Stochastic Optimization With Random Fields

Convergence in RKHS norms

Alois Pichler Faculty of mathematics TU Chemnitz May 23, 2022

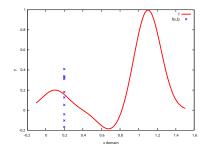


Conditional expectation and stochastic optimization

Problem (Stochastic optimization)

Solve

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

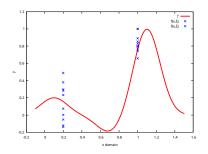


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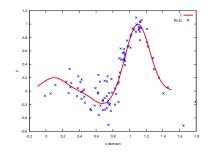


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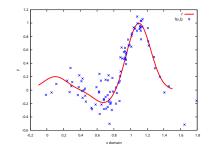


Conditional expectation and stochastic optimization

Problem (Stochastic optimization)

Solve

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



Problem (Optimal control: Hamilton-Jacobi-Bellman)

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

Problem (Time series, learning)

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



Outline

- 1 Deriving RKHS from stochastics
 - Gaussian random fields
 - Traditional realization
 - Representation as RKHS function



- 2 Predictions from Gaussian processes
 - Conditional Gaussians
 - Conditional Gaussians, applied to RKHS
- 3 Perspective from stochastic optimization
 - Stochastic optimization problem
 - Denoising
 - Order of convergence



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Method I: Feature map

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

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



Method I: Feature map

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

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

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

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



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

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

Gaussian like (polynomial, radial) feature map

Example (RBF)

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

realization 1 realization 2 realization 3 realization 4 realization 5 realization 6 realization 6 realization 7 realization 9 realization 9



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Example

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

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



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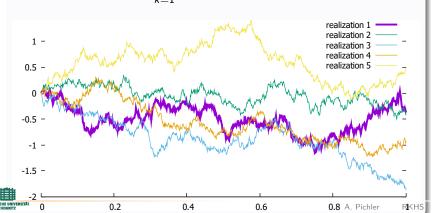


Wiener process

Example

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

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



Brownian bridge

Example

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

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

$$1 - \text{realization 1} - \text{realization 2} - \text{realization 3} - \text{realization 4} - \text{realization 5} - \text{realization$$

0.4

0.6



0.2

0.8

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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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We find the realization

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



Fractional Brownian motion

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

Example Hurst index H = 0.8: increments are positively correlated realization 1 1.5 realization 2 realization 3 realization 4 realization 5 0.5 --0.5 --1 --1.5 ^l 0.2 0.6 0.4 8.0 ^aThe Wiener process has Hurst index H = 1/2.



Fractional Brownian motion

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

Example Hurst index H = 0.2: increments are negatively correlated realization 1 2 realization 2 1.5 realization B realization 0.5 -0.5 -1.5 -0.2 0.4 0.6 0.8



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Method III: RKHS representation

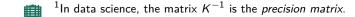
With Gramian
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, choose the

weights¹

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

and set

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



Method III: RKHS representation

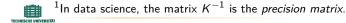
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Proposition

Then

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

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



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and set

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

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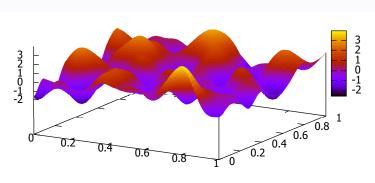


2D process visualizations

Example

Choose the radial Gaussian kernel^a

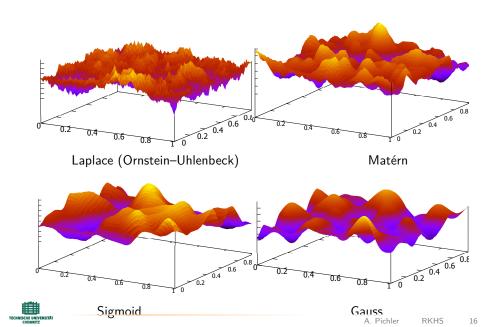
$$k(x,y) = \sigma_f^2 \cdot \exp\left(-\|x - y\|^2/\ell^2\right)$$



 a This is a Matérn- ∞ covariance kernel: all derivatives available everywhere



2D process visualizations



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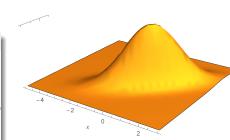


Conditional Gaussians are Gaussian

Theorem (Cf. [Bishop, 2006])

Suppose that

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim \mathcal{N} \left(\begin{pmatrix} \mu_X \\ \mu_Y \end{pmatrix}, \ \begin{pmatrix} K_{XX} & K_{XY} \\ K_{YX} & K_{YY} \end{pmatrix} \right),$$



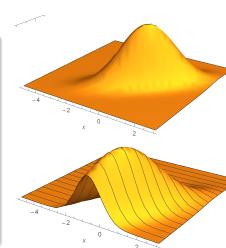


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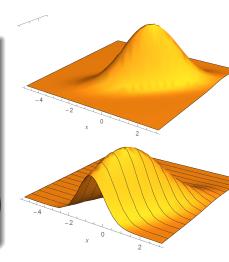
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then the conditional distribution is Gaussian as well:

$$X|Y \sim \mathcal{N}\left(\frac{\mu_X + K_{XY}K_{YY}^{-1}(Y - \mu_Y)}{K_{XX} - K_{XY}K_{YY}^{-1}K_{YX}}\right)$$





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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

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



Signal + noise: predictions

Suppose that

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

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It follows that

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

where

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

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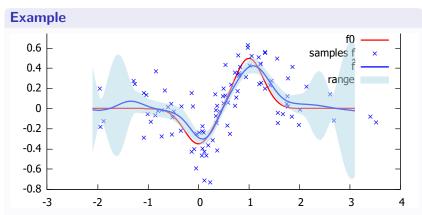
$$\hat{\mu} := k(\hat{X}, X)(k(X, X) + \Lambda)^{-1} f(X)$$

and

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



Quality of the predictor



The local variance

$$var(f_0(x)|f(X_1) = f_1,..., f(X_n) = f_n)$$

$$= k(x,x) - k(x,X)(k(X,X) + \Lambda)^{-1}k(X,x).$$

loes not depend on the samples f_i !

.. Pichler RKHS

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Stochastic filtering

Linear predictor

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

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

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

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

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The variance is

$$\operatorname{var}(f_0(x)|f(X_1) = f_1, \dots, f(X_n) = f_n)$$

$$= k(x, x) - k(x, X)(k(X, X) + \Lambda)^{-1}k(X, x).$$

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



Filtering and splines

Kriging models

Remark (Relation to kriging)

Kriging ...

- \bullet ... employs an unknown variogram instead of k,
 - ... assumes a radial variogram,
 - ... estimates the variogram, or the parameters in a parametric model;
 - typically, the error vanishes, $\Lambda = 0$.
- Design points X_i are known



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Estimator

Problem

For $(X_i, f_i) \in \mathcal{X} \times \mathbb{R} \subset \mathbb{R}^d \times \mathbb{R}$ iid. observations with $X_i \sim P$ (the design measure) we study the estimator

$$\hat{f}_n(\cdot) := \frac{1}{n} \sum_{i=1}^n \hat{w}_i \, k(\cdot, X_i),$$

where

$$\lambda \, \hat{w}_i + \frac{1}{n} \sum_{i=1}^n k(X_i, X_j) \, \hat{w}_j = f_i,$$

 $i=1,\ldots,n$.



Worst case analysis: Generalization (learning) theory, cf.

[Steinwart and Christmann, 2008]

Remark (Relation of norms)

$$\|g\|_2 \le \|g\|_{\infty} \le C_k \cdot \|g\|_k$$

More precisely,

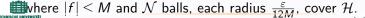
$$\|g\|_2 \le \|K\|^{1/2} \cdot \|g\|_k$$
 and $|g(x)| \le \sqrt{k(x,x)} \cdot \|g\|_k$.

Remark (L^2 -norm, $\|\cdot\|_k$ regularization)

Usual results consider the expected risk,

$$\mathcal{E}(g(\cdot)) := \mathbb{E}(f - g(X))^2 = ||f - g(X)||^2,$$

$$P(\mathcal{E}(f_z) - \mathcal{E}(f_{z;\mathcal{H}}) > \varepsilon) < \mathcal{N}\left(\mathcal{H}, \frac{\varepsilon}{12M}\right) e^{-\frac{n\varepsilon}{300M^2}},$$



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where |f| < M and $\mathcal N$ balls, each radius $\frac{\varepsilon}{12M}$, cover $\mathcal H$.

Mean (integrated) squared error observation T

Density estimation, cf. [Tsybakov, 2008]

• Locally, at $x \in \mathcal{X}$,

$$\operatorname{mse} \hat{f}_n(x) \coloneqq \mathbb{E} \left(\hat{f}_n(x) - f_0(x) \right)^2$$

$$= \left(\operatorname{bias} \hat{f}_n(x) \right)^2 + \operatorname{var} \hat{f}_n(x).$$

• Or globally (L² risk function),

mise
$$\hat{f}_n := \mathbb{E} \int_{\mathbb{R}^d} (\hat{f}_n(x) - f_0(x))^2 dx$$

or $\int_{\mathbb{R}^d} \operatorname{mse} (\hat{f}_n(x)) p(x) dx = \mathbb{E} \|\hat{f}_n(\cdot) - f_0(\cdot)\|_2^2$.

• For convergence in $(\mathcal{H}_k, \|\cdot\|_k)$ and thus uniform convergence,

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Smoothing splines

Predictions in RKHS: $f_i \cdots \longleftrightarrow \dots \hat{f_n}$

Theorem (Representer theorem [Schölkopf et al., 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

$$\hat{f}_n(\cdot) := \frac{1}{n} \sum_{i=1}^n \hat{w}_i \cdot k(\cdot, X_i).$$

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

Proposition ($\hat{\vartheta}_n$ is downwards biased, cf. [Norkin et al., 1998])

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



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

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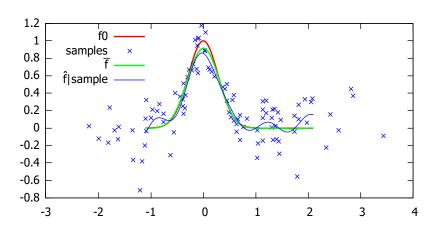
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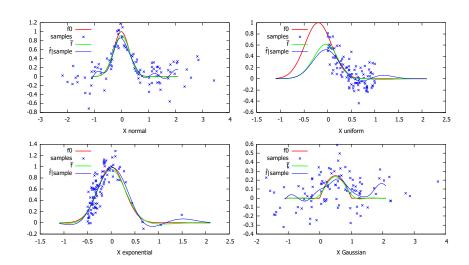
The expectation of \hat{f}_n **BLU Predictions**





Design measure, empirical

BLU Predictions





Law of Large Numbers, LLN

Predictions: $f_i \longleftrightarrow f_0$

Remark

Consider the random variable $(X, f) \sim P$ and the problem

$$\vartheta^* := \min_{f_{\lambda}(\cdot)} \mathbb{E} \left(f - f_{\lambda}(X) \right)^2 + \lambda \|f_{\lambda}\|_{k}^2$$

and note that

$$\vartheta^* = \underbrace{\mathbb{E}\left(f - f_0(X)\right)^2}_{f_{\lambda}(\cdot)} + \min_{f_{\lambda}(\cdot)} \mathbb{E}\left(f_0(X) - f_{\lambda}(X)\right)^2 + \lambda \left\|f_{\lambda}\right\|_{k}^2.$$

By Doob-Dynkin, $f_0(x) = \mathbb{E}(f \mid X = x)$.



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and note that

$$\vartheta^* = \underbrace{\mathbb{E}\left(f - f_0(X)\right)^2}_{\text{irreducible}} + \min_{f_{\lambda}(\cdot)} \mathbb{E}\left(f_0(X) - f_{\lambda}(X)\right)^2 + \lambda \left\|f_{\lambda}\right\|_k^2.$$

By Doob-Dynkin, $f_0(x) = \mathbb{E}(f \mid X = x)$.



The limit: $f_i \longleftrightarrow f_0 \longleftrightarrow f_{\lambda}$

Proposition

The solution of

$$\min_{f_{\lambda}(\cdot)} \mathbb{E} \left(f_{0}(X) - f_{\lambda}(X) \right)^{2} + \lambda \left\| f_{\lambda} \right\|_{k}^{2}$$

is

$$f_{\lambda} = K w_{\lambda}$$
, where $(\lambda I + K)w_{\lambda} = f_0$,

where

$$K w(x) = \int_{\mathcal{X}} k(x, y) w(y) P(dy).$$

Proposition

It holds that $f_0 - f_\lambda = \lambda w_\lambda$ and

$$||f_0 - f_\lambda||_k \le C_0 \lambda$$



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Nyström method

Integral equation

Remark (Inhomogeneous Fredholm equation of the second kind)

Suppose that

$$\lambda \, \tilde{w}_{\lambda}(x) + \frac{p(x)}{p(x)} \cdot \int_{\mathcal{X}} k(x,y) \, \tilde{w}_{\lambda}(y) \, \frac{dy}{dy} = \frac{p(x)}{p(x)} \cdot f_0(x),$$

then

$$f_{\lambda}(x) := \int_{\mathcal{X}} k(x, y) \, \tilde{w}_{\lambda}(y) \, dy$$

satisfies

$$(\lambda I + K) f_{\lambda} = K f_0.$$



Outline

- Deriving RKHS from stochastics
 - Gaussian random fields
 - Traditional realization
 - Representation as RKHS function
- Predictions from Gaussian processes

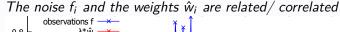
- Conditional Gaussians
- Conditional Gaussians, applied to RKHS
- 3 Perspective from stochastic optimization
 - Stochastic optimization problem
 - Denoising
 - Order of convergence

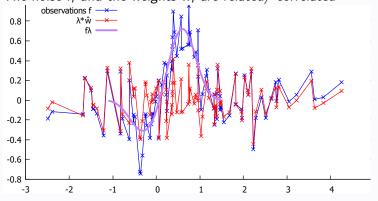


Denoising

Tight relation between noise and weights

Conjecture





$$\lambda \, \hat{w}_i + \underbrace{\frac{1}{n} \sum_{j=1}^n k(X_i, X_j) \, \hat{w}_j}_{j=1} = f_i$$

 $\approx f_{\lambda}(X_i)$



Denoising: the predictor $\tilde{f}_n(\cdot)$

$$f_i \longleftrightarrow f_0 \longleftrightarrow \frac{f_{\lambda} \longleftrightarrow \tilde{f}_n}{\longleftrightarrow \hat{f}_n} \longleftrightarrow \hat{f}_n$$

Definition

With

$$\tilde{w}_i = \frac{f_i - f_\lambda(X_i)}{\lambda}$$

set

$$\widetilde{f}_n(\cdot) := \frac{1}{n} \sum_{i=1}^n k(\cdot, X_i) \, \widetilde{w}_i.$$

Theorem (Unbiased)

Then

$$\operatorname{corr}(f_i, \tilde{w}_i | X = x) = 1$$

and, for every $x \in \mathcal{X}$,

$$\mathbb{E}\,\tilde{f}_n(x)=f_\lambda(x).$$

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$$= \frac{1}{n} \sum_{i=1}^{n} \mathbb{E} k(x, X_i) \frac{f_0(X_i) - f_{\lambda}(X_i)}{\lambda}$$
$$= \mathbb{E} k(x, X_i) \frac{w_{\lambda}(X_i)}{\lambda} = K w_{\lambda}(x) = f_{\lambda}(x)$$



$$f_i \longleftrightarrow f_0 \longleftrightarrow \frac{f_{\lambda} \longleftrightarrow \tilde{f}_n}{f_n} \longleftrightarrow \hat{f}_n$$

Theorem (Consistency for heteroscedastic data)

Further.

$$\mathbb{E}\left\|f_{\lambda}(\cdot)-\tilde{f}_{n}(\cdot)\right\|_{k}^{2}=\frac{C}{n},$$

where

$$C := \frac{1}{\lambda^2} \int_{\mathcal{X}} \left(\left(\underbrace{f_0(x) - f_\lambda(x)}_{\mathcal{X}} \right)^2 + \mathsf{var}(f|x) \right) k(x, x) P(dx) - \|f_\lambda\|_k^2.$$

Here, the data are possibly heteroscedastic,

$$\operatorname{var}(f|x) = \mathbb{E}\left(\left(f - f_0(X)\right)^2 | X = x\right).$$



$$f_i \longleftrightarrow f_0 \longleftrightarrow \frac{f_{\lambda}}{f_{\lambda}} \longleftrightarrow \frac{\tilde{f}_n}{f_n} \longleftrightarrow \hat{f}_n$$

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$$f_i \longleftrightarrow f_0 \longleftrightarrow f_\lambda \longleftrightarrow \frac{\tilde{f}_n \longleftrightarrow \hat{f}_n}{f_n} \longleftrightarrow \hat{f}_n$$

Proposition (Consistency)

•

$$\tilde{f}_n(\cdot) - \hat{f}_n(\cdot) = \frac{1}{n} \sum_{i=1}^n \tilde{r}_n^\top \left(\lambda + \frac{1}{n} K \right)_j^{-1} k(\cdot, X_j),$$

•

$$\|\tilde{f}_n(\cdot) - \hat{f}_n(\cdot)\|_k^2 = \tilde{r}_n^\top \left(\lambda + \frac{1}{n}K\right)^{-1} \frac{1}{n}K \left(\lambda + \frac{1}{n}K\right)^{-1} \tilde{r}_n,$$

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$$\tilde{r}_n = \left(\tilde{f}_n(X_i) - \hat{f}_n(X_i)\right)_{i=1}^n$$
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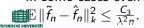
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Theorem

$$\mathbb{E} \|\tilde{f}_n - \hat{f}_n\|_k^2 \le \frac{C_3}{\lambda^3 n},$$

in some cases even



Proof.

$$\left(\lambda + \frac{1}{n}K\right)^{-1}\frac{1}{n}K\left(\lambda + \frac{1}{n}K\right)^{-1} \leq \frac{1}{4\lambda}.$$

Now RKHS

$$f_i \longleftrightarrow f_0 \longleftrightarrow f_\lambda \longleftrightarrow \frac{\tilde{f}_n \longleftrightarrow \hat{f}_n}{f_n}$$

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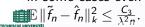
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Outline

- - Gaussian random fields
 - Traditional realization
 - Representation as RKHS

- Conditional Gaussians
- Conditional Gaussians,
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 - Stochastic optimization
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 - Order of convergence



Order of convergence

$$f_i \longleftrightarrow f_0 \longleftrightarrow f_\lambda \longleftrightarrow \tilde{f}_n \longleftrightarrow \hat{f}_n$$

| $ f_i - f_0 $ | irreducible |
|---|---|
| $ f_0 - f_\lambda _k^2$ $\mathbb{E} f_\lambda - \tilde{f}_n _k^2$ $\mathbb{E} \tilde{f}_n - \hat{f}_n _k^2$ | $ \leq C_0 \lambda^2 \leq \frac{C_1}{\lambda^2 n} \leq \frac{C_2}{\lambda^3 n}, \leq \frac{C_2}{\lambda^2 n} $ |

Theorem (Unbiased)

If
$$\lambda_n = \mathcal{O}\!\left(n^{-1/5}\right)$$
, then

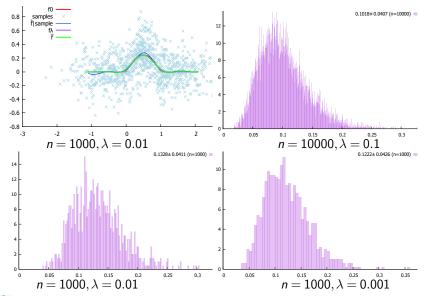
$$\mathbb{E} \|f_0(\cdot) - \hat{f}_n(\cdot)\|_k^2 = \mathcal{O}\left(n^{-2/5}\right).$$

For the best constant, an oracle is needed.



Precision analysis: $f_0 \notin \mathcal{H}_k$

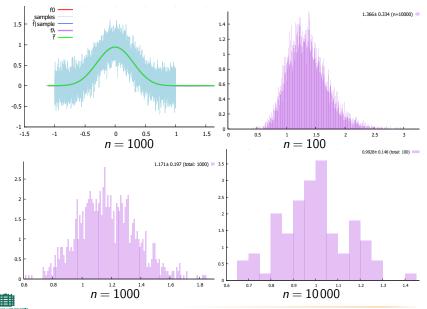
Histogram of $n\lambda \|f_{\lambda}(\cdot) - \hat{f}_{n}(\cdot)\|_{k}^{2}$





Precision analysis (cont): $f_0 \in \mathcal{H}_k$

Histogram of $\sqrt{n} \|f_0(\cdot) - \hat{f}_{\lambda_n}(\cdot)\|_k^2$ for $\lambda_n = n^{-1/2}$



Consistency

Employing Markov's inequality

Proposition (Weak consistency)

For $\varepsilon > 0$ it holds that $f_0(x) = \mathbb{E}[f \mid X = x]$

$$P(\|f_{\lambda}-\hat{f}_{n}\|_{k}\geq\varepsilon)\to 0$$

as $n \to \infty$ (convergence in probability).

Proposition

Consistency of $\hat{\vartheta}_n$: it holds that

$$P(|\vartheta^* - \hat{\vartheta}_n| \ge \varepsilon) \to 0$$

as $n \to \infty$.



Risk

Incorporate risk aversion

Quantile estimation employs the loss function

$$\ell_{\alpha}(y) := \begin{cases} -(1-\alpha)y & \text{if } y \leq 0, \\ \alpha \cdot y & \text{if } y \geq 0. \end{cases}$$

The expectile

$$e_{\alpha}(X) := \operatorname{argmin}_{x \in \mathbb{R}} \mathbb{E} \ell_{\alpha}(X - x),$$

the only *elicitable* risk functional, which is coherent – employs the loss function

$$\ell_{\alpha}(y) := \begin{cases} -(1-\alpha)y^2 & \text{if } y \leq 0, \\ \alpha \cdot y^2 & \text{if } y \geq 0. \end{cases}$$

$$e_{\alpha}(x) := \operatorname{argmin}_{f_{\lambda}(\cdot)} \mathbb{E} \ell_{\alpha}(f - f_{\lambda}(X)) + \lambda \|f_{\lambda}(\cdot)\|_{k}^{2},$$



$$\hat{e}_{\alpha}(x) := \operatorname{argmin}_{f_{\lambda}(\cdot)} \frac{1}{n} \sum_{i=1}^{n} \ell_{\alpha}(f_{i} - f_{\lambda}(X_{i})) + \lambda \|f_{\lambda}(\cdot)\|_{k}^{2}.$$
A. Pichler

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The conditional expectile is

$$e_{\alpha}(x) := \operatorname{argmin}_{f_{\lambda}(\cdot)} \mathbb{E} \ell_{\alpha}(f - f_{\lambda}(X)) + \lambda \|f_{\lambda}(\cdot)\|_{k}^{2},$$

with discretized version



$$\hat{\mathbf{e}}_{\alpha}(x) := \operatorname{argmin}_{f_{\lambda}(\cdot)} \frac{1}{n} \sum_{i=1}^{n} \underbrace{\ell_{\alpha}(f_{i} - f_{\lambda}(X_{i}))}_{A \text{ Pichler}} + \lambda \|f_{\lambda}(\cdot)\|_{k}^{2}.$$

Conditional improvements

Eigenvalues

Theorem

Assume the spectrum of the matrix K decays exponentially, i.e., there are constants α and β such that

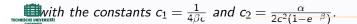
$$\sigma_i \leq \alpha e^{-\beta i}$$
.

Then

$$\mathbb{E}\left\|\frac{1}{n}\sum_{i=1}^{n}w_{i}^{N}k(\cdot,X_{i})\right\|_{k}^{2} \leq \sigma_{\max}^{2}c_{1}\frac{\log n}{p\,n\,\lambda} + c_{2}\frac{\sigma_{\max}^{2}}{\lambda^{2}\,n^{\frac{1}{p}+1}}$$

holds for all $p \ge 1$. Moreover, for $\lambda_n = \frac{c}{\sqrt{n}}$ it holds that

$$\mathbb{E}\left\|\frac{1}{n}\sum_{i=1}^{n}w_{i}^{N}k(\cdot,X_{i})\right\|_{L}^{2} \leq \frac{\sigma_{\max}^{2}c_{1}\frac{\log n}{\sqrt{n}}+c_{2}\frac{\sigma_{\max}^{2}}{\sqrt{n}}}{\sqrt{n}}$$



Remarks and follow-up questions

Invitation for future work

- The results do not depend on the dimension.
- Risk: the expectile is an M-estimator and consistent with this type of optimization,
- cf. [Dentcheva and Lin, 2021]
- \bullet Further implications on machine learning: different loss functions ℓ
- Bandwidth selection
- What is the limiting distribution of $n \cdot ||f_n(\cdot) f_{\lambda}(\cdot)||^2$
- Correct order of convergence in special cases
- Implications on the stochastic optimization problem

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

for smooth functions

- Implications on multistage programs and HJB
- time series analysis, machine learning: predict X_{t+1} , given the past observations $X_t, \ldots, X_{t-\ell}$.



ANOVA

Analysis of variance (ANOVA)

Signal + noise: Iterations on variables

Observations (X_i, f_i) , where $f_i = f_0(X_{i1}, \dots, X_{id}) + \varepsilon$:

$$f_0(x_1,\ldots,x_d)+\varepsilon=\underbrace{\mathbb{E}\,f}_{\hat{f}_0\in\mathbb{R}}+\varepsilon_0$$



Analysis of variance (ANOVA)

Signal + noise: Iterations on variables

Observations (X_i, f_i) , where $f_i = f_0(X_{i1}, \dots, X_{id}) + \varepsilon$:

$$f_0(x_1, \dots, x_d) + \varepsilon = \underbrace{\mathbb{E} f}_{\hat{f}_0 \in \mathbb{R}} + \underbrace{\mathbb{E} (f | X_1 = x_1)}_{\hat{f}_1(x_1)} + \dots + \underbrace{\mathbb{E} (f | X_d = x_d)}_{\hat{f}_d(x_d)} + \varepsilon_1$$

Here,
$$\hat{f}_i(\cdot) = \sum_{i=1}^n \hat{w}_i k(\cdot, X_i)$$
, where

$$\lambda \, \hat{w}_i + \sum_{\ell=1}^n k(X_i, X_\ell) \, \hat{w}_\ell = f_i - \sum_{i < i} \hat{f}_j(X_i).$$



Analysis of variance (ANOVA)

Signal + noise: Iterations on variables

Observations (X_i, f_i) , where $f_i = f_0(X_{i1}, \dots, X_{id}) + \varepsilon$:

$$f_{0}(x_{1},...,x_{d}) + \varepsilon = \underbrace{\mathbb{E} f}_{\hat{f}_{0} \in \mathbb{R}} + \underbrace{\mathbb{E}(f|X_{1} = x_{1})}_{\hat{f}_{1}(x_{1})} + \cdots + \underbrace{\mathbb{E}(f|X_{d} = x_{d})}_{\hat{f}_{d}(x_{d})} + \sum_{i < j} \underbrace{\mathbb{E}(f|X_{i} = x_{i}, X_{j} = x_{j})}_{\hat{f}_{ij}(x_{i}, x_{j})} + \varepsilon_{2}$$

Here,
$$\hat{f}_i(\cdot) = \sum_{i=1}^n \hat{w}_i k(\cdot, X_i)$$
, where

$$\lambda \hat{w}_i + \sum_{\ell=1}^n k(X_i, X_\ell) \hat{w}_\ell = f_i - \sum_{i < i} \hat{f}_j(X_i).$$



Predictions based on temporal lag ℓ

Luftdruck

Observations

$$X_0,\ldots,X_{t-\ell-1},\underbrace{X_{t-\ell},\ldots X_t},X_{t+1},X_{t+2},\ldots,X_n,$$

where

Temperatur +

$$X_{t+1} = f(X_{t-\ell}, \dots, X_t) + \varepsilon.$$
Niederschlag * Wind *

Niederschlag -Temperatur 3.Jul 4.Jul 5.Jul 6.Jul 7.Jul 8.Jul 9.Jul 10.Jul 11.Jul 12.Jul 30 °C 25 °C 20 °C 15 °C 10 °C

A. Pichler

RKHS

48

Predictions based on temporal lag ℓ

Luftdruck

Observations

$$X_0,\ldots,X_{t-\ell-1},\underbrace{X_{t-\ell},\ldots X_t,X_{t+1}},X_{t+2},\ldots,X_n,$$

where

Temperatur +

$$X_{t+1} = f(X_{t-\ell}, \dots, X_t) + \varepsilon.$$
Niederschlag * Wind *

Niederschlag -

Temperatur 3.Jul 4.Jul 5.Jul 6.Jul 7.Jul 8.Jul 9.Jul 10.Jul 11.Jul 12.Jul 30 °C 25 °C 20 °C 15 °C 10 °C A. Pichler RKHS

48

Predictions based on temporal lag ℓ

Observations

$$X_0, \dots, X_{t-\ell-1}, \underbrace{X_{t-\ell}, \dots, X_t, X_{t+1}}_{\text{training}}, X_{t+2}, \dots, X_n,$$

where

$$X_{t+1} = f(X_{t-\ell}, \dots, X_t) + \varepsilon.$$

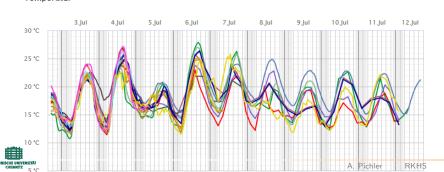
Temperatur -

Luftdruck

Niederschlag ▼

Wind -

Temperatur



48

Predictions based on temporal lag ℓ

Observations

$$X_0, \dots, X_{t-\ell-1}, \underbrace{X_{t-\ell}, \dots, X_t, X_{t+1}}_{\text{training}}, X_{t+2}, \dots, X_n,$$

where

$$X_{t+1} = \frac{f}{f}(X_{t-\ell}, \dots, X_t) + \varepsilon.$$

Here.

$$\hat{f}(x_{-\ell},...,x_0) = \sum_{t=1}^n \hat{w}_t \, k\Big((x_{-\ell},...,x_0),(X_{t-\ell},...,X_t)\Big),$$

where

$$\lambda \hat{w}_t + \sum_{j=1}^n k((X_{t-\ell}, \dots, X_t), (X_{j-\ell}, \dots, X_j) \hat{w}_j = X_{t+1}.$$



Thank you!

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