_E(x,z)$ and

$$\begin{aligned} d_M(x,z) &\leq \frac{d_E(x,z)}{\left(1 - \frac{\kappa^2}{24} d_M(x,z)^2\right)} \\ &\leq \frac{d_E(x,z)}{\left(1 - \frac{\kappa^2}{24}\left(\frac{\pi}{2} d_E(x,z)\right)^2\right)} \\ &\leq d_E(x,z)(1 + C_0 \kappa^2 d_E(x,z)^2) \end{aligned}$$

where the last inequality holds if $\kappa d_E(x,z)$ is small enough. Therefore, it is enough to show that there is $\tau > 0$ s.t.

$$d_M(x,z) \leq \frac{\pi}{\kappa}$$

when $d_E(x,z) \leq \tau$. This is true, because the smoothness of M guarantees that d_M be continuous as a function of the compact set $M \times M$. □

Theorem 2.15. *Suppose $M \subset \mathbb{R}^d$ has the above properties. Consider a sample $Y = \{y_1, \ldots, y_m\} \subset M$. For $r > 0$ from the corresponding r-ball graph. Let c_0 and τ be defined per lemma 2.14 and $\kappa r \leq \frac{1}{3}$. We have*

$$d_M(x,z) \leq (1 + C_0 \kappa^2 r^2) d_G(x,z) \ \forall x, y \in Y$$

Proof. Fix $x, z \in Y$. Let $x = y_{i_0}, \ldots, z = y_{i_s}$ define a shortest path in the graph joining x, z, so that $d_G(x,z) = \sum_{j=0}^{s-1} \Delta_j$, where $\Delta_j = d_E(y_{i_j}, y_{i_{j+1}})$. Define $a = d_M(x,z)$ and $a_j = d_M(y_{i_j}, y_{i_{j+1}})$. Since $\Delta_j \leq r \leq \tau$ by lemma 2.14 we see

$$\Delta_j \min\left(\frac{\pi}{2} c_0 \kappa^2 \Delta_j^2\right) \geq a_j.$$

By assumption, $\kappa r \leq \frac{1}{3}$, and this can be seen to imply $1 + C_0 \kappa^2 r^2 \leq \frac{\pi}{2}$, which then implies that $a_j \leq \Delta_j + C_0 \kappa^2 \Delta_j^3$, we thus have

$$a \leq \sum_{j=1}^{s-1} a_j \leq \sum_{j=0}^{s-1} (\Delta_j + C_0 \kappa^2 \Delta_j^3) \leq \sum_{j=0}^{s-1} \Delta_j (1 + C_0 \kappa^2 r^2) = (1 + C_0 \kappa^2 r^2) d_G(x,z)$$ □

Added remark. *This is the justification for using Isomap. One should consider, that the assumptions are NOT always met in practice, which might result our algorithm to fail. In particular we don't know M in practice, which makes our assumptions hard to check ...*
Luckily the assumptions are often met "naturally".

2.2.1 Parallel transport unfolding

Underlying idea: Systematically overestimating the distance (by doing unnecessary turns on the graph). We then think about the tangent spaces and try to connect the local views of the tangent spaces. Main idea we find a better path (closer to the geodesic).
We will now consider the computational ingredients using discrete parallel transport. We are using a l-nearest neighbor graph.

Start of lecture 18 (20.06.24)

1. Approximate tangent spaces: Take q-NN in the graph, $q \geq k$, denoted

   $$\{\tilde{y}_l^i\}_{l=1}^q, \ \hat{y}_l^i = \tilde{y}_l^i - y_i \ \hat{Y}^i = [\hat{y}_1^i, \ldots, \hat{y}_q^i]$$

   The p left singular vectors of $\hat{Y}^i$ to the p largest singular values give an orthonormal basis for T_i, spanning tje approximate tangent space

   $$T_i = [t_1^i, \ldots, t_p^i] \in \mathbb{R}^{d \times p}$$

   separate k, q to avoid unwanted connection while still getting good approximations

   The space spanned by the columns of T_i

2. Now given y_o and y_j connected in G

   $$R_{j,i} = \underset{R \in O(p)}{\operatorname{argmin}} \|T_i - T_j R\|_F$$

   $R_{j,i}$ is the discrete metric connection between y_i, y_j, it best aligns T_i, T_j. By definition $R_{i,j} = R_{j,i}^{-1} = R_{j,i}^T$. With $T_i^T T_j = U \Sigma V^\intercal$ we can show $R_{j,i} = V U^T$.

   $O(p)$ are the $p \times p$ orthogonal matrices

3. Consider (y_i, y_j, y_k) and start w.l.o.g. y_i. The first edge

$$l_i = y_j - y_i$$

is projected onto T_i: $v_i = T_i^\intercal e_i$. We set $z_i = 0$ and $z_j = z_i + v_i$ defines the first modified edge. Now, $e_j = y_k - y_i$ and $T_j^\intercal e_j$ is parallel transported into the tangent space at y_i

Projected in the L^2 sense

$$v_j = R_{i,j}[T_j^\intercal e_j]$$

and $z_k = z_j + v_j$Under some assumptions

$$\|v_i + v_j\|_2 = d_E(z_i, z_k) \approx d_M(y_i, y_k)$$

4. For longer paths $y_{i_1}, \dots, y_{i_m}$ we iteratively project the edges $l_{i_s} = y_{i_{s+1}} - y_{i_s}$ onto T_{i_j} before parallel transporting back to T_{i_1}

$$V_{i_s} = \left(\prod_{j=1}^{s-1} R_{i_j, i_{j+1}} \right) [T_{i_s}^\intercal l_{i_s}]$$

with $V = \sum_{j=1}^{M} v_{I_S}$ WE GET $\|v\|_2 \approx d_M(y_1, y_{i_m})$

$$(\star)\ 1 - \xi \frac{d_G(y_i, y_j)}{d_M(y_i, y_j)} \leq 1 + \xi$$

We saw in PTU

$$\min_{R \in O(p)} \|Y^\intercal - X^\intercal R\|_F.$$

Generally aligning two point sets using an orthogonal transformation is called **procrustes problem**.
Pointwise:

$$\min_{R \in O(p)} \sum_{i=1}^{N} \|y_i - R x_i\|_2^2.$$

Consider two configurations X, Y, given

which stem from two different EDMs, which are somehow alligned / comparable

$$\|Y^\intercal Y - X^\intercal X\|_F = \epsilon^2$$

and

$$\|X^\dagger\|_2 \epsilon \leq \frac{1}{\sqrt{2}}$$

it holds

$$\min_{R \in O(d)} \|Y^\intercal X^\intercal R\|_F \leq (1 + \sqrt{2}) \|X^\dagger\|_2 \epsilon^2$$

For $D, \tilde{D} \in$ EDM it holds using $\epsilon^2 = \frac{1}{2}\|H(\tilde{D} - D)H\|_F$ a corresponding result.
Using $(\star)$ for Isomap amd X the exact embedding using d_M into $\mathbb{R}^p$ one has

$$\min_{R \in O(p)} \left(\frac{1}{N} \sum_{i=1}^{N} \|z_i - R x_i\|^2 \right)^{\frac{1}{2}} \leq \frac{36\sqrt{p}\rho^3}{w^2} \xi$$

for Z the approximate embedding and ρ, w are singular values of our datamatrix:

$$\rho = \rho(X) = \frac{\sigma_1(X)}{\sqrt{N}}$$

radius of X largest deviations along any direction in space.

$$w = w(X) = \frac{\sigma_p(w)}{\sqrt{N}}$$

half width of X, smallest deviations along any direction in space.

Using kernels again ...

Nonlinear PCA
Reminder: $C = \frac{1}{N} Y \cdot Y^\intercal = \frac{1}{N} \sum_{i=1}^N y_i \cdot_i^T$ we consider some **feature map** $\phi : R^d \to \mathbb{R}^r -: \mathcal{F}$ For simplicity, we assume to be mean-centered on the feature space:

$$\sum_{i=1}^N \phi(y_i) = 0.$$

Now, do PCA in $\mathcal{F}$, $C_\phi = \frac{1}{N} \sum_{i=1}^N \phi(y_i)\phi(y_i)^\intercal = \frac{1}{N} \phi(Y)\phi(Y)^\intercal = \frac{1}{N} \Phi \cdot \Phi^\intercal$.
EVD gives $C_\phi u_i = \lambda_i u_i$ and by theorem 2.3 the nonlinear principal components are

$$X_i = u_i^\intercal \Phi.$$

IGNORE:

$$\Phi\Phi^\intercal \to \Phi^\intercal\Phi$$

$$U^\intercal = V^\intercal \Phi^\intercal$$

$$X = V^\intercal \Phi^\intercal \Phi = \Lambda^{-\frac{1}{2}} \Phi^\intercal \Phi = \Lambda^{-\frac{1}{2}} V^\intercal V \Lambda V^\intercal = \Lambda^{\frac{1}{2}} V^\intercal$$

STOP IGNORING

$$x_I = V^\intercal \Phi^\intercal \Phi(y_i)$$

$$K_{i,j} = \langle \Phi(y_i), \Phi(y_j) \rangle_\mathcal{F} =: K(y_i, y_j)$$

A projection of a point y with image $\phi(y)$ gives

$$\begin{aligned} x &= V^\intercal \Phi^\intercal \phi(y) \\ &= \sum_{i=1}^N v_i \langle \phi(y_i), \phi(y) \rangle_\mathcal{F} \\ &= \sum_{i=1}^N v_i K(y_i, y) \end{aligned}$$

This kernelized form we call **Kernel MDS**, but it is usually called **Kernel PCA** in the literature.

The interpretation step of PCA gets a lot harder. Especiially, since the feature maps are not unique ...

To consider non-centered data, we need to center it:

$$\tilde{\phi}(y_i) \coloneqq \phi(y_i) - \frac{1}{N} \sum_{j=1}^N \phi(y_j)$$

with associated kernel $\tilde{K}$.

$$\tilde{\Phi}(Y) = (\Phi^c(Y) - \frac{1}{N} \Phi(Y) 1) 1^\intercal = \Phi(Y) H$$

Action of H goes through the SP

$$\tilde{K} = K^c = HKH$$

Algorithm 3 Nonlinear PCA

Input: nonlinear data set Y $\phi : \mathbb{R}^d \to \mathbb{R}^r, p$
Output: configuration X in $p \leq \min(r, N)$ dimensions
$K = -H\Phi^\intercal(Y)\Phi H$
$[V_p, \Lambda_p] = \text{EVD}(K, p)$
Return $\Lambda_p^{\frac{1}{2}} V_p^\intercal$

Algorithm 4 Nonlinear MDS

Input: nonlinear data set Y, Kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$
Output: configuration X in $p \leq N$ dimensions

$K_{i,j} = K(y_i, y_j)$
$\hat{K} = HKH$
$[V_p, \Lambda_p] = \text{EVD}(\hat{K}, p)$
Return $\Lambda_p^{\frac{1}{2}} V_p^\intercal$

Appendix

Tutorials

All norms and scalar products w.r.t. H if not specified.

Start of tutorial 02 (23-04-24)

a)

Proof.

$$|h_n(t) - h_m(t)| \overset{\text{Reproduction equality}}{\leq} |\langle h_n - h_m, k(t,)\rangle| \overset{\text{C.S.}}{\leq} \|h_n - h_m\|_H \|k(t,\cdot)\|_H \to 0$$

Therefore $h_n(t)$ is Cauchy $\implies$ $h_n(t)$ converges. □

b)

Proof. Show definition is well defined:
1.: $\langle f, g\rangle \in \mathbb{R}$ for all $f, g \in \mathcal{N}_k$.
f_n, g_n Cauchy sequences, $f_n \to f, g_n \to g$ pointwise.
1.1.:Show that $\lim_{n\to\infty} \|f_n\|_H$ exists in $\mathbb{R}$.

$$|\|f_n\|_H - \|f_m\|_H| \leq \|f_n - f_m\|_H \implies \|f_n\|_H \text{ is Cauchy}$$

and therefore bounded.
1.2.: Show $\langle f, g\rangle_H = \lim_{n\to\infty}\langle t_n, g_n\rangle_H$ exists in $\mathbb{R}$.

$$\begin{aligned}|\langle f_n, g_n\rangle_H - \rangle f_m, g_m\rangle_H| &= |\langle f_n - f_m, g_n\rangle_H + \langle f_m, g_n - g_m\rangle| \\ &\leq \|f_n - f_m\|_H \|g_n\|_H + \|f_n\|_H \|g_n - g_m\|_H\end{aligned}$$

Let f_n, f_n', g_n Cauchy, $f_n \to f, f_n' \to f, g_n \to g$ pointwise.
We need:

$$\begin{aligned}\lim_{n\to\infty}\langle f_n, g_n\rangle_H = \lim_{n\to\infty}\langle f_n', g_n\rangle_H &\iff \lim_{n\to\infty}\langle f_n - f_n', g_n\rangle_H = 0 \\ &\iff f_n \to 0 \text{ pointwise } \implies \langle f_n, g_n\rangle \to 0 \\ &\iff \forall f_n \to 0 \text{ pointwise } \langle f_n, f_n\rangle \to 0 \\ &\iff f = 0 \implies \langle f, f\rangle_H = 0\end{aligned}$$

$h_n = f_n - f_n'$.
1.: f_n is Cauchy in H

$$\|(f_n - f_n') - (f_m - f_m')\|_H \leq \|f_n - f_m\| + \|f_n' - f_m'\|_H$$

2.: h_n bounded by M(follows from Cauchy)
3.: $h_n \to 0$ in H
Fix $l \in \mathbb{N}$ and let $h_l = \sum_{i=1}^{m} a_i k(x, \cdot)$

$$\langle h_n, h_l \rangle = \lambda_{A^{(l)}, x^{(l)}}(h_n) = \sum_{i=1}^{m} a_i h_m(x_i) \to 0$$

$$\implies (\star) : \forall \epsilon > 0 : \exists n_0 \in \mathbb{N} : \forall n \geq n_0 |\langle h_n, h_l \rangle| < \epsilon$$

h_n is Cauchy $\implies \forall \delta > 0 \exists l \in \mathbb{N} \forall n \geq l$:

$$\|h_n - h_l\| < \delta / M.$$

Choose n_0 s.t. $(\star)$ holds with δ

$$\begin{aligned} \|h_n\|_H^2 = \langle h_n, h_n \rangle_H &= \langle h_n, h_l \rangle + \langle h_n, h_n - h_l \rangle \\ &\leq \delta + \|h_n\|_H \|h_n - h_l\| < \delta + M \frac{\delta}{M} \end{aligned}$$

Choose $\delta = \frac{\epsilon}{2}$.
Still have to show $\langle f, f \rangle = 0$:

$$\lim_{n \to \infty} f_n(t) = \lim_{n \to \infty} \langle f_n, k(t, \cdot) \rangle_H \leq \lim_{n \to \infty} \|f_n\| \underbrace{\|k(t, \cdot)\|}_{\text{bounded}}$$

□

c)

Proof. f_n Cauchy:
$f_n \to f$ in $\mathcal{N}_k$ and $f \in \mathcal{N}_k$.
Construct Cauchy sequence in H:
$\lim_{n \to \infty} f_n(k) = f_n$ and $f_n^{(k)} \in H$.
$\forall n \in \mathbb{N}$ choose $k(n)$ such that

$$\|f_n - f_n^{k(n)}\| < \frac{1}{n}$$

$g_n = f_n^{(k(n))}$. Let $\epsilon > 0$, $n_0 = \max\{\frac{3}{\epsilon}, m\}$
$\forall k, l \geq m : \|f_k - f_l\| < \epsilon / 3$

$$\begin{aligned} \|g_n - g_m\| &\leq \|f_n^{(k(n))} - f_n\| + \|f_n - f_m\| + \|f_m - f_m^{(k(n))}\| \\ &\leq \frac{\epsilon}{3} + \frac{\epsilon}{3} + \frac{\epsilon}{3} = \epsilon \end{aligned}$$

for all $n, m \geq n_0$.
Set $f \in \mathcal{N}_k$ as the limit of g_n (because it is a Cauchy sequence in H).
2.: f_n converges to f in $\mathcal{N}_k$.

$$\begin{aligned} \|f_n - f\| &\leq \|f_n - f_{n+1}\| + \|f_{n+1} - f_{n+1}^{(k(n+1))}\| + \|g_{n+1} - f\| \\ &< \frac{\epsilon}{3} + \frac{1}{n+1} + \frac{\epsilon}{3} = \epsilon \end{aligned}$$

□

$$\begin{aligned}\exp(-(x-y)^2) &= \exp(-(x^2-2xy+y^2)) \\ &= \exp(-x^2)\exp(+2xy)\exp(-y^2) \\ &= \sum_{k=0}^{\infty} \frac{(2xy)^k}{k!}\exp(-x^2)\exp(-y^2) \\ &= \sum_{k=0}^{\infty} \underbrace{\frac{2^k}{k!}}_{=\lambda_k} \underbrace{\frac{x^k}{\exp(x^2)}}_{\varphi_k(x)} \underbrace{\frac{y^k}{\exp(y^2)}}_{\varphi_k(y)}\end{aligned}$$

$D_n(x,y) = \sum_{k=-n}^{n} \overline{\exp(-ikx)}\exp(-iky)$

List of Lectures