Quantization with Maximum Mean Discrepancies

Are Reproducing Kernel Hilbert Spaces (RKHS) of any use in Stochastic Optimization?

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Mathematik!
TU Chemnitz

Kernels
Densities and bandwidth selection

- The kernel density estimator of the density f is

$$\hat{f}_n(x) = \frac{1}{n}\sum_{i=1}^{n} k_h\left(x - X_i\right),$$

where

$$k_h(\cdot) = \frac{1}{h} k\left(\frac{\cdot}{h}\right).$$

- Typical examples for kernels k are $k(x) \simeq \max\left\{1 - x^2; 0\right\}$, the Gaussian kernel, or the logistic kernel $k(x) \simeq \frac{1}{(e^x + e^{-x})^2}$.
- The Cauchy kernel $k(x) \simeq \frac{1}{1+x^2}$ does not have moments.

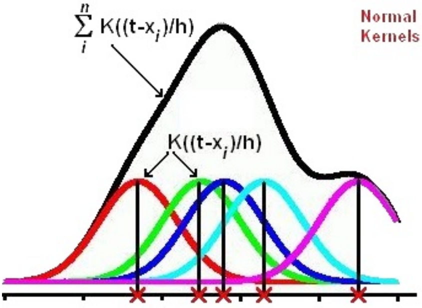


Figure: Normal Kernels

Density estimator
Traditional kernels

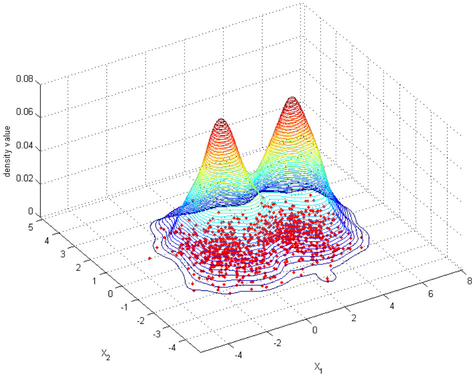


Figure: density

Examples (Density estimation)

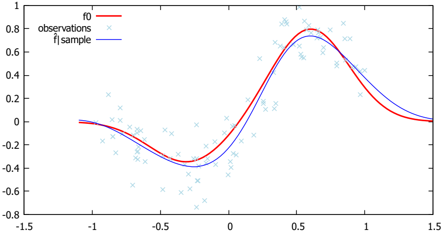
Parzen–Rosenblatt estimator associates with the empirical measure

$$\mu := \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$$

the function

$$\mu_k(x) = \frac{1}{n}\sum_{i=1}^{n} k(x_i, x)$$

in the space $\mathcal{H}_k$.



Problem (Stochastic optimization)

Solve

$$\min_{x\in\mathcal{X}} f_0(x) := \mathbb{E}\, f(x, Y).$$

Motivation (cont.)

Conditional expectation and stochastic optimization

Problem (Optimal control: Hamilton–Jacobi–Bellman)

$$v_t(x) = \sup_u \mathbb{E}\left(\begin{array}{l} c(x, X_{t+1}, u) \\ +\gamma\, v_{t+1}(X_{t+1}) \end{array} \,\middle|\, X_t = x \right);$$

Problem (Time series, learning)

Predict the next X_{t+1}, given the history $X_t, \dots, X_{t-\ell}$.

Outline

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Consider the space $\mathcal{H}$ of functions on $\mathcal{X}$ (usually $\mathcal{X} \subset \mathbb{R}^d$),

$$\begin{aligned} f \colon \mathcal{X} &\to \mathbb{R} \\ z &\mapsto f(z). \end{aligned}$$

In RKHS $(\mathcal{H}, \langle \cdot \mid \cdot \rangle_{\mathcal{H}})$, there is $k_x \in \mathcal{H}$ such that

$$f(x) = \langle f \mid k_x \rangle_{\mathcal{H}} = \langle f(\cdot) \mid k_x(\cdot) \rangle_{\mathcal{H}} \qquad \text{for all} \qquad f \in \mathcal{H},\ x \in \mathcal{X}.$$

We define the kernel

$$\begin{aligned} k \colon \mathcal{X} \times \mathcal{X} &\to \mathbb{R} \\ (x, y) &\mapsto \langle k_x \mid k_y \rangle_{\mathcal{H}}. \end{aligned}$$

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The characterizing property

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Examples

A. Berlinet and C. Thomas-Agnan (2004). *Reproducing Kernel Hilbert Spaces in Probability and Statistics*. Springer US. DOI: 10.1007/978-1-4419-9096-9

A sequence space

$$f=(f_i)_{i=1}^\infty\in\mathbb{R}^{\mathbb{N}},\ \mathcal{X}=\mathbb{N},$$

$$\|f\|:=\sum_{i=1}^\infty\frac{(f_{i+1}-f_i)^2}{\theta^i}$$

$$k(i,j)=\frac{\theta^{\max(i,j)}}{1-\theta}$$

Dirichlet kernel — trigonometric polynomials

$$f(x)=\sum_{k=-N}^N a_k\,e^{ikx},$$

$$\|f\|^2:=\int_{-\pi}^{\pi}f(x)^2\mathrm{d}x$$

$$k(x,y)=\frac{\sin\left(N+\frac12\right)(x-y)}{2\sin\frac{x-y}{2}}$$

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Examples (cont.)

Nice inner product on $[0,1]$ (Payley–Wiener space)

$f, g \in L^2([-1,1])$ and Fourier transform supported in $[0,1]$

$$\langle f | g \rangle_{\mathcal{H}} := \int_{-1}^{1} f(x) g(x) \,\mathrm{d}x$$

$$k(x,y) = \frac{\sin(t-s)}{t-s}$$

Periodic functions

$$\|f\|_{\mathcal{H}}^2 := \int_0^1 f(x)^2 + f(x)^{(m)2} \mathrm{d}x$$

$$k(x,y) = B_{2m}(|x-y|)$$

where B_{2m} is the Bernoulli polynomial of degree $2m$.

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Laplace kernel

$f, g \in L^2(\mathbb{R})$,

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$$\|f\|_{\mathcal{H}} := \int_{\mathbb{R}} f(x)^2 + \frac{1}{\tau^2} f'(x)^2 \mathrm{d}x$$

Connections to ReLU functions

$$f, g \in L^2((0,\infty))$$

$$\langle f | g \rangle_{\mathcal{H}} := \int_{-1}^{1} f'(x) g'(x) \, \mathrm{d}x$$

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Moore–Aronszajn

k is positive definite

With $k_y := k(\cdot, y)$, $\langle k_x | k_y \rangle_{\mathcal{H}} = \langle k_x | k(\cdot, y) \rangle_{\mathcal{H}} = k(x, y)$, and

$$\left\langle \sum_{i=1}^{n} \alpha_i k_{x_i} \middle| \sum_{j=1}^{m} \beta_j k_{x_j} \right\rangle_{\mathcal{H}} = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_i \beta_j \cdot k(x_i, x_j),$$

thus $\big(k(x_i, x_j)\big)_{i,j=1}^{n}$ is a positive definite matrix.

Theorem (Moore–Aronszajn)

If k is positive definite, then there is a space $\mathcal{H}_k$ with kernel k.

The Gaussian kernel

$$k(x, y) := e^{-\|x-y\|^2/\ell^2}$$

is a kernel function (for $\ell > 0$ some fixed length parameter).

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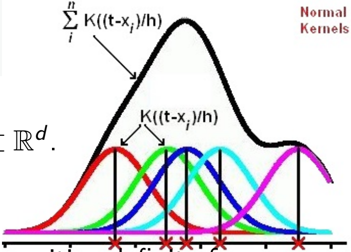
Outline

Stochastic Optimization Problems Involve Uncertainties

Embedding probabilities in RKHS



Consider probabilities on $(\mathcal{X}, \Sigma, P)$ with $\mathcal{X} \subset \mathbb{R}^d$.

$$k\colon \mathcal{X} \times \mathcal{X} \to \mathbb{R}$$

is a kernel, if every $\boldsymbol{K}$ with $\boldsymbol{K}_{ij} := k(x_i, x_j)$ is positive definite for every $x_i, \dots, x_n \in \mathcal{X}$.

Definition (Embedding)

Let μ be a measure on $\mathcal{X}$.
Define the function

$$\mu_k(\cdot) := \int_{\mathcal{X}} k(\cdot, y)\, \mu(\mathrm{d}y).$$

For a probability measure P, then $P_k(\cdot) = \mathbb{E}\, k(\cdot, \xi)$ with $\xi \sim P$.

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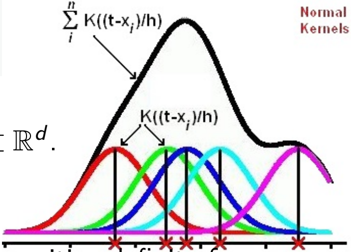

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Embedding:

$$\iota\colon \mathcal{M}(\mathcal{X}) \hookrightarrow \mathcal{H}_k(\mathcal{X})$$

$$\mu \mapsto \mu_k$$

For a probability measure P, then $P_k(\cdot) = \mathbb{E}\, k(\cdot, \xi)$ with $\xi \sim P$.

Outline

Bounded kernel

We shall typically assume that

$$k(x,x) = \|k(x,\cdot)\|^2_{\mathcal{H}_k} \leq C < \infty, \qquad x \in \mathcal{X}.$$

The embedding function

$$\mu_k(\cdot) = \int_{\mathcal{X}} k(\cdot, y)\,\mu(\mathrm{d}y) \in \mathcal{H}_k(\mathcal{X})$$

then is well defined (as Bochner integral, cf. Diestel and Uhl[1]).

[1] J. Diestel and J. J. Uhl Jr. (1977). *Vector Measures*. Mathematical Surveys 15. American Mathematical Society. URL: http://books.google.com/books?id=EQFjD90fXWAC.

Key property of the space $\mathcal{H}_k$ is its inner product, satisfying

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

Reproducing property
Characterization

Key property of the space $\mathcal{H}_k$ is its inner product, satisfying

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

If $\mu_k(\cdot) = \int_{\mathcal{X}} k(\cdot,y)\,\mu(\mathrm{d}y)$, by linearity

$$\begin{aligned}
\langle k(\cdot,x) | \mu_k(\cdot)\rangle_k &= \int_{\mathcal{X}} \langle k(\cdot,x) | k(\cdot,y)\rangle_{\mathcal{H}_k}\,\mu(\mathrm{d}y) \\
&= \int_{\mathcal{X}} k(x,y)\,\mu(\mathrm{d}y) \\
&= \mu_k(x).
\end{aligned}$$

Maximum Mean Discrepancy

A new distance for probability measures

Definition

The *Maximum Mean Discrepancy* of measures $\mu, \gamma \in \mathcal{M}(\mathcal{X})$ is

$$\mathrm{MMD}(\mu,\gamma) := d_k(\mu,\gamma) := \|\mu_k - \gamma_k\|_{\mathcal{H}_k}.$$

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- MMD is a distance
- on $\mathcal{M}(\mathcal{X})$, not just $\mathcal{P}(\mathcal{X})$;
- $$\begin{aligned}\mathrm{MMD}(\mu,\eta)^2 &= \langle \mu_k - \gamma_k |\ \mu_k - \gamma_k \rangle_k \\ &= \iint_{\mathcal{X}\times\mathcal{X}} k(x,y)\mu(\mathrm{d}x)\mu(\mathrm{d}y) \\ &\qquad - 2\iint_{\mathcal{X}\times\mathcal{X}} k(x,y)\mu(\mathrm{d}x)\gamma(\mathrm{d}y) \\ &\qquad + \iint_{\mathcal{X}\times\mathcal{X}} k(x,y)\gamma(\mathrm{d}x)\gamma(\mathrm{d}y).\end{aligned}$$

Let $f \in \mathcal{H}_k(\mathcal{X})$. Then

$$\begin{aligned}
\mathbb{E}_P f - \mathbb{E}_Q f &= \int_{\mathcal{X}} f(x)\, P(\mathrm{d}x) - \int_{\mathcal{X}} f(x)\, Q(\mathrm{d}x) \\
&= \int_{\mathcal{X}} \langle k(x,\cdot) | f(\cdot)\rangle_k\, P(\mathrm{d}x) - \int_{\mathcal{X}} \langle k(x,\cdot) | f(\cdot)\rangle_k\, Q(\mathrm{d}x) \\
&= \langle P_k(\cdot) | f(\cdot)\rangle_k - \langle Q_k(\cdot) | f(\cdot)\rangle_k \\
&\le \|P_k - Q_k\|_k \cdot \|f\|_k \qquad (1) \\
&= \|f\|_k \cdot \mathrm{MMD}(P,Q),
\end{aligned}$$

with Cauchy–Schwartz in (1).

Of Interest In Stochastic optimization?
Optimal Transport and MMD

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$$\mathbb{E}_P f - \mathbb{E}_Q f \leq Lip(f) \cdot w(P, Q).$$

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For $x \in \mathcal{X}$,

$$\delta_x(A) := \mathbb{1}_A(x)$$

is the Dirac measure. Its embedding is

$$\delta_{xk}(\cdot) = k(x,\cdot).$$

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For $x, y \in \mathcal{X}$,

$$\begin{aligned}\mathrm{MMD}(\delta_x, \delta_y) \\ &= \|k(x,\cdot) - k(y,\cdot)\|_{\mathcal{H}_k} \\ &=: d_k(x,y)\end{aligned}$$

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It holds that

$$\mathrm{MMD}(\delta_x, \delta_y) = \sqrt{k(x,x) - 2k(x,y) + k(y,y)}.$$

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Recall

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For the Gaussian kernel $k(x,y)=e^{-\|x-y\|^2/\ell^2}$,

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For the Laplacian kernel $k(x,y)=e^{-\|x-y\|/\ell}$,

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Optimal transport and MMD
Relation

Proposition

Let P and Q be probability measures. Suppose that

$$k(x,x) - 2k(x,y) + k(y,y) \le c^2 \cdot d(x,y)^{2\alpha}, \qquad x, y \in \mathcal{X},$$

for some $c > 0$ and $\alpha \ge 1/2$. Then it holds that[a]

$$\mathrm{MMD}(P,Q) = \|P_k - Q_k\|_{\mathcal{H}_k} \le c \cdot w_\alpha(P,Q)^\alpha.$$

[a] R. Lakshmanan and A. P. (2024). "Unbalanced Optimal Transport and Maximum Mean Discrepancies: Interconnections and Rapid Evaluation". In: *Journal of Scientific Computing* 100.72. DOI: 10.1007/s10915-024-02586-2.

	Kernel	Hölder α	constant c
Gauss	$e^{-\|x-y\|^2/\ell^2}$	1	$2/\ell^2$
Laplace	$e^{-\|x-y\|/\ell}$	$1/2$	$2/\ell$
Inverse multiquadratic	$1/\sqrt{\|x-y\|^2+c^2}$	1	$2/c^4$

Outline

Problem statement

Problem (General measures)

$$\text{minimize } \operatorname{MMD}(\mu, \mu^n) = \|\mu_k - \mu_k^n\|_k$$
$$\text{in } \boldsymbol{\mu} = (\mu_1, \dots, \mu_n)$$
$$\text{and } \boldsymbol{x} = (x_1, \dots, x_n),$$

where $\mu^n = \sum_{i=1}^n \mu_i \cdot \delta_{x_i}$.

Here,
$\boldsymbol{\mu} = (\mu_1, \dots, \mu_n) \in \mathbb{R}^n$
are the weights, and
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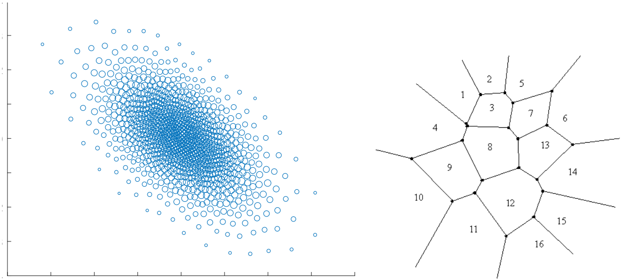

(a) Optimal weights and locations **(b)** Voronoi tessellation

Figure: Quantization in Wasserstein distance

Locations given, optimal weights

Proposition

Let $x_1, \dots, x_n$ be fixed. Then the optimal weights $\boldsymbol{\mu} = (\mu_1, \dots, \mu_n)$ satisfy

$$\boldsymbol{K}\boldsymbol{\mu} = \boldsymbol{m},$$

where $\boldsymbol{K} = \begin{pmatrix} k(x_1, x_1) & \dots & k(x_1, x_n) \\ \vdots & & \vdots \\ k(x_n, x_1) & \dots & k(x_n, x_n) \end{pmatrix}$ *and*

$$\boldsymbol{m}_i = \mathbb{E}\, k(x_i, \cdot) = \int_{\mathcal{X}} k(x_i, \xi)\, P(\mathrm{d}\xi).$$

Further, $\mathrm{MMD}_k(\mu, \mu^n)^2 = \iint_{\mathcal{X}^2} k(\xi, \xi')\mu(\mathrm{d}\xi)\mu(\mathrm{d}\xi') - \boldsymbol{m}^\top \boldsymbol{K}^{-1}\boldsymbol{m}$.

In general,

$$\mu(\mathcal{X}) \neq \mu^n(\mathcal{X}).$$

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Optimal weights

Problem (Probability measures)

$$\text{minimize } \|P_k - P_k^n\|_k$$
$$\text{where } P^n = \sum_{i=1}^{n} p_i\, \delta_{x_i} \text{ and } p_1 + \dots + p_n = 1.$$

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Outline

Problem (General measures)

$$\text{minimize } \iint_{\mathcal{X}^2} k(\xi,\xi')\mu(\mathrm{d}\xi)\mu(\mathrm{d}\xi') - \boldsymbol{m}^\top \boldsymbol{K}^{-1}\boldsymbol{m} + \frac{\left(\mathbb{1}^\top \boldsymbol{K}^{-1}\boldsymbol{m} - 1\right)^2}{\mathbb{1}^\top \boldsymbol{K}^{-1}\mathbb{1}},$$

$$\text{where } \boldsymbol{m}_i = \mathbb{E}\, k(x_i,\cdot) = \int_{\mathcal{X}} k(x_i,\xi)\, P(\mathrm{d}\xi).$$

Define

$$c(\boldsymbol{x},\xi,\xi') := k(\xi,\xi') - k(\xi,\boldsymbol{x})^\top \boldsymbol{K}(\boldsymbol{x})^{-1} k(\xi',\boldsymbol{x}) + \frac{\left(1 - \mathbb{1}^\top \boldsymbol{K}(\boldsymbol{x})^{-1} k(\xi,\boldsymbol{x})\right)^2}{\mathbb{1}^\top \boldsymbol{K}(\boldsymbol{x})^{-1}\mathbb{1}}.$$

Then

$$\min_{\boldsymbol{x}=(x_1,\dots,x_n)} \mathbb{E}_{(\xi,\xi')\sim P\otimes P}\; c(\boldsymbol{x},\xi,\xi').$$

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To solve

$$\min_{\boldsymbol{x}=(x_1,\dots,x_n)} \mathbb{E}_{(\xi,\xi')\sim P\otimes P}\; c(\boldsymbol{x},\xi,\xi'),$$

repeat

generate independent $\xi,\xi'\sim P\otimes P$,

$$\text{update } \boldsymbol{x} \leftarrow \boldsymbol{x} - \eta_t\cdot\nabla c(\boldsymbol{x},\xi,\xi') \text{ and}$$

$$\boldsymbol{m} \leftarrow \frac{1}{t+1}\left(t\cdot\boldsymbol{m} + \frac{1}{2}\big(k(\xi,\boldsymbol{x}) + k(\xi',\boldsymbol{x})\big)\right),$$

with $\sum_{t=1}^\infty \eta_t = \infty$ and $\sum_{t=1}^\infty \eta_t^2 < \infty$.

Non-negativity constraints

Problem (Probability measures)

$$\begin{aligned} &\text{minimize } \|P_k - P_k^n\|_k \\ &\text{where } P^n = \sum_{i=1}^n p_i\,\delta_{x_i},\; p_1 + \dots + p_n = 1, \\ &\text{and } p_1 \geq 0, \dots, p_n \geq 0. \end{aligned}$$

Instead of solving

$$\begin{aligned} &\text{minimize } f(\boldsymbol{x}) \\ &\text{subject to } \boldsymbol{x} \in \mathcal{X} \end{aligned}$$

minimize $f\big(\pi_{\mathcal{X}}(\boldsymbol{x})\big) + \|\boldsymbol{x} - \pi_{\mathcal{X}}(\boldsymbol{x})\|$,

with projection $(\pi_{\mathcal{X}} \circ \pi_{\mathcal{X}} = \pi_{\mathcal{X}})$

$$\pi_{\mathcal{X}}(\boldsymbol{x}) \begin{cases} = \boldsymbol{x} & \text{if } \boldsymbol{x} \in \mathcal{X}, \\ \cdots & \text{if } \boldsymbol{x} \notin \mathcal{X} \end{cases}$$

for example (Norkin and P. (2024))

$\pi_{\mathcal{X}}(\boldsymbol{x}) := \arg\min_{\boldsymbol{y} \in \mathcal{X}} \|\boldsymbol{y} - \boldsymbol{x}\|$.

Example

Suppose that $P \sim \mathcal{N}(\mu, \sigma^2)$, and $k(x,y) = \frac{1}{\sqrt{2\pi\ell^2}} e^{-\frac{1}{2}|x-y|^2}$, then

$$\mathrm{MMD}_k(P, P^n)^2 = \frac{1}{\sqrt{2\pi(2\sigma^2+\ell^2)}}.$$

$$- \frac{1}{\sqrt{2\pi(2\sigma^2+\ell^2)}} \sum_{i,j=1}^{n} e^{-\frac{(x_i-\mu)^2+(x_j-\mu)^2}{2(\sigma^2+\ell^2)}} \boldsymbol{K}(\boldsymbol{x})_{ij}^{-1}.$$

Outline

Proof of concept
Normal distribution

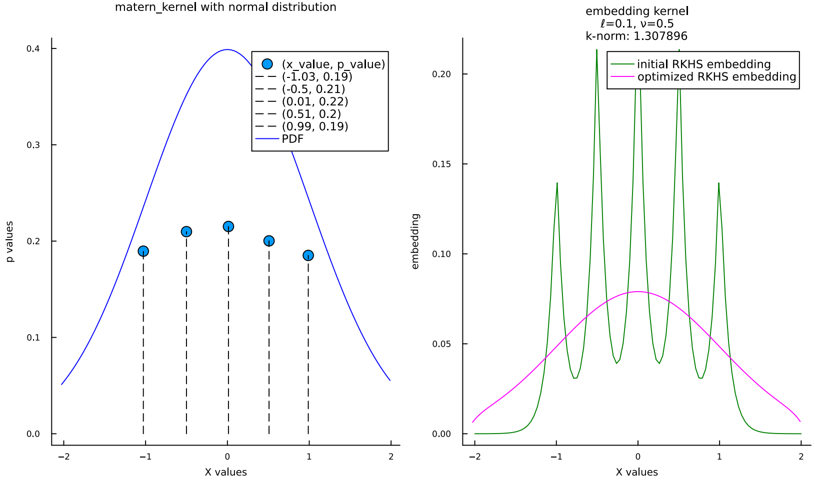


Figure: Normal distribution with Laplace kernel

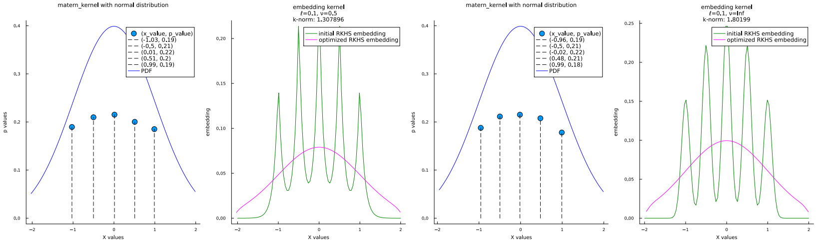


Figure: Normal distribution with smooth kernels

Numerical approximations
Uniform and exponential distribution

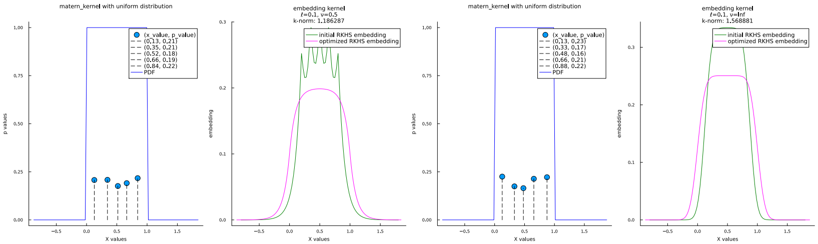


Figure: Uniform with varying kernels

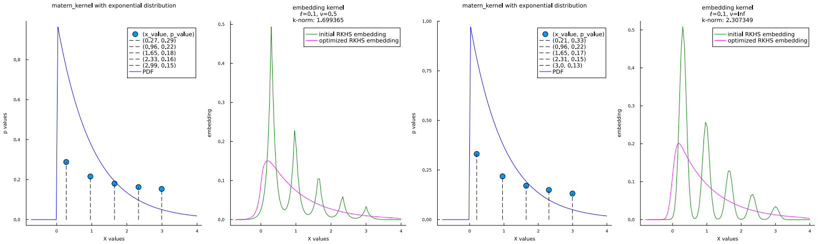
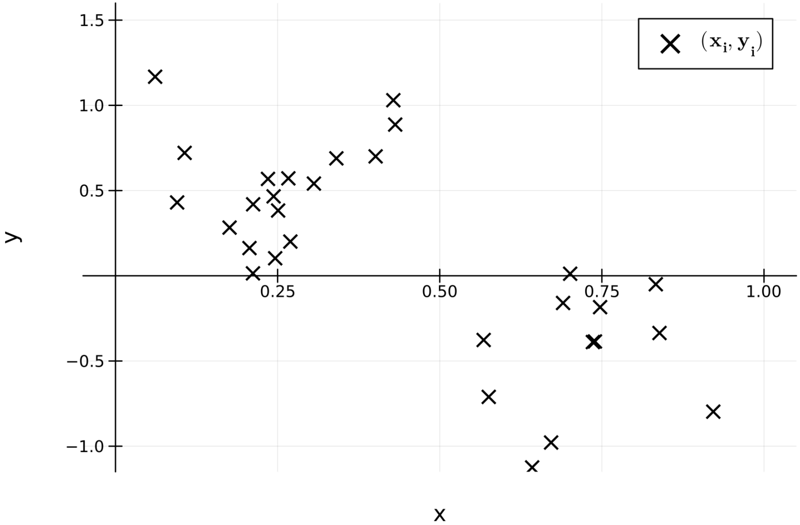


Figure: Exponential with varying kernels

Outline

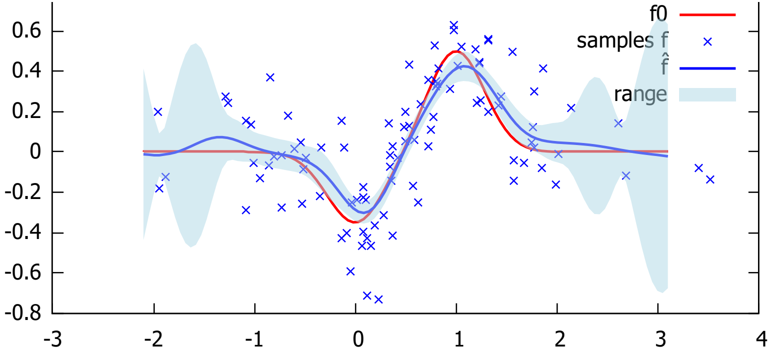
TECHNISCHE UNIVERSITÄT CHEMNITZ

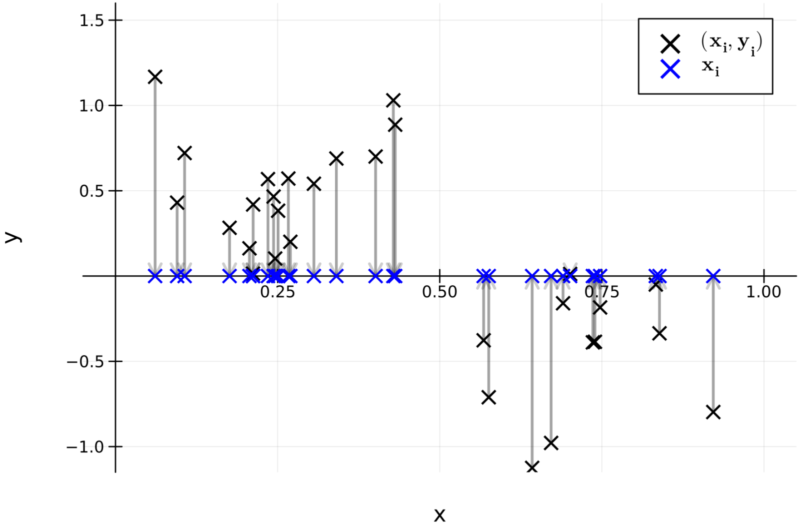
Quality of the predictor



random iid samples from $(x_1, y_1), \dots, (x_n, y_n) \sim (X, Y) \in \mathcal{X} \times \mathbb{R}$ with $\mathcal{X} \in \mathbb{R}^d$.

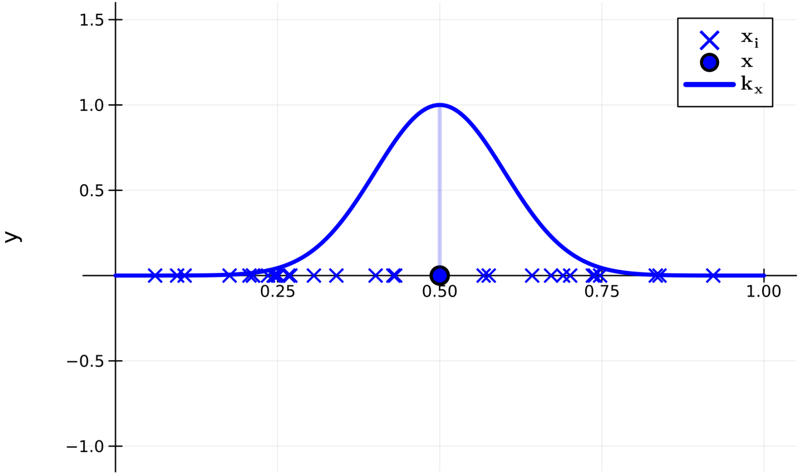
Quality of RKHS approximations
Probability measure on $\mathcal{X}$





The first component, $x_1, \ldots, x_n \sim X$ represent a measure on $\mathcal{X}$.

Approximating elementary functions
by combining translates



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Approximate an elementary function
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Best approximation

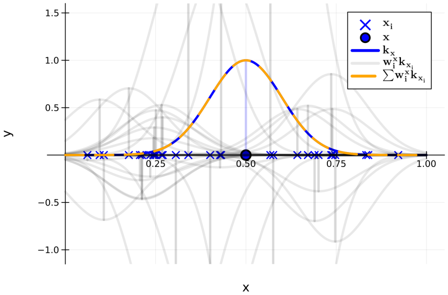
The solution of

$$\min_{w_1,\dots,w_n} \left\| k(\cdot,x) - \sum_{i=1}^{n} w_i\, k(\cdot,x_i) \right\|_k$$

is

$$\boldsymbol{K} w = f,$$

where $\boldsymbol{K}_{ij} = k(x_i,x_j)$ and $f_i = k(x,x_i)$.



Highly oscillating weights :-(

Smoothing splines

Theorem (Representer theorem Schölkopf, Herbrich, and Smola 2001)

The solution of the problem

$$\hat{\vartheta}_n := \min_{f_\lambda(\cdot)\in\mathcal{H}_k} \frac{1}{n}\sum_{i=1}^n \ell(f_i, f_\lambda(X_i)) + \lambda \|f_\lambda(\cdot)\|_k^2$$

takes the form

$$\hat{f}_n(\cdot) := \frac{1}{n}\sum_{j=1}^n \hat{w}_j \cdot k(\cdot, X_j).$$

For $\ell(x,y) = (x-y)^2$, *the weights are* $\hat{w} = \left(\lambda + \frac{1}{n}K\right)^{-1} f$.

Proposition ($\hat{\vartheta}_n$ is downwards biased)

It holds that (irrespective of $\ell(\cdot)$*)*

$$\mathbb{E}\,\hat{\vartheta}_n \le \mathbb{E}\,\hat{\vartheta}_{n+1} \le \vartheta^*.$$

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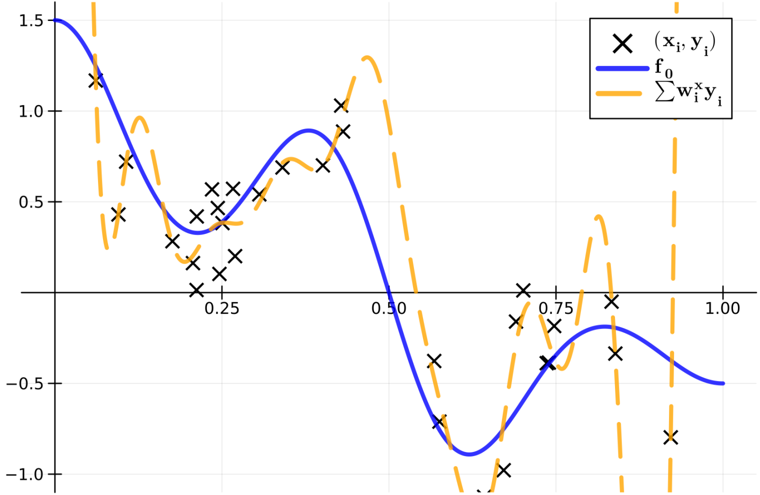
Noisy observations



Overfitting

If the data an had error. . .

Covariance operator

Discrete problem (random)

Analyzing the problem

$$\min_{w\in\mathbb{R}^n} \lambda\|w\|_2^2 + \left\| k(\cdot,x) - \sum_{i=1}^n k(\cdot,x_i)w_i \right\|_k^2$$

is difficult, due to the dependence of the support points $x_1,\dots,x_n$.

Discrete problem (random)

Continuous counterpart is

$$\min_{w\in\mathbb{R}^n} \lambda\|w\|_{L^2}^2 + \left\| k(\cdot,x) - L_k w \right\|_k^2$$

with

$$L_k\colon L^2 \to \mathcal{H}_k$$
$$f \mapsto \int_{\mathcal{X}} k(x,z)\, f(z)\, P(\mathrm{d}z)$$

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Definition (Covariance operator)

The covariance operator is

$$L_k\colon \mathcal{H}_k \to \mathcal{H}_k$$
$$L_k = \int_{\mathcal{X}} k(\cdot,x)\otimes k(\cdot,x)\,P(\mathrm{d}x),$$

where $(k_x\otimes k_x)(f) := \langle f \mid k_x\rangle\, k_x$.

Remark (Trace class)

It holds that

$$trace(k_x\otimes k_x) = k(x,x)$$

and $trace(L_k) = \int_{\mathcal{X}} k(x,x)\,P(\mathrm{d}x) \le \sup_{x\in\mathcal{X}} k(x,x)$.

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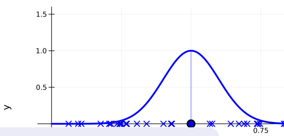
Maximal marginal degrees of freedom
Approximation quality



Definition

The *maximal marginal degrees of freedom* is the worst case value[a]

$$\mathcal{N}_\infty(\lambda) := \lambda^{-1} \sup_{x\in\mathcal{X}} \min_{w\in L^2} \lambda\|w\|_{L^2}^2 + \|k(\cdot,x) - L_k w\|_k^2 .$$

[a] A. Rudi, R. Camoriano, and L. Rosasco (2015). "Less is more: Nyström computational regularization". In: *Proceedings of the 28th International Conference on Neural Information Processing Systems - Volume 1*. NIPS'15. Montreal, Canada: MIT Press, pp. 1657–1665.

The quantity is related to the effective dimension,

$d_{\mathrm{eff}}(\lambda) := \mathbb{E}\left\|(L_k+\lambda)^{-1/2}\right\|^2.$

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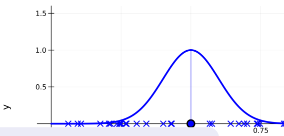

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Concentration inequality

Linking the discrete and the continuous problem

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Concentration inequality between discrete and continuous problem ("On the Approximation of Kernel functions")

Let $\tau > 0$. If $\lambda > 0$ is chosen such that

$$\frac{4\tau\mathcal{N}_\infty\left(\frac{\lambda}{n}\right)\ln\mathcal{N}_\infty\left(\frac{\lambda}{n}\right)}{3n} + \sqrt{\frac{2\tau\mathcal{N}_\infty\left(\frac{\lambda}{n}\right)\ln\mathcal{N}_\infty\left(\frac{\lambda}{n}\right)}{n}} \leq \frac{1}{2}$$

is satisfied, it holds, with probability at least $1-2e^{-\tau}$, that

$$\min_{w\in\mathbb{R}^n} \lambda\|w\|_2^2 + \left\|k(\cdot,x) - \sum_{i=1}^n w_i\, k(\cdot,x_i)\right\|_k^2 \leq \frac{4\lambda}{n}\mathcal{N}\left(\frac{\lambda}{n}\right).$$

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Outline

Research questions

Question

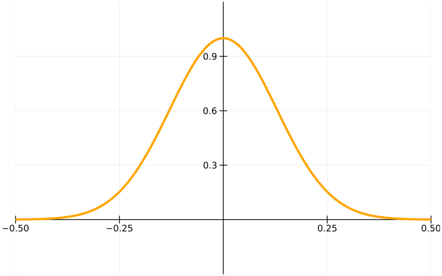
- What are powerful bounds on $\mathcal{N}_\infty(\lambda)$?
- $\hat{f}_{\lambda_n} \to f_0$ in L^2, if $n \to \infty$?
- $\hat{f}_{\lambda_n} \to f_0$ in L^∞, if $n \to \infty$?

Setting

- The sample space is $\mathcal{X} = [0,1]^d$?
- The kernel is

$$k(x,y) = e^{-a\|x-y\|_2^2}$$

with fixed precision parameter $a > 0$.



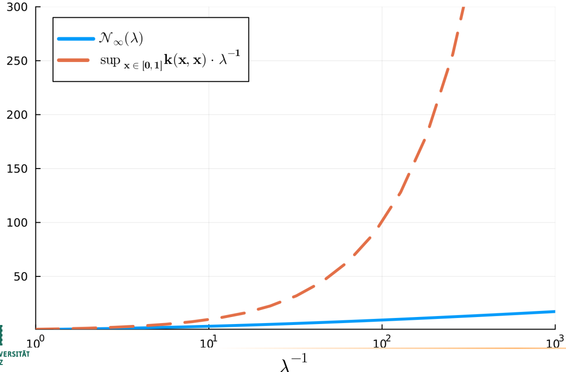
Behavior of $\mathcal{N}_\infty(\lambda)$

Proposition (A priori bound for Maximal marginal degrees of freedom)

The obvious bound is (cf. Rudi, Camoriano, and Rosasco (2015))

$$\mathcal{N}_\infty(\lambda) \le \lambda^{-1} \sup_{x\in\mathcal{X}} k(x,x),$$

which does not reflect the actual behavior.



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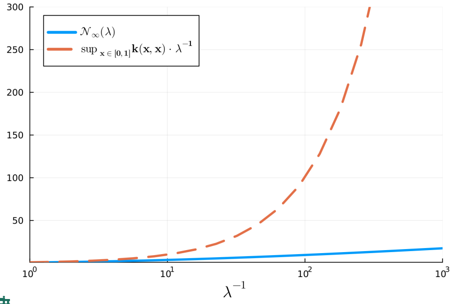


Problem

This bound implies that

$$\lambda_n \ge c_0 > 0 \quad \text{for all } n \in \mathbb{N},$$

which gives convergence rates of $\left\|\hat f_{\lambda_n} - f_0\right\|_{L^2} = \mathcal{O}\left((\ln n)^{-\alpha}\right)$ for some $\alpha > 0$.

For the Gaussian kernel only

Proposition

The minimizer of

$$\min_{w\in L^2} \lambda \|w\|_{L^2}^2 + \|k_x - L_k w\|_k^2$$

is

$$w_\lambda^x = (\lambda + L_k)^{-1} k_x.$$

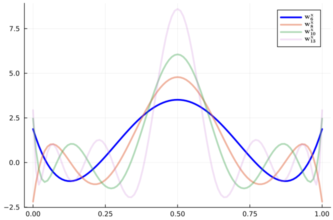


Figure: $x = 0.5$

Lemma

A good proxy is

$$w_\lambda^x(z) \approx \sum_{i=0}^{m-1} Q_i(x) Q_i(z)$$

with Q_i (scaled) Legendre polynomials.

Reason:

$$k(\cdot, a) = \sum_{i=0}^{\infty} \frac{(-a)^i}{i!} \|\cdot - x\|_2^2.$$

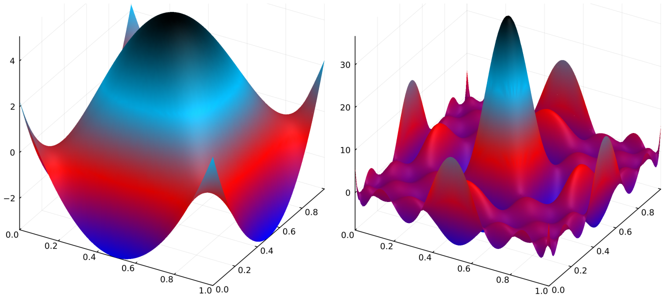
For the Gaussian kernel only

Proposition

For the Gaussian kernel, there is a constant $C>0$ such that[a]

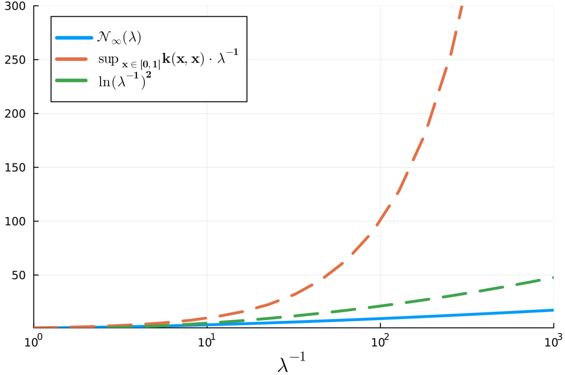
$$\mathcal{N}_\infty(\lambda) \le C \cdot \ln\left(\lambda^{-1}\right)^{2d}.$$

[a] Dommel and P., 2025.



(a) $m=4$, $x=(0.5,0.5)$ **(b)** $m=10$, $x=(0.5,0.5)$

Discussion



Notes

1. The new bound on $\mathcal{N}_\infty(\lambda)$ is significantly *tighter* than the initial bound;
2. The approach works for kernels with polynomial expansions;
3. The bound might still be improved.

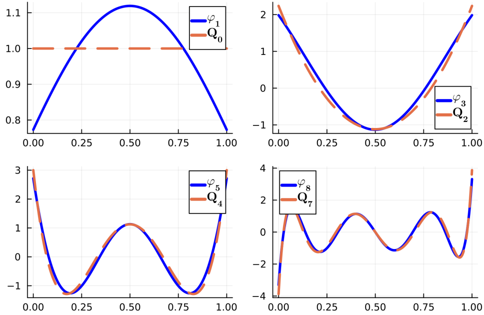
Outline

Consequences on Eigenfunctions

Proposition (Mercer)

The covariance operator L_k is compact and thus

$$(L_k f)(y) = \int_{\mathcal{X}} k(y,z)\,\mu(\mathrm{d}z) = \sum_{\ell=1}^{\infty} \mu_\ell \, \langle \varphi_\ell \mid f \rangle_{L^2} \cdot \varphi_\ell(y).$$



Why?

A bound on

$$\|\varphi_\ell\|_{L^\infty}$$

is essential for deriving uniform convergence for $f_0 \notin \mathcal{H}_k$.

Eigenfunctions
For Gaussian kernels

Relation

The eigenfunctions φ_ℓ and the eigenvalues μ_ℓ are related by

$$\sup_{x\in\mathcal{X}} |\varphi_\ell(x)| \le 4\sqrt{\mathcal{N}_\infty(\mu_\ell)} \le 4C\cdot\left(\ln \mu_\ell^{-1}\right)^d.$$

Proposition

There is a constant $C > 0$ such that

$$\|\varphi_\ell\|_{L^\infty} = \sup_{x\in[0,1]^d} |\varphi_\ell(x)| \le C\,\ell^2$$

for all $\ell \in \mathbb{N}$.

[2] P. Dommel and A. P. (2025). "On the Approximation of Kernel functions". In: *Journal of Machine Learning Research* 26.41, pp. 1–30. URL: http://jmlr.org/papers/v26/24-0270.html.

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Details[2] (2025)

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Relation of norms

$$\|f\|_{L^2} \le \|f\|_{L^\infty} \le C_k \cdot \|f\|_{\mathcal{H}_k}.$$

More precisely,

$$\|f\|_{L^2} \le \|L_k\|^{1/2} \cdot \|f\|_k \quad \text{and} \quad |f(x)| \le \sqrt{k(x,x)} \cdot \|f\|_{\mathcal{H}_k}.$$

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$$\|f\|_{L^2} \leq \|f\|_{L^\infty} \leq C_k \cdot \|f\|_{\mathcal{H}_k}$$

Theorem

For every function $f(\cdot) = \sum_{\ell=1}^{\infty} c_\ell \varphi_\ell(\cdot)$ *such that* $\sum_{\ell=1}^{\infty} \frac{c_\ell^2}{\ell^{-2\alpha}} < \infty$ *for some* $\alpha > 3$*, it holds that*

$$\|f\|_{L^\infty} \leq C \frac{\pi}{\sqrt{6}} \left(\sum_{\ell=1}^{\infty} \frac{c_\ell^2}{\ell^{-2\alpha}} \right)^{3/\alpha} \cdot \|f\|_{L^2}^{1-\frac{3}{\alpha}}.$$

Remark

1. The condition $\sum_{\ell=1}^{\infty} \frac{c_\ell^2}{\ell^{-2\alpha}} < \infty$ can be verified for functions $f \in \mathcal{H}_k$.
2. If $f \in H^s$ for $s > \frac{7d}{2}$, then $\sum_{\ell=1}^{\infty} \frac{c_\ell^2}{\ell^{-2\alpha}} < \infty$.

Theorem (Approximation of smooth functions)

It holds – with high probability – that

$$\left\|\hat{f}_{\lambda_n}-f_0\right\|_{L^2}^2=\mathcal{O}\left(n^{-\frac{2s}{2s+d}+\delta}\right)$$

and

$$\left\|\hat{f}_{\lambda_n}-f_0\right\|_{L^\infty}^2=\mathcal{O}\left(n^{-\frac{s-\frac{7d}{2}}{2s+d}+\delta}\right)$$

$(\delta>0)$ *where* $f_0\in H^s$*.*

Remark

Note the convergence for $s=\infty$, that is, $f\in C^\infty$.

Conclusions & Consequences

Theorem (Approximation of smooth functions)

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$(\delta > 0)$ *where* $f_0 \in H^s$.

Remark

Note the convergence for $s = \infty$, that is, $f \in C^\infty$.

Conclusions & Consequences, cont.

Approximations in lower dimensions: "Less is more: Nyström computational regularization"

The Nyström method

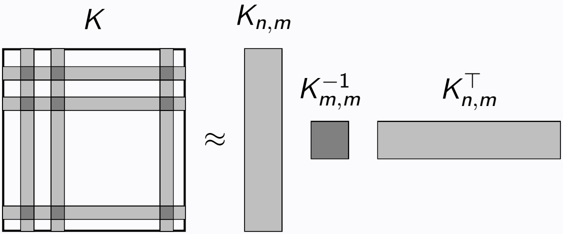

Figure: Approximation of the kernel matrix by lower rank matrices

Outline

RKHS. Useful in Stochastic Optimization?

Pros and potential future research

- Less functions (smooth)
- Faster empirical convergence
- Simpler to compute than Wasserstein
- Less curse of dimensionality
- Performance on real-world data
- Distributionally robust optimization: with MMD instead of Wasserstein
- What is the right kernel?
- Bandwidth selection à la Norkin
- Extend the results to multistage (nested) MMD

Thank you.
Literature

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Outline

TECHNISCHE UNIVERSITÄT CHEMNITZ

Gaussian random fields

Method I: Feature map

Let $\varphi_k\colon \mathcal{X} \to \mathbb{R}$ be functions, $\sigma_k \in \mathbb{R}$. Set

$$f(x) := \sum_{k=0}^{\infty} \quad \sigma_k \varphi_k(x), \qquad x \in \mathcal{X}, \omega \in \Omega,$$

Gaussian random fields

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$$f(x) := \sum_{k=0}^{\infty} \xi_k \sigma_k \varphi_k(x), \qquad x \in \mathcal{X}, \omega \in \Omega,$$

with $\xi_k \sim \mathcal{N}(0,1)$ iid. Note, that $\mathbb{E}\,\xi_k = 0$ and $\mathbb{E}\,\xi_k \xi_\ell = \delta_{k\ell}$. It follows that $\mathbb{E}\,f(x) = 0$ and

$$\operatorname{cov}\big(f(x), f(y)\big) = \sum_{k=0}^{\infty} \sigma_k^2 \varphi_k(x) \varphi_k(y), \qquad x, y \in \mathcal{X}.$$

Let $\varphi_k\colon \mathcal{X} \to \mathbb{R}$ be functions, $\sigma_k \in \mathbb{R}$. Set

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$$k(x,y) := \operatorname{cov}\big(f(x), f(y)\big) = \sum_{k=0}^{\infty} \sigma_k^2 \varphi_k(x) \varphi_k(y), \qquad x, y \in \mathcal{X}.$$

Hence,

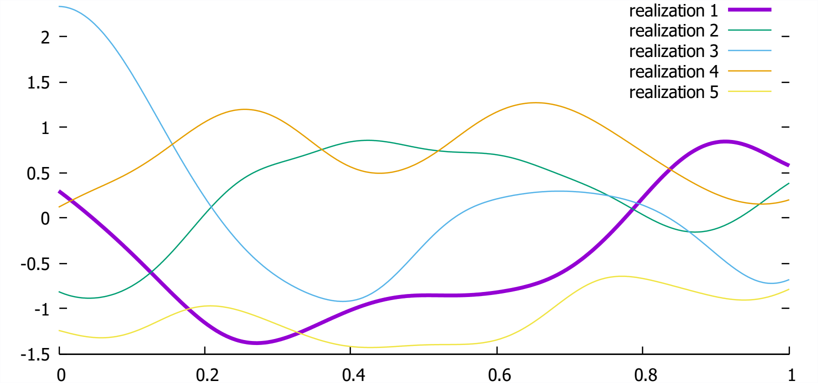
$$\begin{pmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} k(x_1,x_1) & \dots & k(x_1,x_n) \\ \vdots & & \vdots \\ k(x_n,x_1) & \dots & k(x_n,x_n) \end{pmatrix} \right);$$

in particular, $f(x) \sim \mathcal{N}\big(0, \sum_{k=0}^{\infty} \sigma_k^2 \varphi_k(x)^2\big)$.

Example
Gaussian like (polynomial, radial) feature map

Example (RBF)

Feature map: $\varphi_k(x) := \left({}^{x}/_{\ell}\right)^k \cdot e^{-x^2/2\ell^2}$, $\sigma_k^2 := \frac{1}{k!}$



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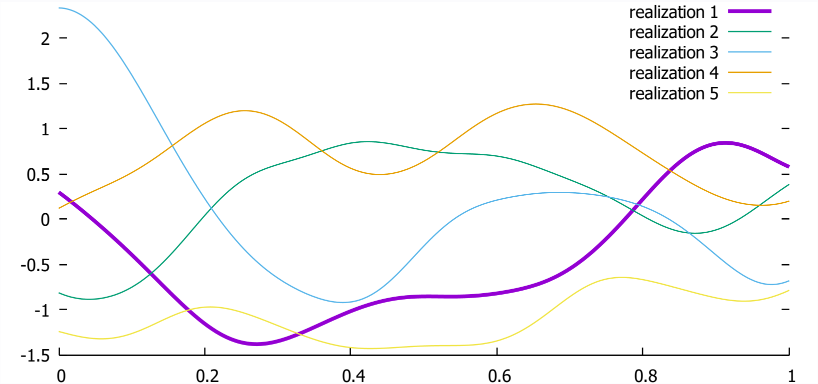

$$k(x,y) = \sum_{k=0} \sigma_k^2 \varphi_k(x) \varphi_k(y) = \exp\left(-\frac{1}{2\ell^2}(x-y)^2\right)$$

TECHNISCHE UNIVERSITÄT CHEMNITZ

Example

Feature map: $\varphi_k(x) := \sqrt{2}\sin\left((k-\frac{1}{2})\pi x\right)$, $\sigma_k := \frac{1}{(k-\frac{1}{2})\pi}$

$$k(x,y) = \sum_{k=1} \sigma_k^2 \varphi_k(x)\varphi_k(y) = \min(x,y)$$

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TECHNISCHE UNIVERSITÄT CHEMNITZ

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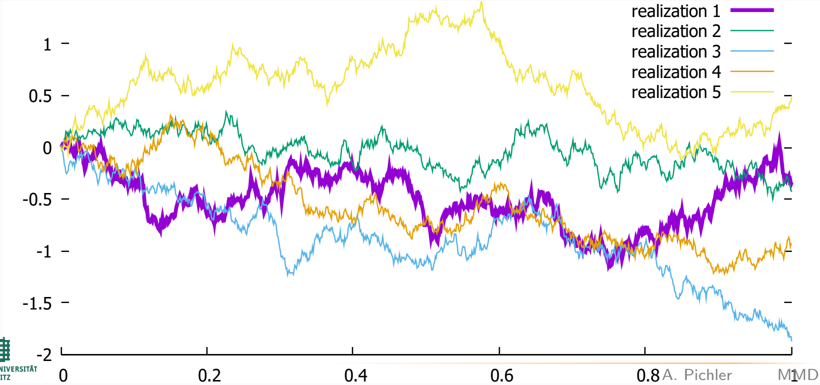
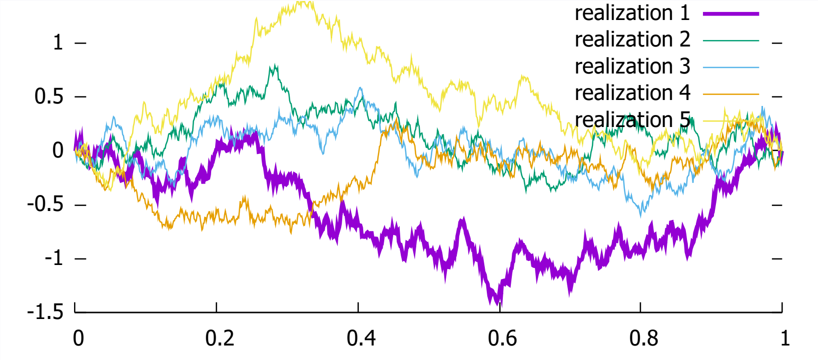


Example
Brownian bridge

Example

Choose $\varphi_k(x) := \sqrt{2}\sin(k\pi x)$, $\sigma_k := \frac{1}{k\pi}$

$$k(x,y) = \min(x,y) - x\,y = \sum_{k=1} \sigma_k^2 \varphi_k(x)\varphi_k(y)$$



Outline

TECHNISCHE UNIVERSITÄT CHEMNITZ

Gaussian random fields

Method II: Gramian

If $\xi_i \sim \mathcal{N}(0,1)$ are iid and

$$K = \begin{pmatrix} k(x_1,x_1) & \dots & k(x_1,x_n) \\ \vdots & & \vdots \\ k(x_n,x_1) & \dots & k(x_n,x_n) \end{pmatrix} = \Phi\Phi^\top$$

(for example $\Phi = K^{1/2}$), then

$$X := \mu + \Phi \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix} \sim \mathcal{N}(\mu, K).$$

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(for example $\Phi = K^{1/2}$), then

$$X := \mu + \Phi \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix} \sim \mathcal{N}(\mu, K).$$

We find the realization

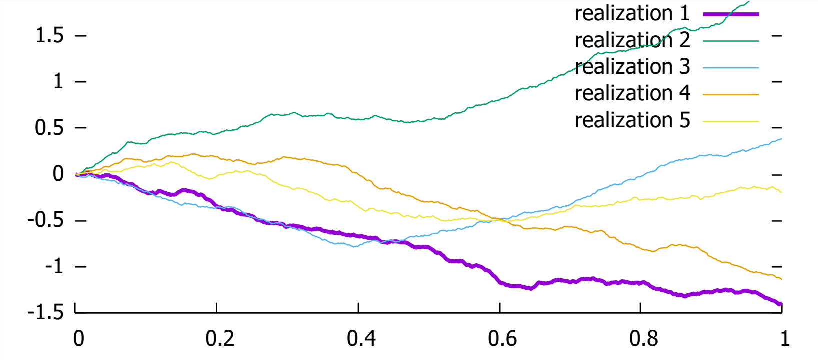
$$\begin{pmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix} := X \sim \mathcal{N}(0, K).$$

Example
Fractional Brownian motion

Choose $2k(x,y) = x^{2H} + y^{2H} - |x-y|^{2H}$

Example

Hurst index $H = 0.8$:[a] increments are positively correlated

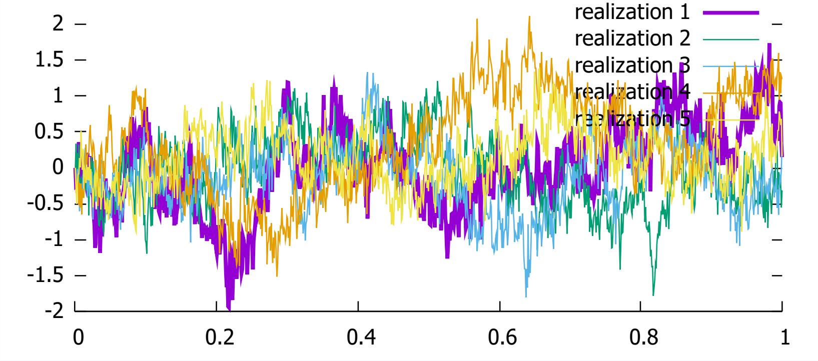


[a] The Wiener process has Hurst index $H = 1/2$.

Choose $2k(x,y) = x^{2H} + y^{2H} - |x-y|^{2H}$

Example

Hurst index $H = 0.2$: increments are negatively correlated



Outline

With Gramian $K := \begin{pmatrix} k(x_1,x_1) & \dots & k(x_1,x_n) \\ \vdots & & \vdots \\ k(x_n,x_1) & \dots & k(x_n,x_n) \end{pmatrix}$, choose the weights[3]

$$w \sim \mathcal{N}(0, K^{-1})$$

and set

$$f(\cdot) := \sum_{i=1}^{n} w_i \cdot k(\cdot, x_i)$$

[3] In data science, the matrix K^{-1} is the *precision matrix*.

Gaussian random fields

Method III: RKHS representation

With Gramian $K := \begin{pmatrix} k(x_1,x_1) & \dots & k(x_1,x_n) \\ \vdots & & \vdots \\ k(x_n,x_1) & \dots & k(x_n,x_n) \end{pmatrix}$, choose the weights[3]

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and set

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Proposition

Then

$$\begin{pmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix} \sim \mathcal{N}(0, K).$$

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With Gramian $K := \begin{pmatrix} k(x_1,x_1) & \dots & k(x_1,x_n) \\ \vdots & & \vdots \\ k(x_n,x_1) & \dots & k(x_n,x_n) \end{pmatrix}$, choose the weights[3]

$$w \sim \mathcal{N}(0, K^{-1})$$

and set

$$f(\cdot) := \sum_{i=1}^n w_i \cdot k(\cdot, x_i) \in \mathcal{H}_k: \ \text{RKHS}, \text{ with } \langle k(\cdot,x), k(\cdot,y)\rangle_k = k(x,y)$$

Proposition

Then

$$\begin{pmatrix} f(x_1) \\ \vdots \\ f(x_n) \end{pmatrix} \sim \mathcal{N}(0, K).$$

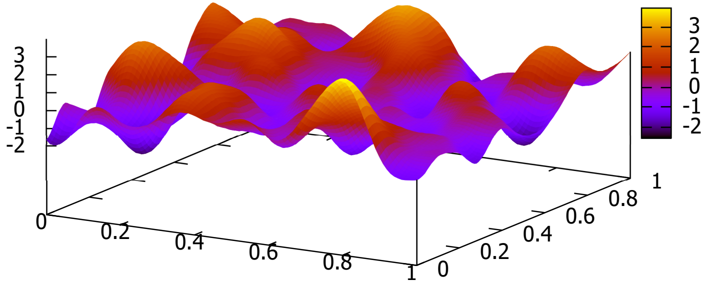
[3] In data science, the matrix K^{-1} is the *precision matrix*.

2D process visualizations

Example

Choose the radial Gaussian kernel[a]

$$k(x,y) = \sigma_f^2 \cdot \exp\left(-\|x-y\|^2/\ell^2\right)$$



[a] This is a Matérn-∞ covariance kernel: all derivatives available everywhere a.s.

2D process visualizations

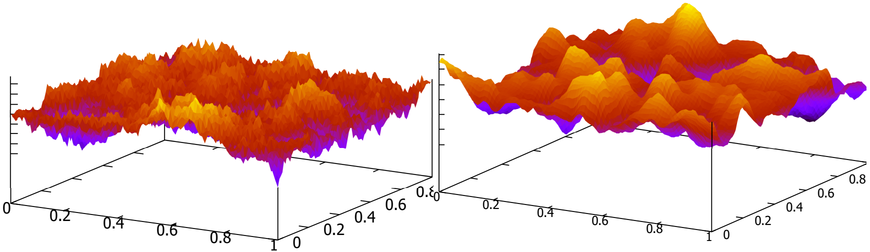


Figure: Laplace (Ornstein–Uhlenbeck) Matérn

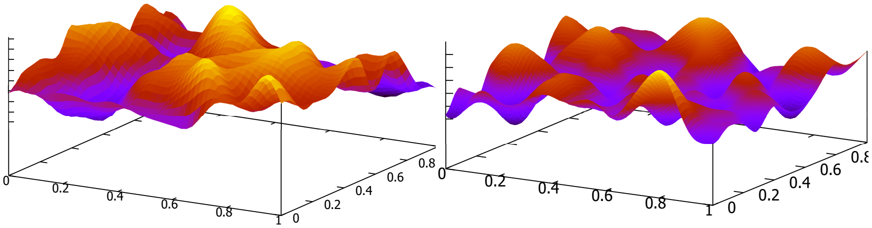


Figure: Sigmoid Gauss

Outline

TECHNISCHE UNIVERSITÄT CHEMNITZ

Suppose that

$$f_i = f_0(\hat{x}_i) + \varepsilon.$$

Let $\hat{X} := (\hat{x}_1, \dots, \hat{x}_m) \in \mathcal{X}^m$ and $X = (x_1, \dots, x_n) \in \mathcal{X}^n$ be sequences of points and $\varepsilon \sim \mathcal{N}(0, \Lambda)$ independent. The joint distribution is

$$\begin{pmatrix} f_0(\hat{X}) \\ f(X) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} k(\hat{X}, \hat{X}) & k(\hat{X}, X) \\ k(X, \hat{X}) & k(X, X) + \Lambda \end{pmatrix} \right).$$

Now RKHS

Signal + noise: predictions

Suppose that

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TECHNISCHE UNIVERSITÄT CHEMNITZ

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It follows that

$$f_0(\hat{X}) \mid f(X) \sim \mathcal{N}(\hat{\mu}, \hat{K}),$$

where

$$\hat{\mu} := k(\hat{X}, X) \big(k(X, X) + \Lambda\big)^{-1} f(X)$$

and

$$\hat{K} := k(\hat{X}, \hat{X}) - k(\hat{X}, X) \big(k(X, X) + \Lambda\big)^{-1} k(X, \hat{X}).$$

Now RKHS

Signal + noise: predictions

Suppose that

$$f_i = f_0(\hat{x}_i)+\varepsilon.$$

Let $\hat{X} := (\hat{x}_1, \dots, \hat{x}_m) \in \mathcal{X}^m$ and $X = (x_1, \dots, x_n) \in \mathcal{X}^n$ be sequences of points and $\varepsilon \sim \mathcal{N}(0,\Lambda)$ independent. The joint distribution is

$$\begin{pmatrix} f_0(\hat{X}) \\ f(X) \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} k(\hat{X},\hat{X}) & k(\hat{X},X) \\ k(X,\hat{X}) & k(X,X)+\Lambda \end{pmatrix}\right).$$

It follows that

$$f_0(\hat{X}) \mid f(X) \sim \mathcal{N}(\hat{\mu}, \hat{K}),$$

where

$$\hat{\mu} := k(\hat{X},X)\big(k(X,X)+\Lambda\big)^{-1} f(X)$$

and

$$\hat{K} := k(\hat{X},\hat{X}) - k(\hat{X},X)\big(k(X,X)+\Lambda\big)^{-1} k(X,\hat{X}).$$

Now RKHS
Signal + noise: predictions

Suppose that

$$f_i = f_0(\hat{x}_i) + \varepsilon.$$

Let $\hat{X} := (\hat{x}_1, \dots, \hat{x}_m) \in \mathcal{X}^m$ and $X = (x_1, \dots, x_n) \in \mathcal{X}^n$ be sequences of points and $\varepsilon \sim \mathcal{N}(0, \Lambda)$ independent. The joint distribution is

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It follows that

$$f_0(\hat{X}) \mid f(X) \sim \mathcal{N}(\hat{\mu}, \hat{K}),$$

where

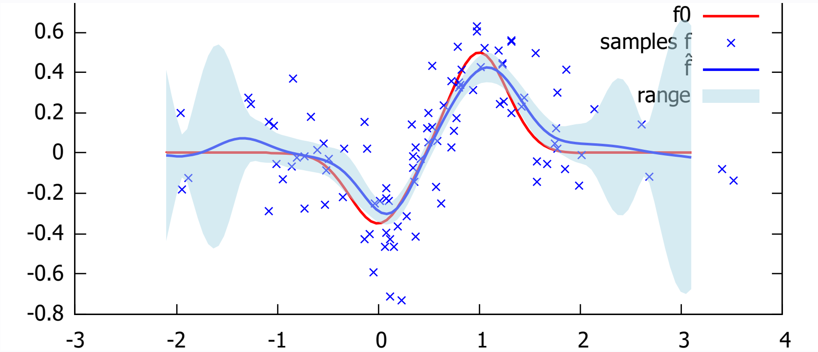
$$\hat{\mu} := k(\hat{X}, X)\big(k(X, X) + \Lambda\big)^{-1} f(X)$$

and

$$\hat{K} := k(\hat{X}, \hat{X}) - k(\hat{X}, X)\big(k(X, X) + \Lambda\big)^{-1} k(X, \hat{X}).$$

Quality of the predictor

Example



The local variance

$$\operatorname{var}\left(f_0(x) \middle| f(X_1) = f_1, \ldots, f(X_n) = f_n\right)$$
$$= k(x,x) - k(x,X)\left(k(X,X) + \Lambda\right)^{-1} k(X,x).$$

does *not* depend on the samples f_i!

In other words, the prediction for a single new point x is

$$\mathbb{E}\big(f_0(\cdot)\big|\, f(x_1)=f_1,\dots,f(x_n)=f_n\big)=\sum_{i=1}^n \hat{w}_i\cdot k(\cdot,x_i),$$

where $\hat{w}$ solves the linear system of equations

$$\sum_{j=1}^n \big(k(x_i,x_j)+\Lambda_{ij}\big)\,\hat{w}_j=f_i,\quad i=1,\dots,n.$$

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The variance is

$$\begin{aligned}&\operatorname{var}\big(f_0(x)\big|\, f(X_1)=f_1,\dots,f(X_n)=f_n\big)\\&\qquad=k(x,x)-k(x,X)\big(k(X,X)+\Lambda\big)^{-1}k(X,x).\end{aligned}$$

If $\Lambda=0$, then $\operatorname{var}\big(f_0(X_i)\big|\, f(X_1)=f_1,\dots,f(X_n)=f_n\big)=0$.