Welcome to LIKE22!

LIKE22 (“Lifting Inference with Kernel Embeddings”) is a winter school and workshop starting today (Monday January 10th 2022) and lasting until Friday January 14th 2022, with main topics

- kernel embeddings from theory to applications,
- recent advances in Gaussian Process modelling,
- active learning for accelerated inference.

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- recent advances in Gaussian Process modelling,
- active learning for accelerated inference.

The first day of the event (today!) aims at covering basics of the aforementioned topics over four introductory courses.

From tomorrow on, various speakers will present and discuss ongoing research and state of the art results. See program for a complete schedule.

Contributed videos by early-stage researchers

On Tuesday from 3PM to 4PM (Swiss time) we will have a first time slot dedicated to contributed video presentations by early-stage researchers (6 at the graduate student level and 3 at the postdoc level).

Subsequently, the Scientific Committee will elect finalists in each category. A specific Questions & Answers session with the finalists will take place on Thursday (from 2.45PM on).

500 Swiss Francs will be awarded for the top-ranked video in each category, announced on Friday.

Legacy and acknowledgements

LIKE22 is part of a powerful flow of local and global events related to its core topics. These include two reading groups (summers 2020 and 2021) on kernel methods, as well as the recent Axtis workshop.

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Also, many of us have had a chance to participate to events belonging to the series of Gaussian Process Summer Schools (GPSS) originally emanating from the University of Sheffield.

GPSS organizers are warmly thanked for their efforts to compile and transfer knowledge on GPs year after year, and we refer to the GPSS website for a highly valuable collection of talks and tutorials!

Legacy and acknowledgements

Many thanks to all colleagues from UniBE (IMSV, ILUB, etc.) and further institutions who have participated in setting up LIKE22 in one way or another. The boundary between organizers and speakers was sometimes blurry, special acknowledgements to participants having served in several capacities!

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Also, let us mention that LIKE22 is among the first events labelled by the Bern Data Science Initiative. More to come!

A few practicalities

- LIKE22 is now a fully online event (webinar)
- The Zoom link should normally remain the same for all sessions
- By default, presentations are recorded and meant to be archived and publically available on Switchtube
- Presentation time slots are long, meant to allow for questions and interactions: please do not hesitate to use discussion and Q&A tools!

Flexible, probabilistic function modelling with Gaussian Processes

Athénaïs Gautier (tutorial) and David Ginsbourger (slides)

[1] IMSV, Mathematics and Statistics Department, University of Bern, Switzerland

Acknowledgements: a number of co-authors, notably appearing via citations!

LIKE22: Lifting Inference with Kernel Embeddings
Day 1: Introductory talks
Online, January 10. 2022

Outline

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Preamble

We investigate i) a complex system represented by a deterministic function $f : \mathbf{x} \in E \mapsto f(\mathbf{x}) \in F$, ii) and/or quantities relying on f, based on a limited number of evaluations of f.

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Two typical example classes

- Engineering Design: $\mathbf{x}$ is a vector parametrizing some system and f returns an indicator of performance or dangerousness. It is then crucial to understand which $\mathbf{x}$'s lead to "high" values of $f(\mathbf{x})$.

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Two typical example classes

- Engineering Design: $\mathbf{x}$ is a vector parametrizing some system and f returns an indicator of performance or dangerousness. It is then crucial to understand which $\mathbf{x}$'s lead to "high" values of $f(\mathbf{x})$.
- Environmental modelling: $\mathbf{x}$ stands e.g. for the medium, boundary conditions, etc. and f returns the evolution of a contaminant and/or a measure of discrepancy between simulation results and given observation results.

Bayesian approach with GP models

Typical situation : f evaluated at $\mathbf{x}_1, \ldots, \mathbf{x}_n \in D \subset E$; one wishes to estimate a quantity relying on f / run new evaluations to improve its estimation.

NB: See today's courses by Dario & Cédric and ST + Dario's and Mark's talks for other types of query to f (latent models / indirect measurements).

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$\Rightarrow$ legitimate to rely on some approximation(s) of f knowing $f(\mathbf{x}_i) + \epsilon_i$ $(1 \leq i \leq n)$. A number of approaches do exist...

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Principles of the GP approach: suppose that, *a priori*, f is a realization of a GP $(Z_{\mathbf{x}})_{\mathbf{x} \in D}$ and approximate f and/or the quantities of interest via the **conditional distribution** of Z knowing $Z_{\mathbf{x}_i} + \varepsilon_i = f(\mathbf{x}_i) + \epsilon_i$.

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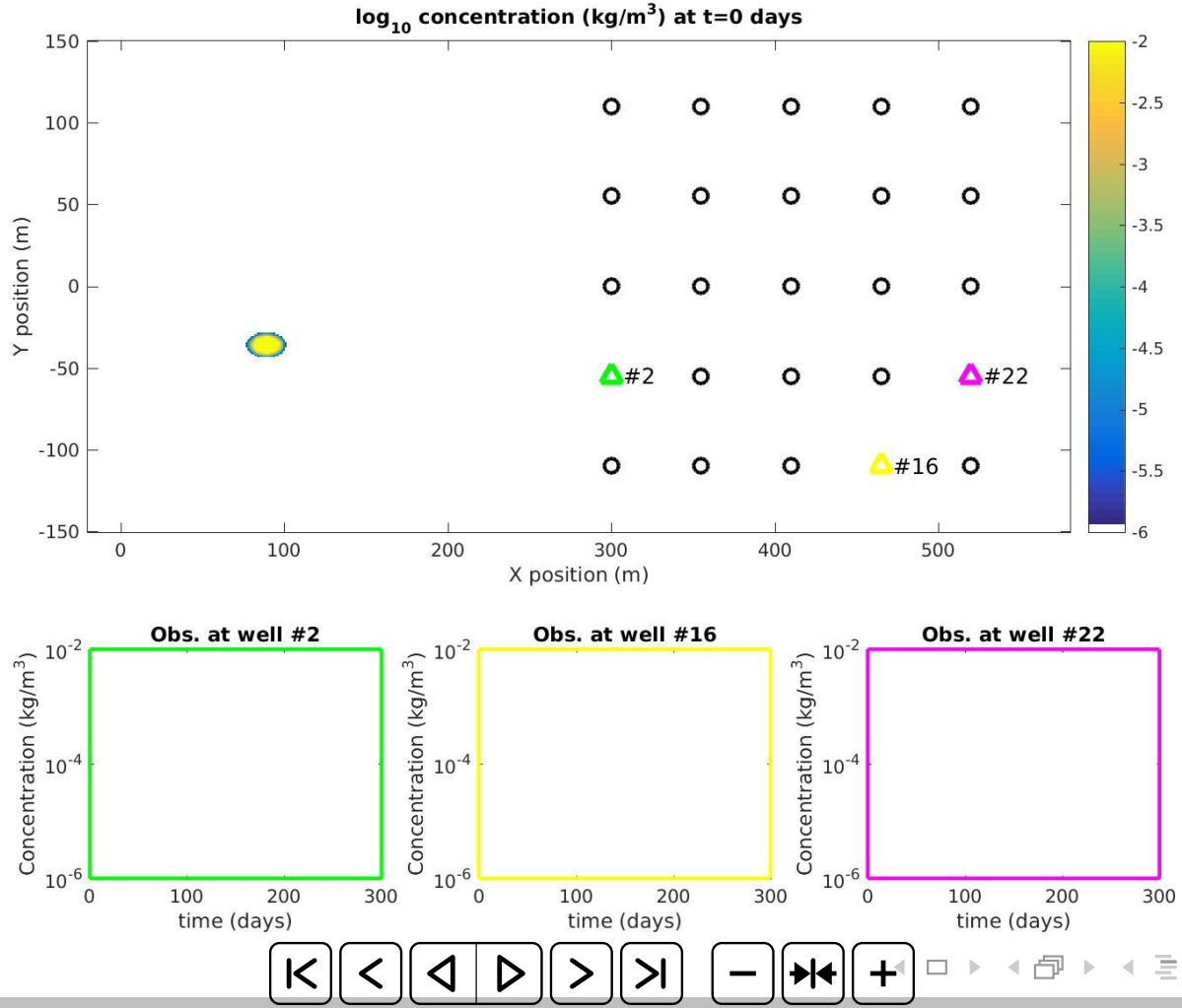
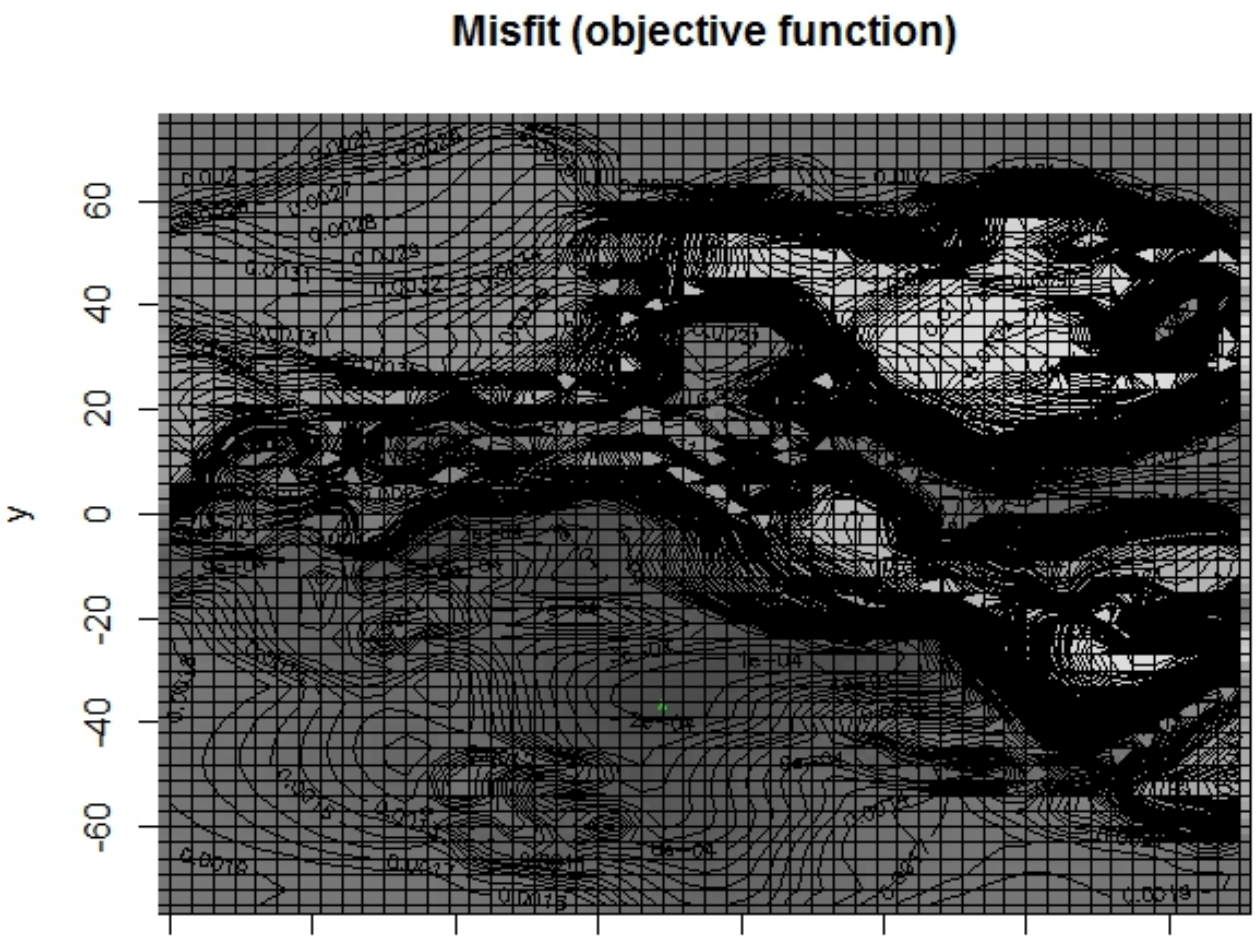
$\Rightarrow$ very practical for sequential design of experiments.

Example inverse problem in hydrogeology



A costly full factorial experimental design!



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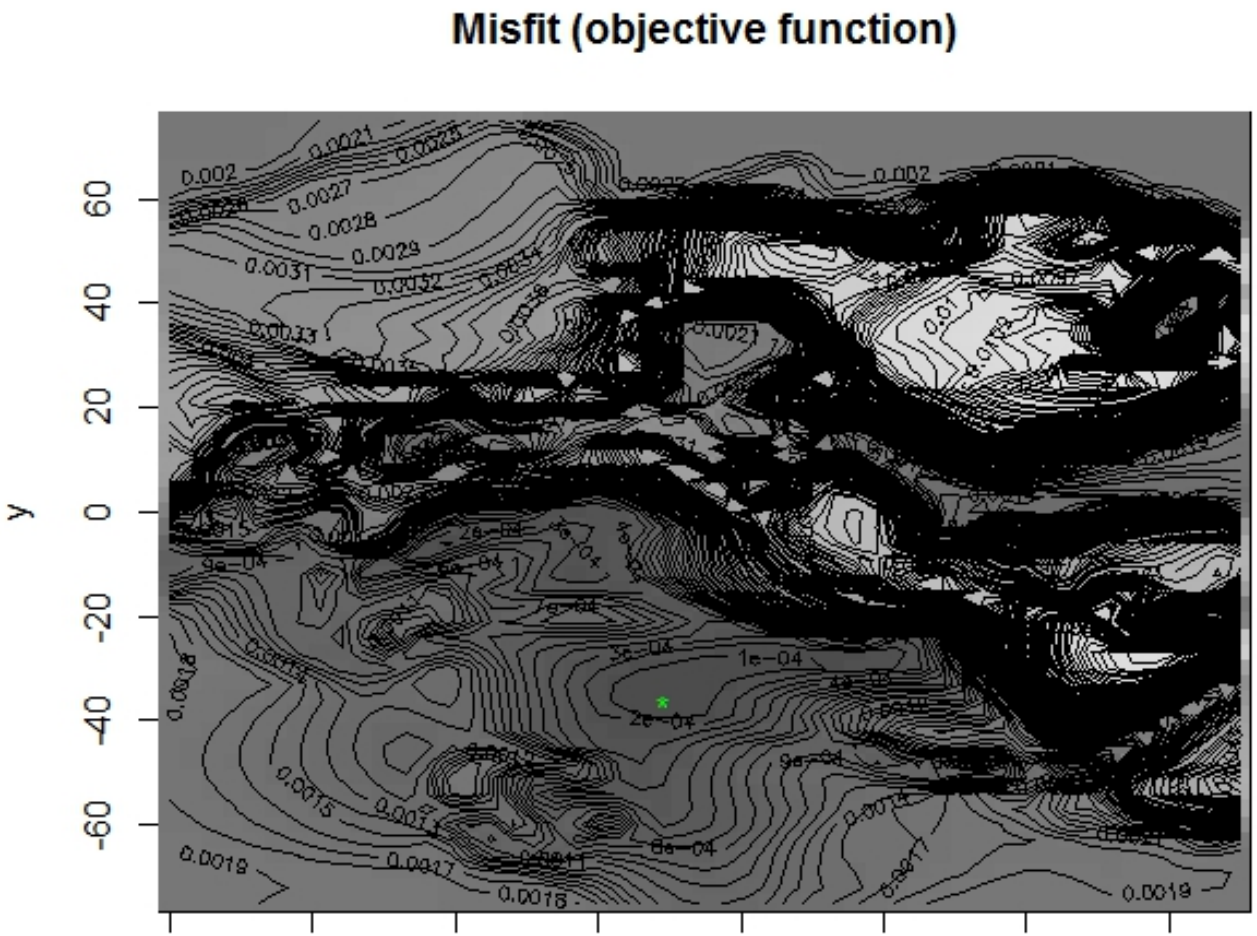
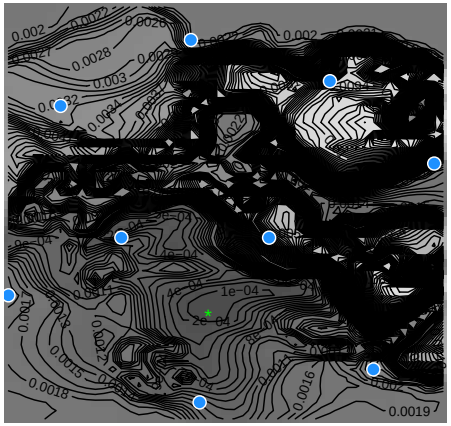
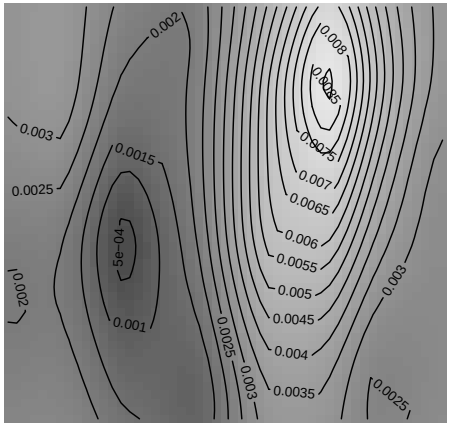


Application of Bayesian optimization

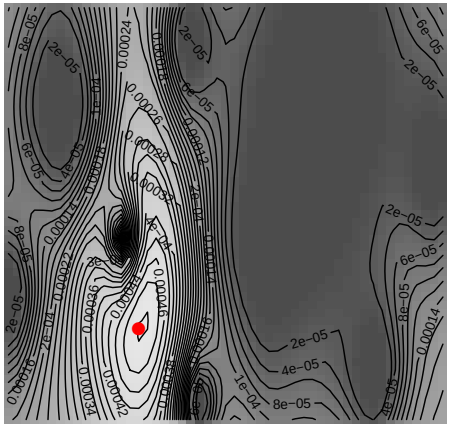
Misfit (objective function)



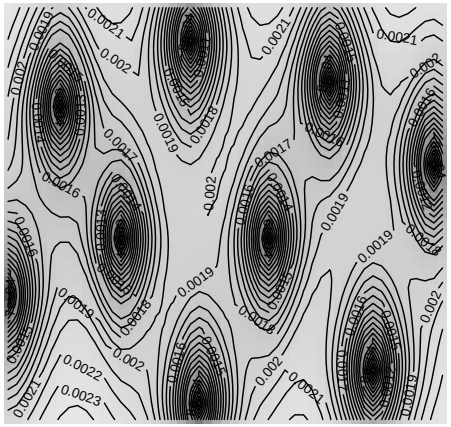
GP mean prediction



Expected Improvement



GP standard deviation



The previous example was produced in the framework of a collaboration with G. Pirot (now at UWA), T. Krityakierne (now at Mahidol University) and P. Renard (University of Neuchâtel).

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Main focus in the following of this presentation/tutorial

Give an insight on probabilistic kernel methods underlying such algorithms...

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Give an insight on probabilistic kernel methods underlying such algorithms...

...thanks to a short and rather informal introduction to GP models, with a focus on the great flexibility that they inherit from their underlying kernels.

A few references on GP modelling...

A. O'Hagan (1978).

Curve fitting and optimal design for prediction.

Journal of the Royal Statistical Society, Series B, 40(1):1-42.

J. Sacks, W.J. Welch, T.J. Mitchell, and H. P. Wynn (1989).

Design and Analysis of Computer Experiments

Statist. Sci. 4(4), 409-423.

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Mathematical Geology, 22 (7):767-786.

M. S. Handcock and M. L. Stein (1993).

A bayesian analysis of kriging.

Technometrics, 35(4):403-410.

A.W. Van der Vaart and J. H. Van Zanten (2008).

Rates of contraction of posterior distributions based on Gaussian process priors.

Annals of Statistics, 36:1435-1463.

. . . and on (GP-based) Bayesian Optimization

H.J. Kushner (1964).

A new method of locating the maximum of an arbitrary multi-peak curve in the presence of noise.
Journal of Basic Engineering, 86:97-106.

J. Mockus (1972).

On Bayesian methods for seeking the extremum.
Automatics and Computers (Avtomatika i Vychislitel'naya Tekhnika), 4(1):53-62.

J. Mockus, V. Tiesis, and A. Zilinskas (1978).

The application of Bayesian methods for seeking the extremum.
In Dixon, L. C. W. and Szegö, G. P., editors, Towards Global Optimisation, volume 2, pages 117-129. Elsevier Science Ltd., North Holland, Amsterdam.

J.M. Calvin (1997).

Average performance of a class of adaptive algorithms for global optimization.
The Annals of Applied Probability, 7(3):711-730.

M. Schonlau, W.J. Welch and D.R. Jones (1998).

Efficient Global Optimization of Expensive Black-box Functions.
Journal of Global Optimization.

What the rest of this presentation is about

- How do GPs relate to Gaussian variables and vectors?
- Discussing the great generality of GP modelling and related pitfalls
- Demonstrating the use of GPs on a few examples
- Getting introduced to selected families of kernels
- Preparing the ground for further talks on neighbouring topics

What the rest of this presentation is not about

- Asymptotic/concentration results on GP modelling
- Indepth results on Bayesian Optimization
- Links to the theory of Gaussian measures in Banach spaces

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  See LIKE22 presentations by Niklas, Florence, George, Johanna

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Outline

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Let us first focus on an arbitrary point $\mathbf{x} \in D$ and think of the unknown response value $f(\mathbf{x})$ as a Gaussian random variable, denoted here $Z_{\mathbf{x}}$.

Of course, how the mean and variance of $Z_{\mathbf{x}}$ are specified is crucial. A simple option is to set them to constant values (e.g. 0 mean and $\sigma^2 > 0$ variance) ...

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... However, a white noise assumption would not be very constructive! The crux in GP modelling is to assume that the $Z_{\mathbf{x}}$'s for different $\mathbf{x}$'s are correlated.

Reminder: n-dimensional Gaussian distribution

More precisely, we will appeal to the multivariate Gaussian distribution. Let us forget about $\mathbf{x}$ for now and consider a random vector $\mathbf{Z} = (Z_1, \ldots, Z_n)$.

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Such $\mathbf{Z}$ is characterized by its mean $\boldsymbol{\mu} \in \mathbb{R}^n$ and covariance matrix $K \in \mathbb{R}^{n \times n}$ (with $\mathbb{E}[Z_i]$ and $\mathrm{Cov}[Z_i, Z_j] = \mathbb{E}[(Z_i - \mu_i)(Z_j - \mu_j)]$ entries, respectively).

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We use the notation:

$$\mathbf{Z} \sim \mathcal{N}(\boldsymbol{\mu}, K).$$

Note that while μ can take any value, K must be symmetric positive semi-definite (i.e. symmetric with non-negative eigenvalues).

Reminder: n-dimensional Gaussian distribution

In case of invertible K, $\boldsymbol{Z}$ possesses the probability density function:

$$p_{\mathcal{N}(\boldsymbol{\mu},K)}(\boldsymbol{z}) = (2\pi)^{-n/2} \det(K)^{-1/2} \exp\left(-\frac{1}{2}(\boldsymbol{z}-\boldsymbol{\mu})' K^{-1} (\boldsymbol{z}-\boldsymbol{\mu})\right)$$

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Besides that, denoting by $\boldsymbol{Z}_a$ and $\boldsymbol{Z}_b$ two subvectors of $\boldsymbol{Z}$ such that $\boldsymbol{Z} = (\boldsymbol{Z}_a, \boldsymbol{Z}_b)$, by $\boldsymbol{\mu}_a, \boldsymbol{\mu}_b$ the corresponding means, and defining the corresponding blocks of $\boldsymbol{Z}$'s covariance matrix by

$$K = \begin{pmatrix} K_a & K_{ab} \\ K_{ba} & K_b \end{pmatrix},$$

then (assuming invertibility of K_a), the conditional probability distribution of $\boldsymbol{Z}_b$ knowing that $\boldsymbol{Z}_a = \mathbf{z}_a$ is (multivariate) Gaussian with

$$\mathcal{L}(\boldsymbol{Z}^{(b)}|\boldsymbol{Z}_a = \mathbf{z}_a) = \mathcal{N}(\boldsymbol{\mu}_b + K_{ba}K_a^{-1}(\mathbf{z}_a - \boldsymbol{\mu}_a), K_b - K_{ba}K_a^{-1}K_{ab}).$$

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Good news from probability theory (Kolmogorov's extension theorem): random processes on D (a.k.a. random fields in case of multivariate D) can be defined through finite-dimensional distributions, i.e. through distributions of the random vectors $(Z_{\mathbf{x}_1}, \ldots, Z_{\mathbf{x}_n})$ for any finite $n \geq 1$ and $\mathbf{x}_1, \ldots, \mathbf{x}_n \in D$.

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Gaussian Processes (a.k.a. Gaussian Random Fields)

A GP (GRF) Z with index set D is a collection of random variables $(Z_{\mathbf{x}})_{\mathbf{x} \in D}$ (defined over the same probability space $(\Omega, \mathcal{A}, \mathbb{P})$) such that for any finite set of points $\mathbf{x}_1, \ldots, \mathbf{x}_n \in D$, $(Z_{\mathbf{x}_1}, \ldots, Z_{\mathbf{x}_n})$ is multivariate Gaussian

Mean and covariance functions of a GP

Hence a GP is Z defined by specifying the mean and the covariance matrix of any random vector of the form $(Z_{\mathbf{x}_1}, \ldots, Z_{\mathbf{x}_n})$, so that Z is characterized by

$$\mu : \mathbf{x} \in D \longrightarrow \mu(\mathbf{x}) = \mathbb{E}[Z_{\mathbf{x}}] \in \mathbb{R}$$
$$k : (\mathbf{x}, \mathbf{x}') \in D \times D \longrightarrow k(\mathbf{x}, \mathbf{x}') = \mathrm{Cov}[Z_{\mathbf{x}}, Z_{\mathbf{x}'}] \in \mathbb{R}$$

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While μ can be any function, k is constrained since $(k(\mathbf{x}_i, \mathbf{x}_j))_{1 \leq i \leq n, 1 \leq j \leq n}$ must be symmetric positive semi-definite for any set of points.

k satisfying such properties are referred to as **p.d. kernels**.

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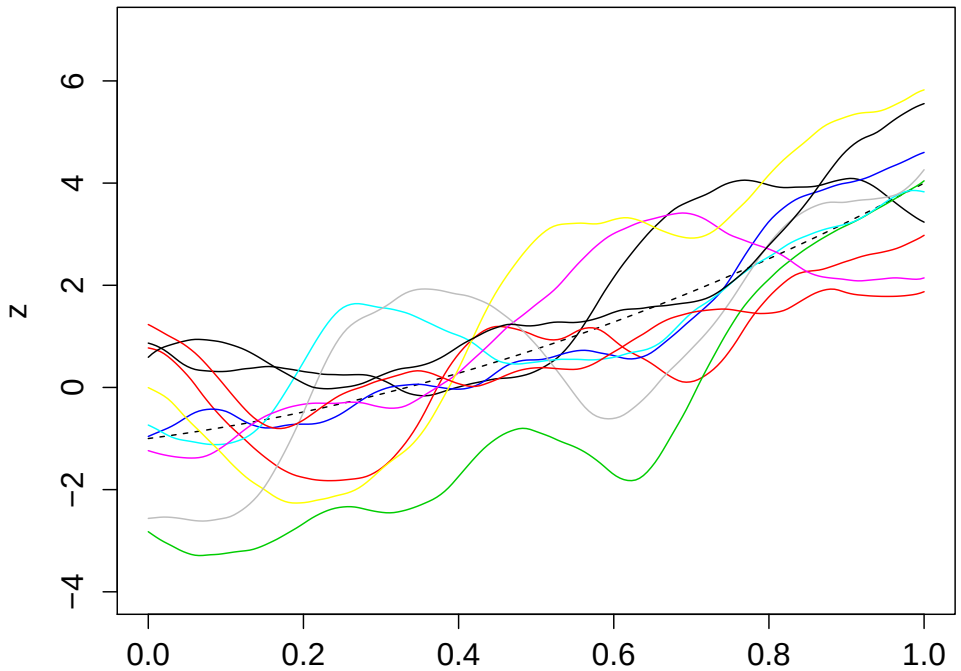
[See third part of this talk + Soham's talk today]

Some GRF R simulations (d=1) with *DiceKriging*

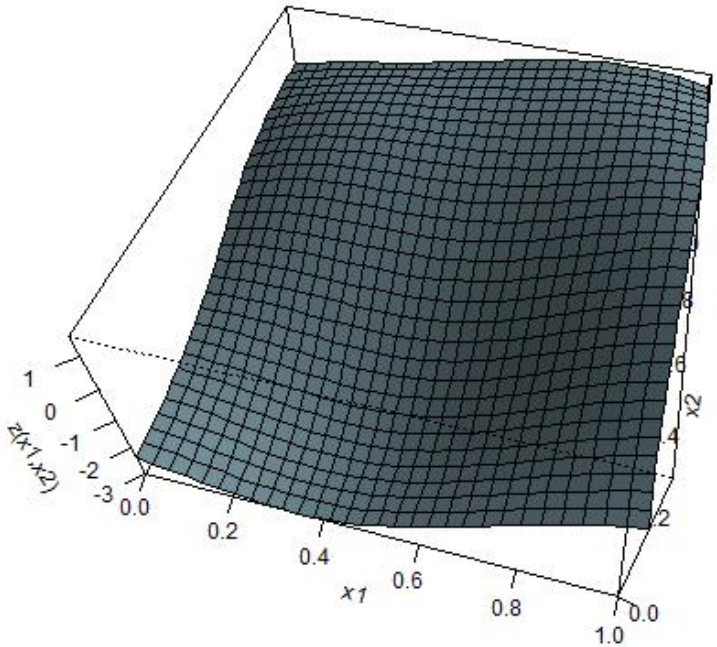
Here $k(t,t') = \sigma^2 \left(1 + |t'-t|/\ell + (t-t')^2/(3\ell^2)\right) \exp\left(-|t'-t|/\ell\right)$ (*Matérn kernel* with regularity parameter $5/2$) where $\ell = 0.4$ and $\sigma = 1.5$.

Furthermore, here trend is a trend $\mu(t) = -1 + 2t + 3t^2$.



Some GRF R simulations (d=2) with *DiceKriging*

Now take a tensorized version of Matérn kernel and a constant trend $\mu = 0$.



Approximating functions using GP models

Let us now consider a deterministic function $f : D \longrightarrow \mathbb{R}$, which response values are measured at n points $\mathbf{X}_n = (\mathbf{x}_1, \ldots, \mathbf{x}_n) \in D^n$.

Putting a GP prior Z on f and updating it with respect to f's values at the $\mathbf{x}_i$ points, we can work out a posterior distribution.

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Indeed, finite-dimensional distributions of this posterior can be obtained by looking at the conditional distribution of $(Z_{\mathbf{x}_{n+1}}, \ldots, Z_{\mathbf{x}_{n+q}})$ knowing $(Z_{\mathbf{x}_1}, \ldots, Z_{\mathbf{x}_n})$ for arbitrary points $\mathbf{x}_{n+1}, \ldots, \mathbf{x}_{n+q} \in D$.

By Gaussianity, it turns out that such conditional distributions are Gaussian and so the posterior $Z|$ measurements is a GP.

Approximating functions using GP models

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NB: the same applied in noisy cases when considering $(Z_{\mathbf{x}_1} + \varepsilon_1, \ldots, Z_{\mathbf{x}_n} + \varepsilon_n)$ with Gaussian ε_i's independent of Z).

Reminder: GP/Kriging equations

The GP/Kriging prediction amounts to calculating the conditional expectation and covariance of $Z_{\mathbf{x}}$ knowing $Z_{\mathbf{X}_n} = \mathbf{z}_n$, with $\boldsymbol{z}_n = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))'$:

$$\begin{cases} m_n(\mathbf{x}) = \mathbb{E}[Z_{\mathbf{x}} | Z_{\mathbf{X}_n} = \mathbf{z}_n] = \mu(\mathbf{x}) + k(\mathbf{x}, \mathbf{X}_n) k(\mathbf{X}_n, \mathbf{X}_n)^{-1} (\mathbf{z}_n - \mu(\boldsymbol{X}_n)) \\ \\ k_n(\mathbf{x}, \mathbf{x}') = \mathrm{Cov}[Z_{\mathbf{x}}, Z_{\mathbf{x}'} | Z_{\mathbf{X}_n} = \mathbf{z}_n] = k(\mathbf{x}, \mathbf{x}') - k(\mathbf{x}, \mathbf{X}_n) k(\mathbf{X}_n, \mathbf{X}_n)^{-1} k(\mathbf{X}_n, \mathbf{x}), \end{cases}$$

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where $k(\mathbf{X}_n, \mathbf{X}_n), = \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & \ldots & k(\mathbf{x}_1, \mathbf{x}_n) \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & \ldots & k(\mathbf{x}_2, \mathbf{x}_n) \\ \ldots & \ldots & \ldots. & \ldots. \\ k(\mathbf{x}_n, \mathbf{x}_1) & \ldots & \ldots. & k(\mathbf{x}_n, \mathbf{x}_n) \end{pmatrix}$ and $k(\mathbf{X}_n, \mathbf{x}) = \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}) \\ k(\mathbf{x}_2, \mathbf{x}) \\ \ldots \\ k(\mathbf{x}_n, \mathbf{x}) \end{pmatrix}$.

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For given m and k ($\exists$ generalizations to μ known up to linear trend coefficients), Z knowing $Z_{\mathbf{X}_n} = \mathbf{z}_n$ is a GP with mean m_n and covariance k_n.

Outline

Tutorial time!

Let us now shift the focus to some concrete implementation examples.

Outline

From p.d. kernels to function approximation

For an introduction to the mathematical foundations of p.d. kernels and their use in function approximation, see notably the following references:


C. Berg, J. P. R. Christensen and P. Ressel (1984)
Harmonic Analysis on Semigroups. Theory of Positive Definite and Related Functions
Springer-Verlag


A. Berlinet, C. Thomas-Agnan (2004)
Reproducing Kernel Hilbert Spaces in Probability and Statistics
Kluwer Academic Publishers

Choosing p.d. kernels?

In practice, choosing an adapted k for an objective f (about which limited information may be available) is both a crucial and difficult task.

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Typically, k is chosen among some well-known p.d. kernel families, often among "shift-invariant" (a.k.a. "stationary") kernels, i.e. functions of $\mathbf{x} - \mathbf{x}'$.

Examples: Generalized Exponential (including Gaussian) kernels, Matérn kernels, and more generally kernels obtained via the Bochner theorem.

Bochner theorem

By a slight abuse of notation, we denote stationary kernels on $D = \mathbb{R}^d$ ($d \geq 1$) by $k : \mathbf{h} \in \mathbb{R}^d \longrightarrow k(\mathbf{h}) \in \mathbb{C}$.

Theorem (Bochner's theorem)

A continuous $k : \mathbf{h} \in \mathbb{R}^d \longrightarrow k(\mathbf{h}) \in \mathbb{C}$ is positive definite if and only if it is the Fourier transform of a finite non-negative Borel measure ν on $\mathbb{R}^d$, i.e.

$$k(\mathbf{h}) = \hat{\nu}(\mathbf{h}) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} e^{-i\langle \mathbf{h}, \boldsymbol{\omega} \rangle} d\nu(\boldsymbol{\omega})$$

See for instance Wendland 2005 (Chap. 6) for a proof.

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By playing on the "spectral measure" ν one can hence generate all continuous stationary p.d. kernels on $\mathbb{R}^d$. For the absolutely continuous case, k is hence characterized by its *spectral density* $q(\boldsymbol{\omega}) = \frac{\mathrm{d}\nu}{\mathrm{d}\lambda}(\boldsymbol{\omega})$.

A few 1-dimensional examples

- Triangular: $k(h) := c(a - |h|)^+$ $\left(q(\omega) \sim \frac{c(1-\cos(a\omega))}{\pi\omega^2}\right)$
- Matérn $\nu = 3/2$: $k(h) \sim \alpha^{-3} e^{-\alpha|h|}(1 + \alpha|h|)$ $(q(\omega) \sim (\alpha^2 + \omega^2)^{-2})$
- Gauss: $k(h) \sim e^{-(\frac{h}{\theta})^2}$ $(q(\omega) \sim e^{-\theta^2\omega^2})$

M. Stein (Springer, 1999)

Interpolation of Spatial Data. Some Theory for Kriging

More on spectral densities of Matérn kernels ($d \geq 1$)

Matérn kernels can be characterized using the Hancock and Wallis parametrization (1994) mentioned in Stein (1999) (here $\sigma = 1$):

$$q(\omega) = \frac{c(\nu, \rho)}{\left(\frac{4\nu}{\rho^2} + ||\omega||^2\right)^{\nu + d/2}}$$

where $c(\nu, \rho) = \frac{\Gamma\left(\nu + \frac{d}{2}\right)(4\nu)^\nu}{\pi^{d/2}\Gamma(\nu)\rho^{2\nu}}$.

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$$k(\mathbf{h}) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\frac{2\nu^{1/2}||\mathbf{h}||}{\rho}\right)^\nu \mathcal{K}_\nu \left(\frac{2\nu^{1/2}||\mathbf{h}||}{\rho}\right)$$

where $\mathcal{K}_\nu$ is a *modified Bessel function of the third kind*. More tractable expressions can be obtained for $\nu = \frac{1}{2}, \frac{3}{2}, \frac{5}{2} \ldots$

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More on isotropic p.d. kernels in $\mathbb{R}^d$

The Matérn (class of) kernels considered previously are one among many *isotropic p.d. kernels on* $\mathbb{R}^d$, i.e. p.d. kernels that write as

$$k(\mathbf{x}, \mathbf{x}') = \kappa(r)$$

where $r = ||\mathbf{x} - \mathbf{x}'||_{\mathbb{R}^d}$, and $\kappa : \mathbb{R}_+ \longrightarrow \mathbb{R}$ is also often (by a slight abusive of language) referred to as positive definite. Such k's are also called *radial*.

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Definition (Cf. Wendland 2005): A function $\Phi : \mathbb{R}^d \longrightarrow \mathbb{R}$ is said to be *radial* if there exists $\phi : [0, +\infty) \longrightarrow \mathbb{R}$ such that $\Phi(\mathbf{h}) = \phi(||\mathbf{h}||_2)$ for all $\mathbf{h} \in \mathbb{R}^d$.

A number κ leading to radial p.d. kernels in $\mathbb{R}^d$ do exist and have been studied by generations of mathematicians. Some depend on d, some do not!

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Let us review of few examples.

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Is it possible to characterize radial p.d. functions defined in terms of one κ valid in any dimension? Yes, thanks to completely monotone functions!

More on isotropic p.d. kernels in $\mathbb{R}^d$

Definition (Cf. Wendland 2005): A function ϕ is called completely monotone on $(0, +\infty)$ if it satisfies $\phi \in C^\infty(0, +\infty)$ and

$$(-1)^\ell \phi^{(\ell)}(r) \geq 0$$

for all $\ell \in \mathbb{N}$ and all $r > 0$. The function ϕ is called completely monotone on $[0, +\infty)$ if it is in addition in $C[0, +\infty)$.

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Theorem (Schoenberg, Cf. Wendland 2005)

A function $\phi : [0, +\infty) \longrightarrow \mathbb{R}$ is completely monotone on $[0, +\infty)$ if and only if $\Phi := \phi(|| \cdot ||_2^2)$ is positive definite on every $\mathbb{R}^d$.

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Application: the inverse multiquadrics is p.d. in any dim. for $c, \beta > 0$.

Nota Bene: geometric anisotropy

Starting from any isotropic p.d. kernel, it is always possible to generalize it and obtain *(geometric) anisotropic* p.d. kernels through orthogonal transformations and dilatations, by defining

$$k(\mathbf{x}, \mathbf{x}') = \kappa\left((\mathbf{x} - \mathbf{x}')^T \Sigma (\mathbf{x} - \mathbf{x}')\right)$$

where Σ is a real-valued symmetric (strictly!) positive definite matrix.

Other ways of defining p.d. kernels: overview

Kernels that write as functions of $\langle \mathbf{x}, \mathbf{x}' \rangle$ (as the previously presented radial p.d. kernels on the sphere) are also called *zonal kernels* in G. E. Fasshauer's review paper below, were examples of zonal kernels are discussed:

Fasshauer, G. E. (2011)
Positive definite kernels: past, present and future
Dolomites Research Notes on Approximation, 4:21-63

The following paper also includes alternative classes of p.d. kernels:

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Overall, the notion of **scalar product** plays a crucial role in p.d. kernels.

Other ways of defining p.d. kernels: Mercer theorem

For continuous p.d. kernels –say real-valued, defined on a compact set $D \subset \mathbb{R}^d$– a fruitful approach is to consider the following operator T_k on $L^2(D)$:

$$g \longrightarrow T_k(g)(\cdot) = \int_D g(\mathbf{x}')k(\cdot, \mathbf{x}')\mathrm{d}\lambda(\mathbf{x}')$$

where λ refers to the Lebesgue measure (generalizations do exist) on $\mathbb{R}^d$.

Under our continuity and compactness conditions on T_k there exist $(\varphi_j(\cdot))_{j\in\mathbb{N}^*}$ forming an orthonormal system of $L^2(D)$ and $(\lambda_j)_{j\in\mathbb{N}^*}$ non-negative such that

$$\forall j \in \mathbb{N}\ T_k(\varphi_j) = \lambda_j\varphi_j$$

and this leads to the Mercer decomposition (1909):

$$k(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{\infty} \lambda_j\varphi_j(\mathbf{x})\varphi_j(\mathbf{x}').$$

See Adler & Taylor, Steinwart and more for detail on the convergence, etc.

Basic principle of the Karhunen-Loève expansion

Assuming D compact and k continuous, the Mercer theorem ensures the existence of an orthonormal basis $(\varphi_j)_{j\geq 1}$ of $L^2(D)$ such that

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$$k(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{+\infty} \lambda_j \varphi_j(\mathbf{x}) \varphi_j(\mathbf{x}')$$

The KL expansion of a GRF Z then consists in representing it under the form

$$Z_{\mathbf{x}} = \sum_{j=1}^{+\infty} \sqrt{\lambda_j} \zeta_j \varphi_j(\mathbf{x})$$

where the ζ_j's are i.i.d. standard Gaussian random variables.

Deriving the eigenfunctions: a Fredholm problem

Given a GRF Z of covariance kernel k, finding the basis functions φ_j ($j \geq 1$) is the key to the KL decomposition of Z.

This is done by solving the following integral equation:

$$\int_D k(\mathbf{x}, \mathbf{x}')g(\mathbf{x})d\mu(\mathbf{x}) = \lambda g(\mathbf{x}'),$$

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called a *Fredholm problem*.

When possible, the latter is solved analytically by using calculus.

Example: KL expansion of the Brownian Motion

For the covariance kernel of the BM, $k(t, t') = \min(t, t')$, the eigenvalues and eigenfunctions are solutions to the following Fredholm problem:

$$\int_0^1 \min(t, t')\varphi(t)dt = \lambda\varphi(t')$$

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It can be shown by solving a differential equation that the solutions are

$$\lambda_j = \frac{1}{\pi^2(j - \frac{1}{2})^2}$$

$$\varphi_j(t) = \sqrt{2}\sin\left(\left(j - \frac{1}{2}\right) \times \pi t\right)$$

R.J. Adler and J.E. Taylor (Springer, 2007)

Random Fields and Geometry

Example: KL expansion of the Brownian Motion

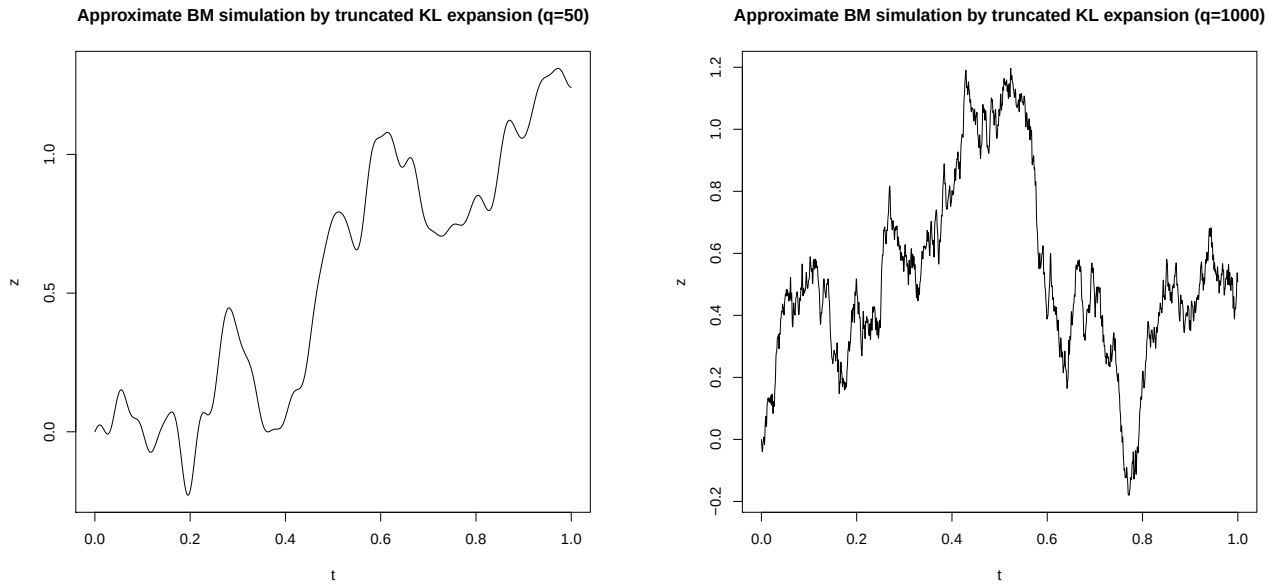
Let us simulate the Brownian Motion using a truncated KL expansion:

```
m <- 10000
t <- seq(0,1,,m)
v <- function(t,k){sqrt(2)*sin((k-0.5)*pi*t)}
lambda <- function(k){1/(pi*(k-0.5))^2}

q <- 1000
KL <- rep(0,m)
for(i in seq(1,q)){
KL <- KL + sqrt(lambda(i))*rnorm(1)*v(t,i)}
```

Example: KL expansion of the Brownian Motion

Here are two simulation results based on the truncated KL expansion of the Brownian Motion, respectively with $q = 50$ and $q = 1000$:



The simulations are not exact, but can be performed at a continuous set. The ζ_j's can be stored, and the corresponding path evaluated at a new point later.

A few selected references

M.L. Stein (1999).
Interpolation of Spatial Data, Some Theory for Kriging
Springer

M. Scheuerer (2009).
A Comparison of Models and Methods for Spatial Interpolation in Statistics and Numerical Analysis
PhD thesis of Georg-August Universität Göttingen

C. E. Rasmussen and C.K.I. Williams (2006).
Gaussian Processes for Machine Learning
MIT Press

R. Adler and J. Taylor (2007).
Random Fields and Geometry
Springer

I. Steinwart (2017).

Convergence Types and Rates in Generic Karhune–Loève Expansions with Applications to Sample Path Properties
arXiv:1403.1040v3 [math.PR]

Outline

In GP models and RKHS regularization with known (e.g., constant) mean, prior assumptions on f are implicitly accounted for through the choice of k.

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Classical notions of invariance for k

- 2nd order stationarity (*k invariant wrt simult. translations of* $\mathbf{x}$ *and* $\mathbf{x}'$)
- Isotropy (*k invariant wrt simultaneous rigid motions of* $\mathbf{x}$ *and* $\mathbf{x}'$).

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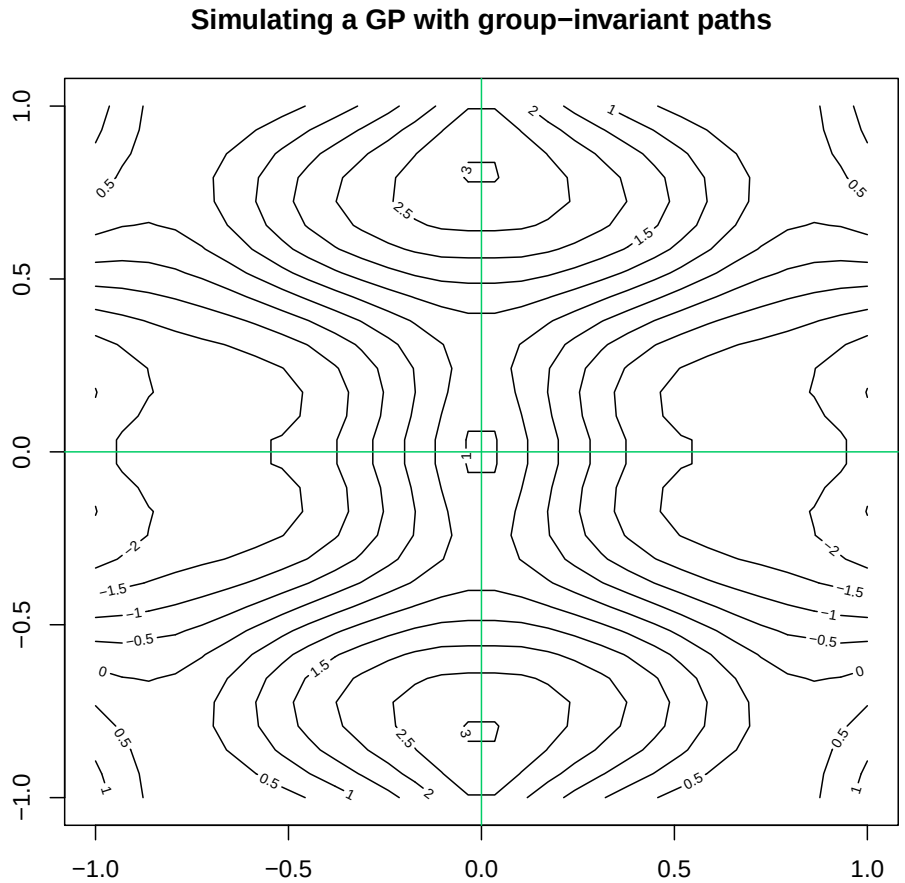
- Isotropy (k *invariant wrt simultaneous rigid motions of* $\mathbf{x}$ *and* $\mathbf{x}'$).

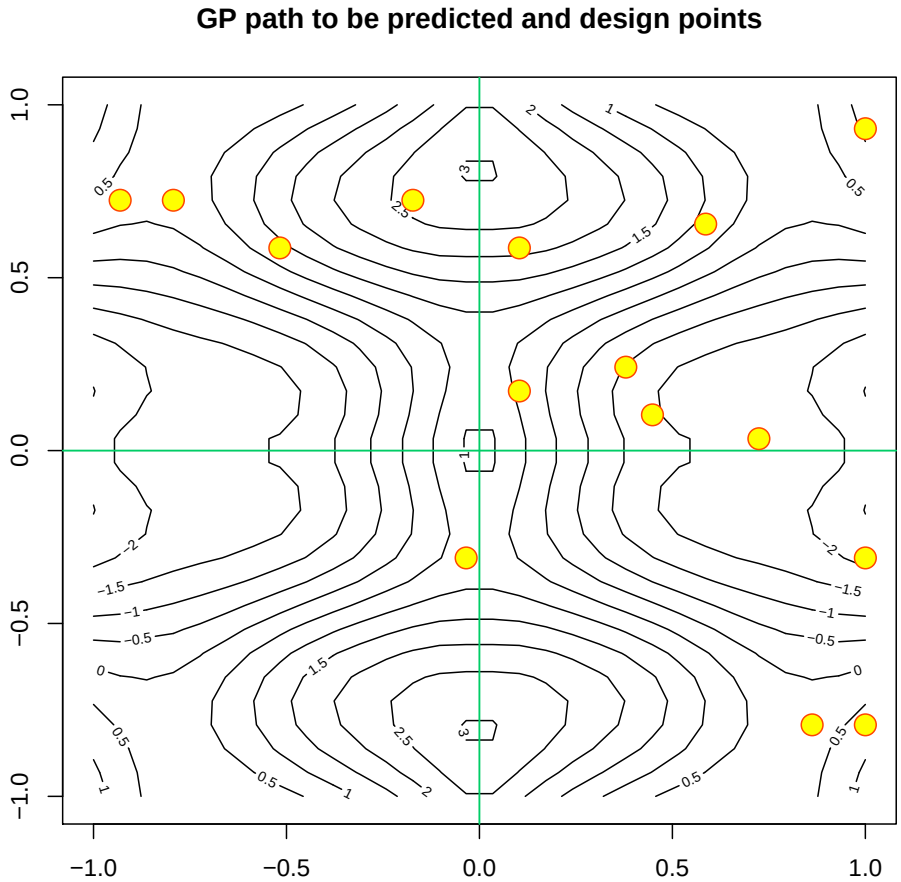
We rather investigate some functional properties driven by k, with a main focus on the stochastic case (+ some links to RKHSs).
This part follows to a large extent the paper below and references therein:

D. G., O. Roustant and N. Durrande (2016)
On degeneracy and invariances of random fields paths with applications in Gaussian Process modelling
Journal of Statistical Planning and Inference, 170:117-128.

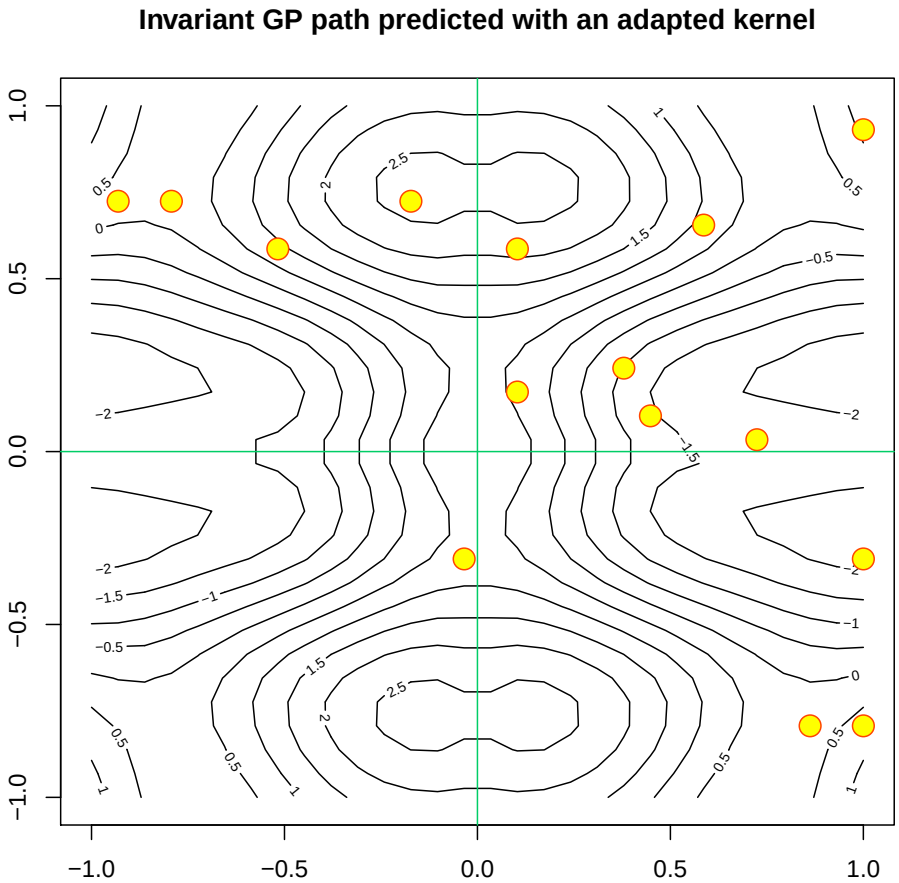
Simulating a GP with group-invariant paths



Towards invariant prediction: set-up



Predicting with an (argumentwise) invariant kernel



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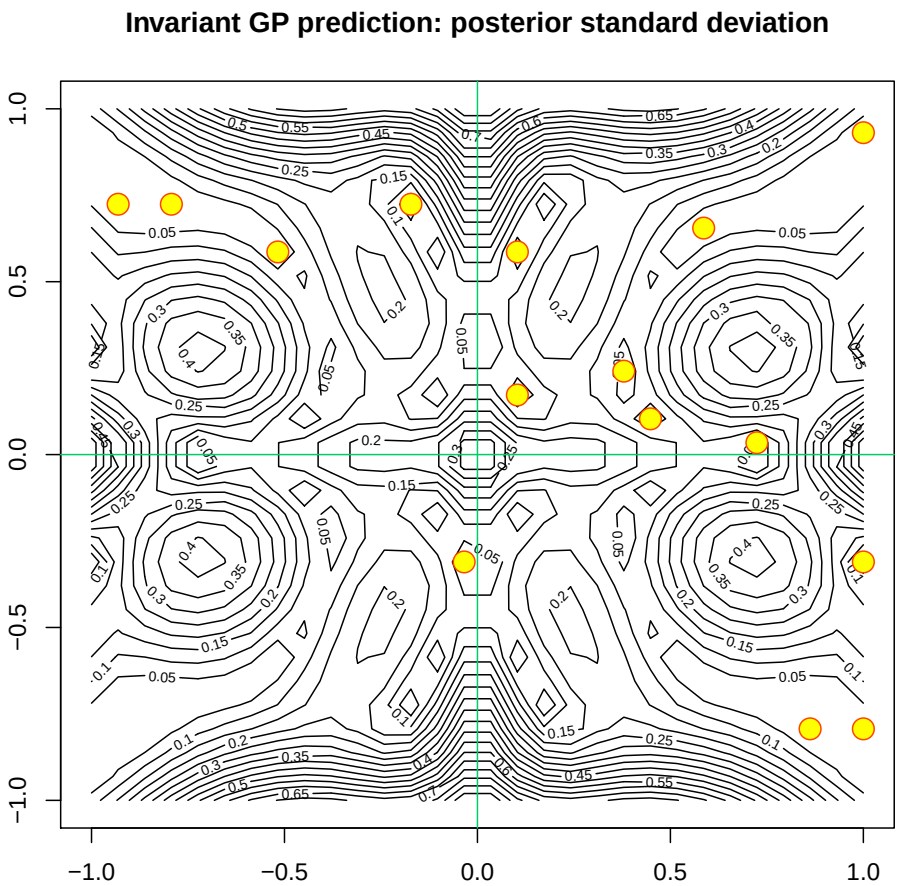
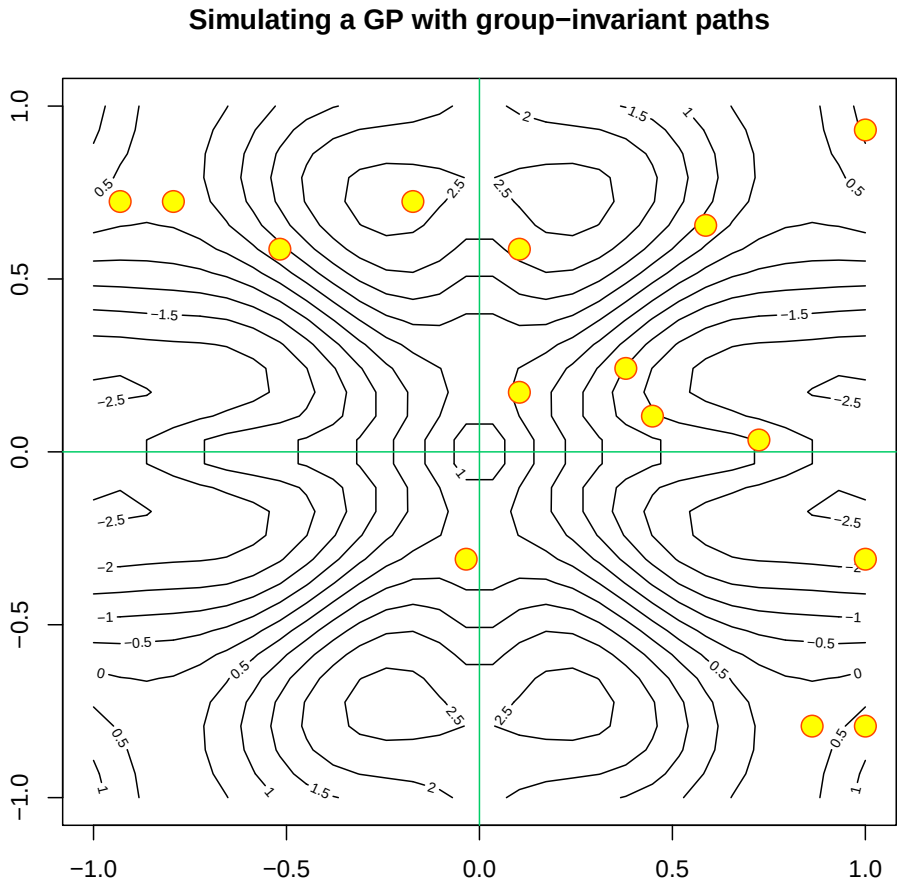


Invariant conditional simulations



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D. G., X. Bay, O. Roustant and L. Carraro (2012)
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Annales de la Faculté des Sciences de Toulouse, 21(3):501-527


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Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies
Journal of Chemical Theory and Computation 9, 3404-3419


Y. Mroueh, S. Voinea, T. Poggio (2015)
Learning with Group Invariant Features: A Kernel Perspective
Advances in Neural Information Processing Systems, 1558-1566

Another invariance: random fields with additive paths

Let $D = \prod_i^d D_i$ where $D_i \subset \mathbb{R}$. $f \in \mathbb{R}^D$ is called additive when there exists $f_i \in \mathbb{R}^{D_i}$ $(1 \leq i \leq d)$ such that $f(\mathbf{x}) = \sum_{i=1}^d f_i(x_i)$ $(\mathbf{x} = (x_1, \ldots, x_d) \in D)$.

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GP models possessing additive paths (with $k(\mathbf{x}, \mathbf{x}') = \sum_{i=1}^d k_i(x_i, x_i')$) have been considered in Nicolas Durrande's Ph.D. thesis (2011):

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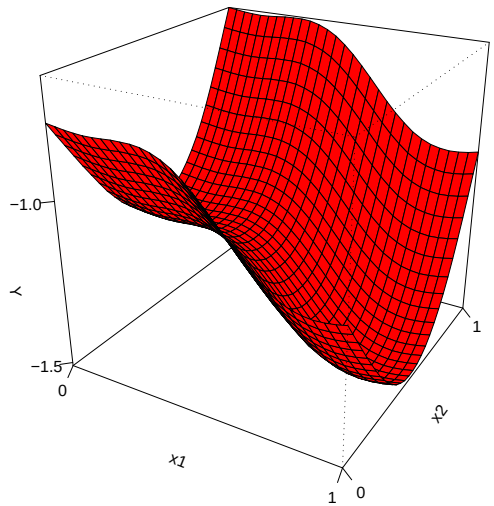

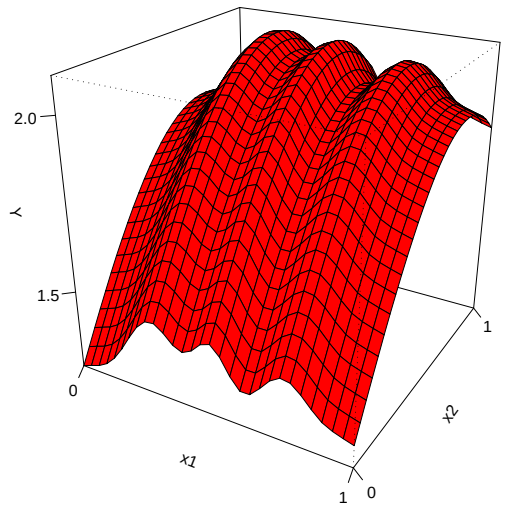

A few selected references related to additive kernels


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PhD thesis, Ecole des Mines de Saint-Etienne


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Additive Covariance kernels for high-dimensional Gaussian Process modeling
Annales de la Faculté des Sciences de Toulouse, 21(3):481-499


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Kernels and designs for modelling invariant functions: From group invariance to additivity.
In mODa 10 - Advances in Model-Oriented Design and Analysis. Contributions to Statistics

Further examples of degeneracies and invariances

a) Let ν be a measure on D s.t. $\int_D \sqrt{k(\mathbf{u},\mathbf{u})} d\nu(\mathbf{u}) < +\infty$. Then a centred Z (Gaussian or not) has centred paths iff $\int_D k(\mathbf{x},\mathbf{u}) \mathrm{d}\nu(\mathbf{u}) = 0, \forall \mathbf{x} \in D$.

For instance, given any p.d. kernel k, k_0 defined by

$$k_0(\mathbf{x},\mathbf{y}) = k(\mathbf{x},\mathbf{y}) - \int k(\mathbf{x},\mathbf{u}) \mathrm{d}\nu(\mathbf{u}) - \int k(\mathbf{y},\mathbf{u}) \mathrm{d}\nu(\mathbf{u}) + \int k(\mathbf{u},\mathbf{v}) \mathrm{d}\nu(\mathbf{u}) \mathrm{d}\nu(\mathbf{v})$$

satisfies the above condition.

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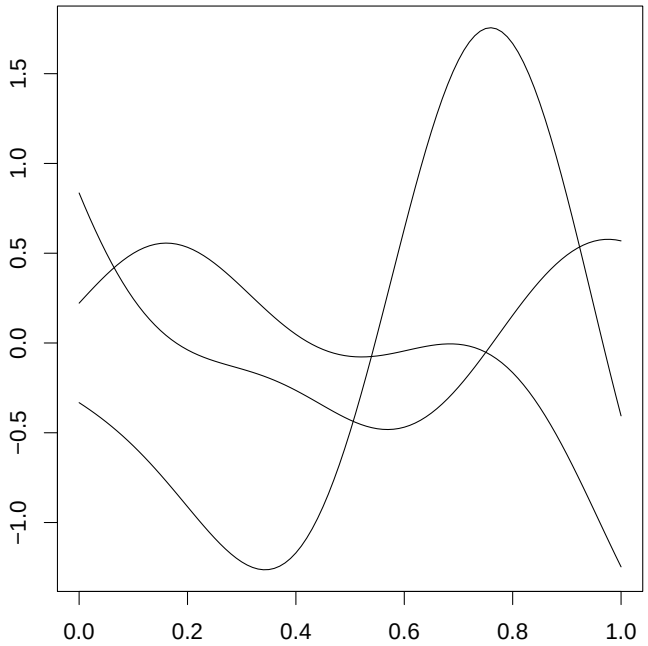
satisfies the above condition.

b) Solutions to the *Laplace equation* are called harmonic functions. Let us call harmonic any p.d. kernel solving the Laplace equation argumentwise: $(\Delta k(\cdot, \mathbf{x}')) = 0$ $(\mathbf{x}' \in D)$.

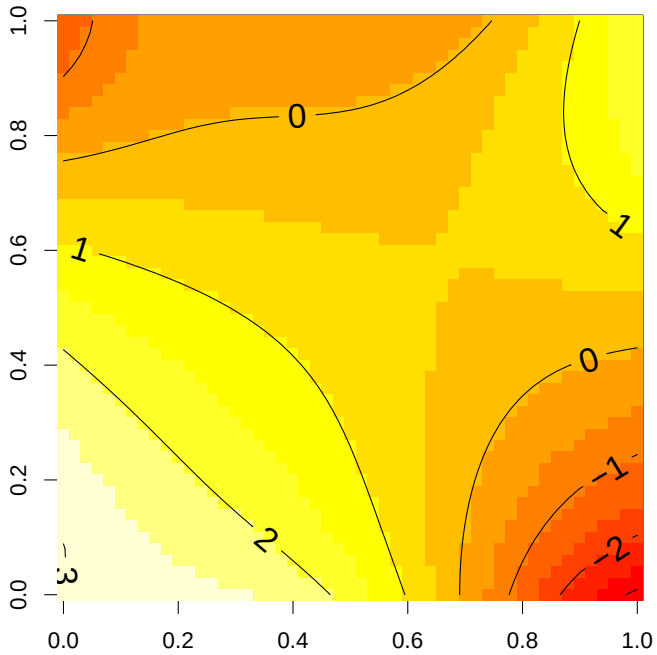
An example of such harmonic kernel over $\mathbb{R}^2 \times \mathbb{R}^2$ can be found in the recent literature (Schaback et al. 2009):

$$k_{harm}(\mathbf{x},\mathbf{y}) = \exp\left(\frac{x_1 y_1 + x_2 y_2}{\theta^2}\right) \cos\left(\frac{x_2 y_1 - x_1 y_2}{\theta^2}\right).$$

Example sample paths invariant under various T's



(a) Zero-mean paths of the centred GP with kernel k_0.



(b) Harmonic path of a GRF with kernel k_{harm}.

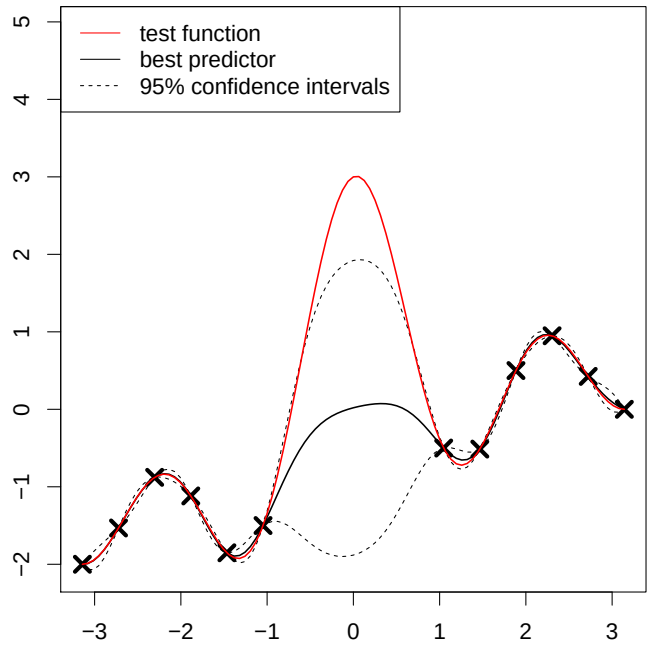
Some "stability of invariances by conditioning" result

Proposition

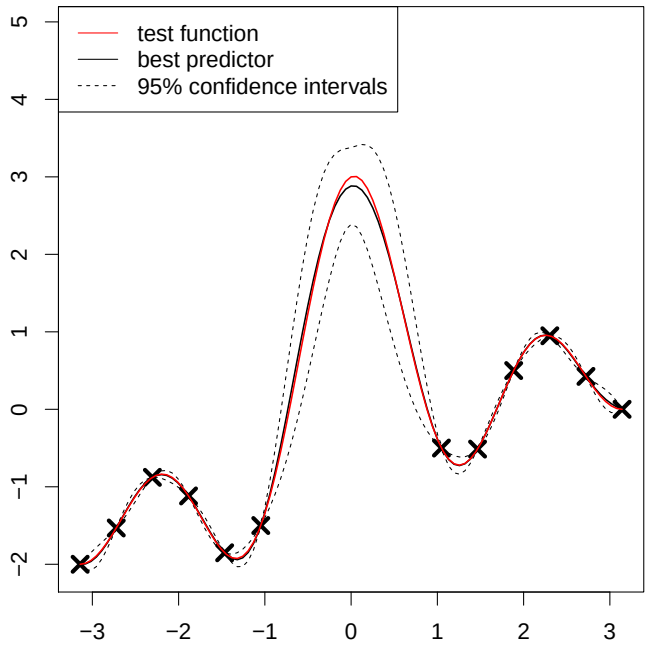
- *Let $\mathcal{F}, \mathcal{G}$ be real separable Banach spaces,*
- *μ be a Gaussian measure on $\mathcal{B}(\mathcal{F})$ with mean zero and covariance operator C_μ*
- *$T : \mathcal{F} \longrightarrow \mathcal{F}$ be a bounded linear operator such that $TC_\mu T^\star = 0_{\mathcal{F}^\star \longrightarrow \mathcal{F}}$*
- *$A : \mathcal{F} \longrightarrow \mathcal{G}$ be another bounded linear operator,*
- *and $A_\sharp \mu$ be the image of μ under A.*

Then there exist a Borel measurable mapping $m : \mathcal{G} \longrightarrow \mathcal{F}$, a Gaussian covariance $R : \mathcal{F}^\star \longrightarrow \mathcal{F}$ with $R \leq C_\mu$ and a disintegration $(q_y)_{y \in \mathcal{G}}$ of μ on $\mathcal{B}(\mathcal{F})$ with respect to A such that for any fixed $y \in \mathcal{G}$, q_y is a Gaussian measure with mean m and covariance operator R satisfying $T(m) = 0_{\mathcal{F}}$ and $TRT^\star = 0_{\mathcal{F}^\star \longrightarrow \mathcal{F}}$.

GP prediction with invariant kernels: example a)



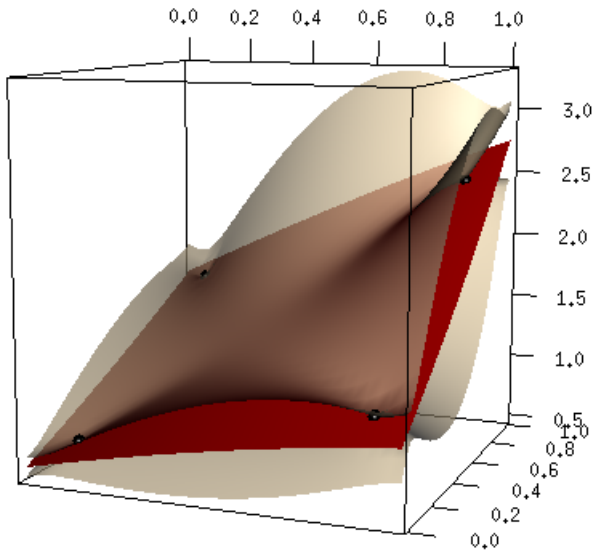
(a) GPR with kernel k



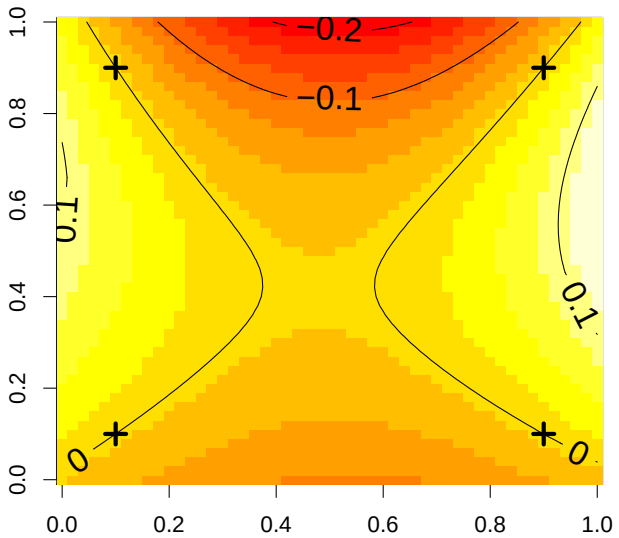
(b) GPR with kernel k_0

Figure: Comparison of two GP models. The left one is based on a Gaussian kernel. The right one incorporates the zero-mean property.

GP models with invariant kernels: example b)



(a) Mean predictor and 95% prediction intervals

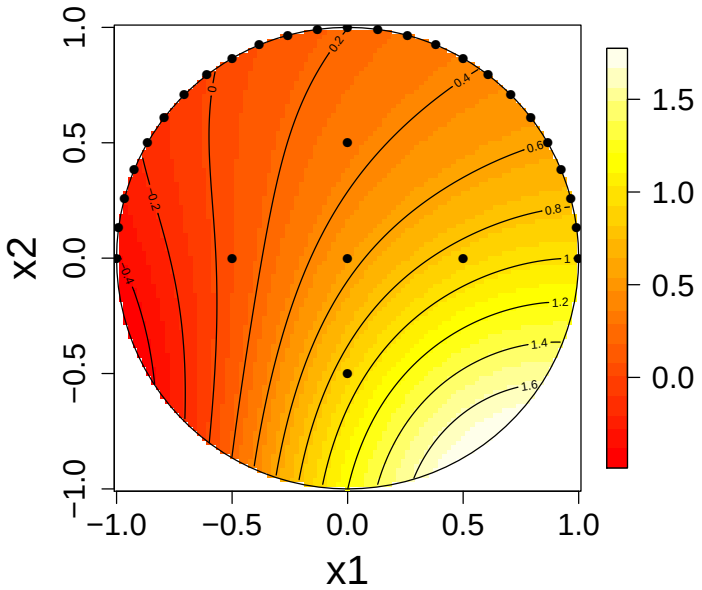


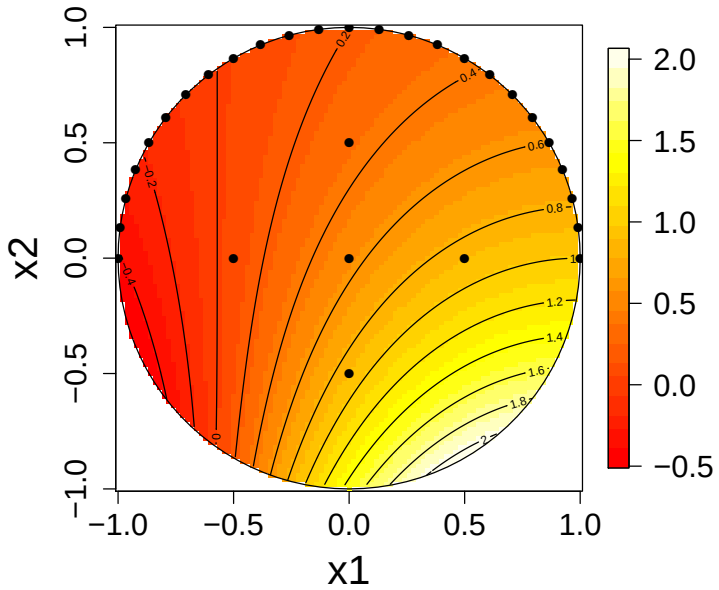
(b) prediction error

Figure: Example of GP model based on a harmonic kernel.

Numerical application: maximum of a harmonic *f*

Here we consider approximating a harmonic function (left/right: Gaussian/harmonic kernels) and estimating its maximum by GRF modelling.





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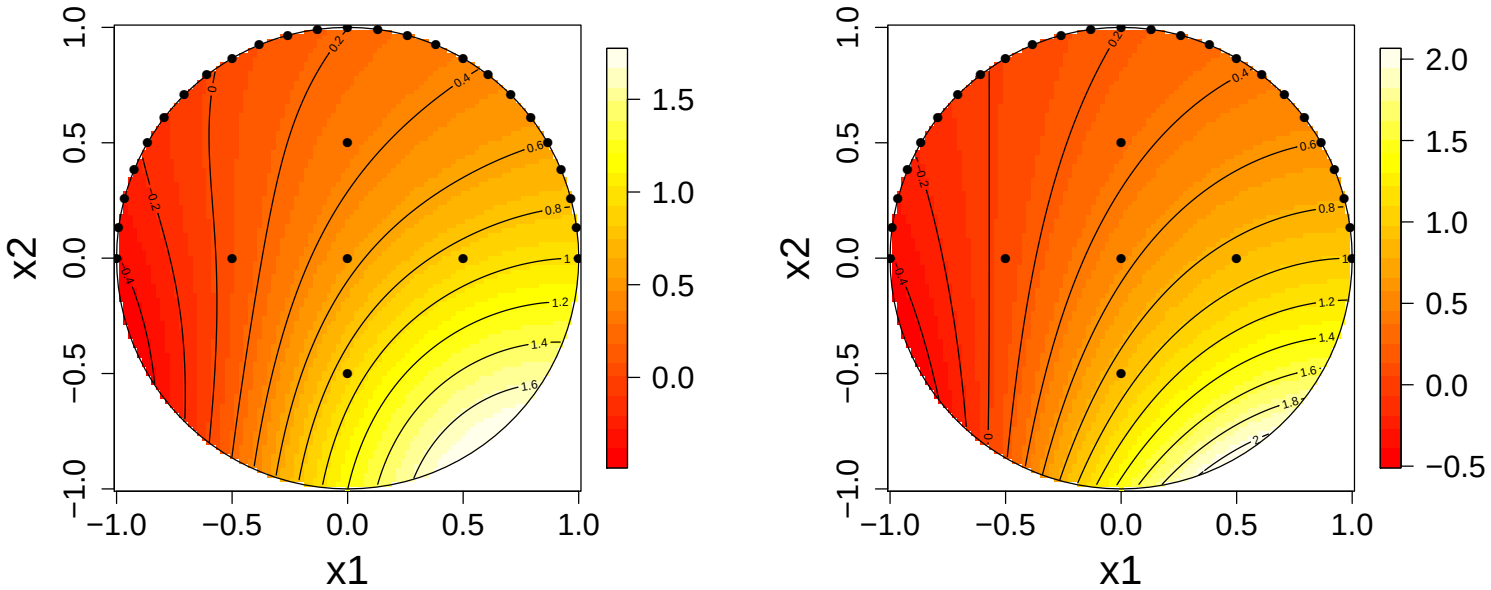

Extracted from “On degeneracy and invariances of random fields paths with applications in Gaussian Process modelling” (DG, O.Roustant & N.Durrande, Journal of Statistical Planning and Inference, 170:117-128, 2016)

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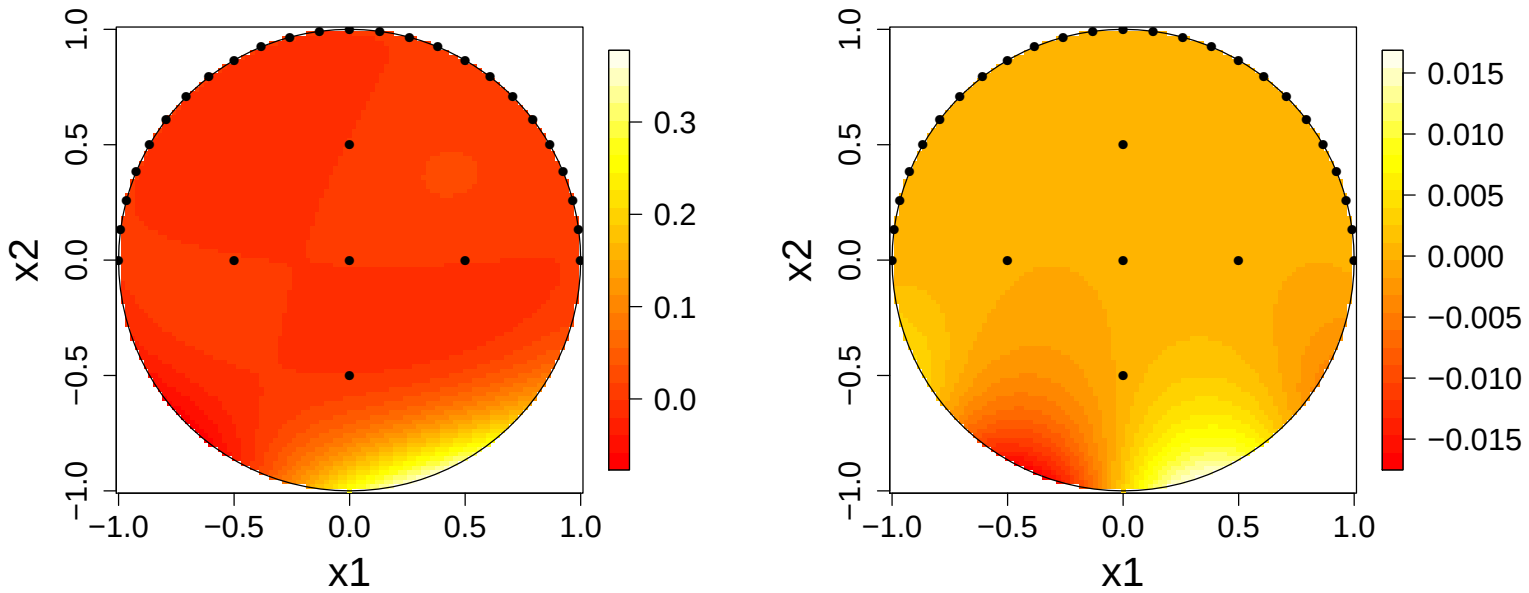

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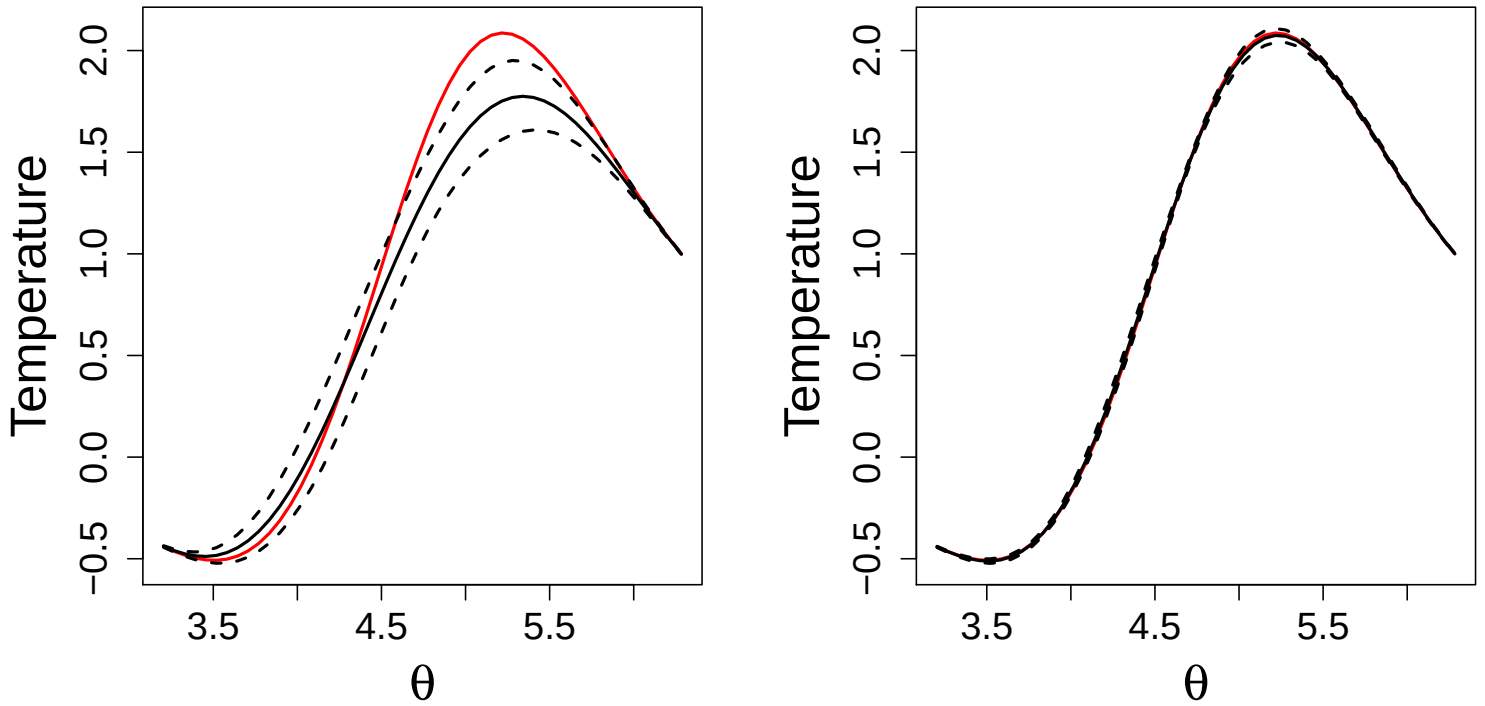
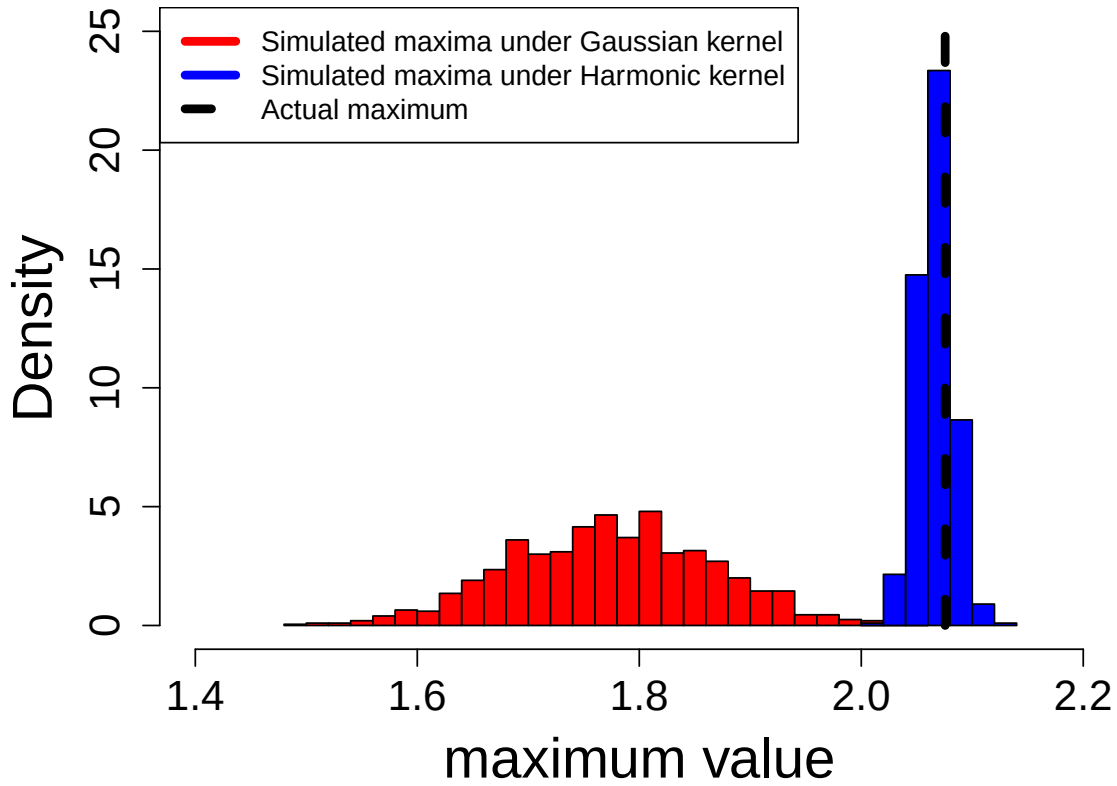
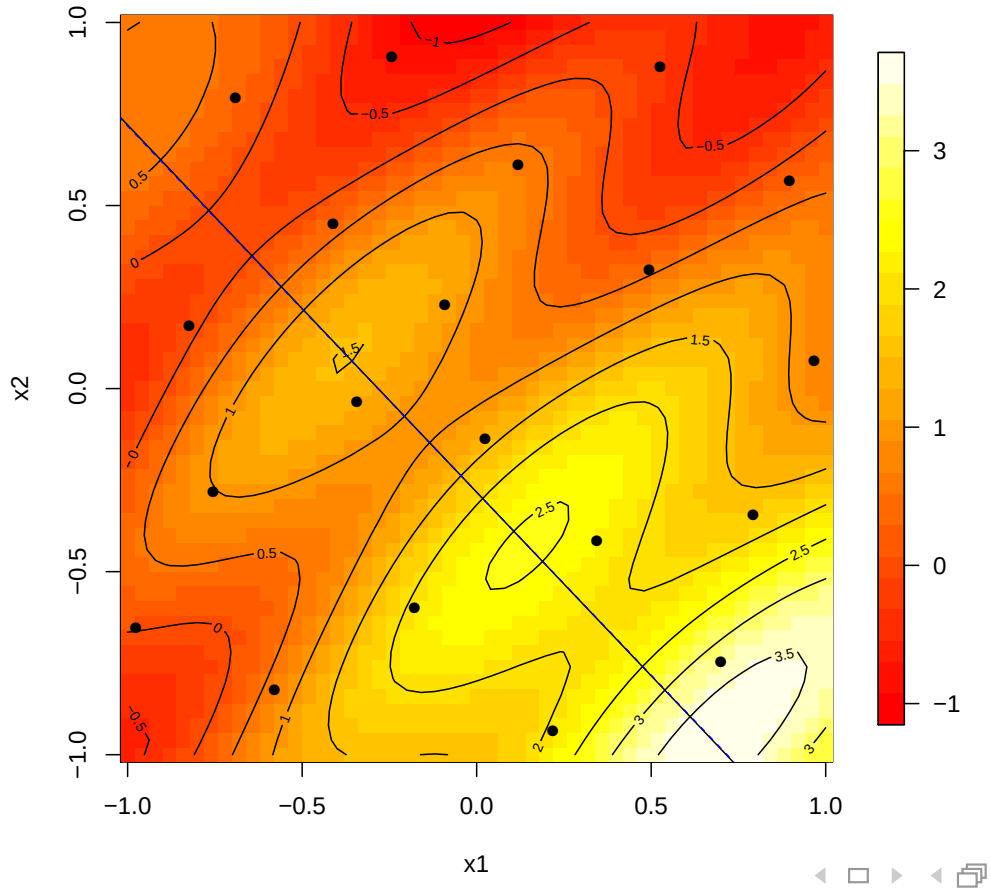


Numerical application: maximum of a harmonic *f*

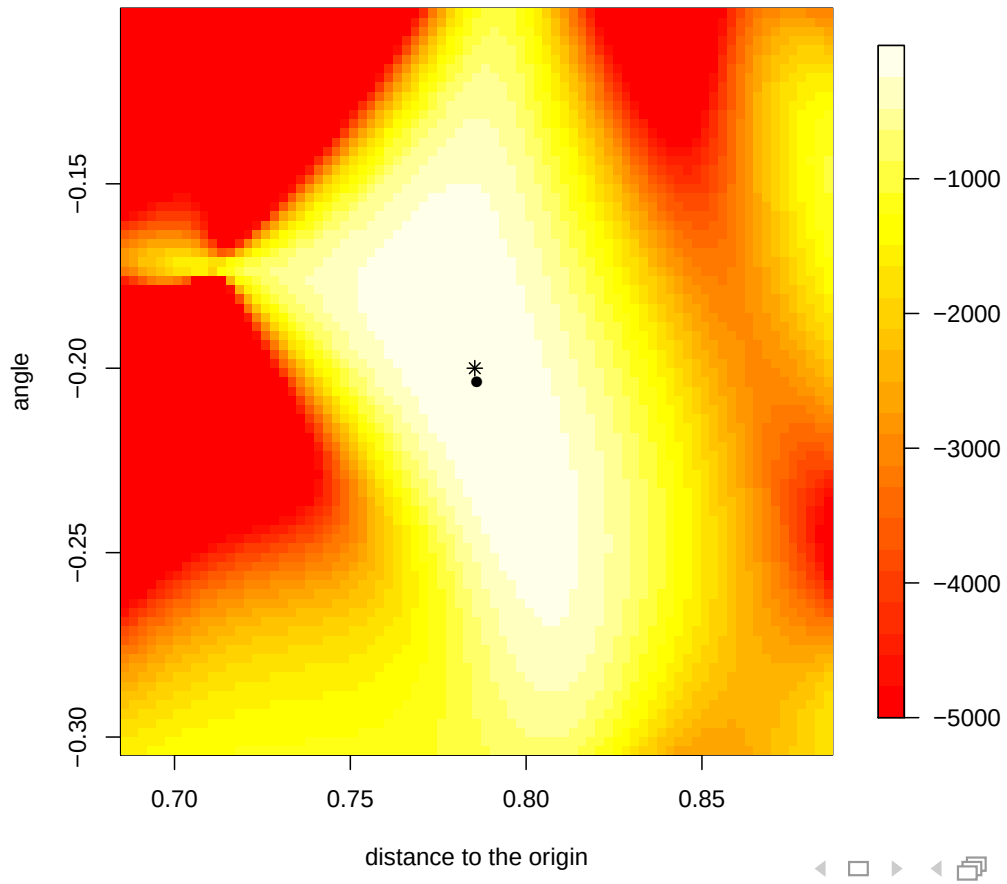
Conditional simulations of the maximum under the two GRF models.



Numerical application: recovering a symmetry axis



Numerical application 2: recovering a symmetry axis



Discussion

Function approximation approaches based on p.d. kernels enable incorporating degeneracies and invariances under linear operators including

- Symmetries and further invariances under group actions [See works of Mark et al. for larger scale investigations in computer vision]
- Additivity and further multivariate sparsity properties towards high-dimensional GP modelling [See works of Andrew et al.]
- Harmonicity but also, e.g., divergence-free properties for vector fields (See, e.g., Scheuerer and Schlather 2012) and more [presentation of Niklas]

In the Gaussian set up, such properties are inherited by conditional distributions, which is clearly convenient but also comes withs risks.

Perspectives

- Developing further the inference of degeneracy/invariance properties based on data and investigating consistency,

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- Creating classes of kernels that incorporate some invariant components and non-invariant components,
- Explore further the potential of invariant kernels based on real-world applications (e.g., from physics, biology, engineering).

Thank you very much for your attention!

Further references


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PhD thesis, University of Cambridge


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High Dimensional Bayesian Optimisation and Bandits via Additive Models
International Conference on Machine Learning (ICML) 2015


D. G., O. Roustant, D. Schuhmacher, N. Durrande and N. Lenz (2016)
On ANOVA decompositions of kernels and Gaussian random field paths.
Monte Carlo and Quasi-Monte Carlo Methods

Kernels are at the heart of various methods

Kernels are a crucial ingredient in a number of mathematical and statistical methods for function approximation, data classification and beyond:

- Support Vector Machines,
- Gaussian Process Modelling,
- Regularization in Reproducing Kernel Hilbert Spaces,
- Kernel Principal Component Analysis,
- Embedding of measures in RKHS,
- Etc.

The implementation of any of these methods require a valid kernel k.

What are (complex- and real-valued) p.d. kernels?

Let D be a set and $k : D \times D \longrightarrow \mathbb{C}$.

k is called a *positive definite* kernel when

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i \overline{a}_j k(\mathbf{x}_i, \mathbf{x}_j) \in [0, +\infty)$$

for all $n \geq 1$, $a_1, \ldots, a_n \in \mathbb{C}$, and $\mathbf{x}_1, \ldots, \mathbf{x}_n \in D$.

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Follow directly from this definition (More here):

- $k(\mathbf{x}, \mathbf{x}) \in [0, +\infty)$ for all $\mathbf{x} \in D$
- $k(\mathbf{x}', \mathbf{x}) = \overline{k(\mathbf{x}, \mathbf{x}')}$ for all $\mathbf{x}, \mathbf{x}' \in D$ (k is hermitian)
- Non-negative combinations and limits of p.d. kernels are p.d.

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NB: $k : D \times D \longrightarrow \mathbb{R}$ is p.d. when both $\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j k(\mathbf{x}_i, \mathbf{x}_j) \in [0, +\infty)$ for all $n \geq 1$, $a_1, \ldots, a_n \in \mathbb{R}$ and $\mathbf{x}_1, \ldots, \mathbf{x}_n \in D$, and k is symmetric.

Further properties of p.d. kernels (back)

Further general properties can be derived for p.d. kernels, including:

- Products of p.d. kernels are p.d. kernels
- If $\sigma : D \longrightarrow D$ is a bijection, $k(\mathbf{x}, \mathbf{x}')$ is a p.d. kernel if and only if $k(\sigma(\mathbf{x}), \sigma(\mathbf{x}'))$ is a p.d. kernel
- For all $\mathbf{x}, \mathbf{x}' \in D$ $|k(\mathbf{x}, \mathbf{x}')| \leq \sqrt{k(\mathbf{x}, \mathbf{x})}\sqrt{k(\mathbf{x}', \mathbf{x}')}$
- The function

$$d_k : (\mathbf{x}, \mathbf{x}') \in D^2 \longrightarrow d_k(\mathbf{x}, \mathbf{x}') = \sqrt{k(\mathbf{x}, \mathbf{x}) + k(\mathbf{x}', \mathbf{x}') - 2\Re(k(\mathbf{x}, \mathbf{x}'))}$$

defines a (pseudo-)distance on D.

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Note also that positive definiteness can be generalized as follows: $k : (\mathbf{x}, \mathbf{x}') \in D^2 \longrightarrow \mathbb{C}$ is called *conditionally positive definite* (*c.p.d.*) if it is hermitian and $\sum_{i=1}^{n} \sum_{j=1}^{n} a_i \overline{a_j} k(\mathbf{x}_i, \mathbf{x}_j) \in [0, +\infty)$ for all $n \geq 1$, $\mathbf{x}_1, \ldots, \mathbf{x}_n \in D$ and $a_1, \ldots, a_n \in \mathbb{C}$ s.t $\sum_{\mathbf{i=1}}^{\mathbf{n}} \mathbf{a_i} = \mathbf{0}$. *C.n.d.* is defined similarly with $(-\infty, 0]$.

Considered kernel methods for function approximation

Here we focus on two classes of kernel methods for the approximation of functions based on observational/evaluation data:

- Gaussian Process (GP) modelling/interpolation/regression
- Interpolation/Regularization in Reproducing Kernel Hilbert Spaces

Typical settings of interest are those of an objective function $f : D \longrightarrow \mathbb{R}$ (e.g. with $D \subset \mathbb{R}^d$, $d \geq 1$) that one wishes to approximate relying on a limited number $n \geq 1$ of evaluations at points $\mathbf{x}_i \in D$ ($1 \leq i \leq n$).

About Gaussian Process modelling

GP modelling basically consists in postulating that f is a realization of a real-valued Gaussian random field $Z = (Z_{\mathbf{x}})_{\mathbf{x} \in D}$ and to do inferences on f by using the conditional distribution of Z given the available evaluation results.

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As we know, in the Gaussian case the mean and covariance functions (say m and k, here) characterize Z's distribution, so choosing them is crucial.

Reminder: GP/Kriging equations

The GP/Kriging prediction amounts to calculating the conditional expectation and covariance of $Z_{\mathbf{x}}$ knowing $Z_{\mathbf{X}_n} = \mathbf{z}_n$, with $\boldsymbol{z}_n = (f(\mathbf{x}_1), \ldots, f(\mathbf{x}_n))'$:

$$\begin{cases} m_n(\mathbf{x}) = \mathbb{E}[Z_{\mathbf{x}} | Z_{\mathbf{X}_n} = \mathbf{z}_n] = m(\mathbf{x}) + k(\mathbf{x}, \mathbf{X}_n) k(\mathbf{X}_n, \mathbf{X}_n)^{-1} (\mathbf{z}_n - m(\boldsymbol{X}_n)) \\ \\ k_n(\mathbf{x}, \mathbf{x}') = \mathrm{Cov}[Z_{\mathbf{x}}, Z_{\mathbf{x}'} | Z_{\mathbf{X}_n} = \mathbf{z}_n] = k(\mathbf{x}, \mathbf{x}') - k(\mathbf{x}, \mathbf{X}_n) k(\mathbf{X}_n, \mathbf{X}_n)^{-1} k(\mathbf{X}_n, \mathbf{x}), \end{cases}$$

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For given m and k (possible generalizations to m known up to linear combination coefficients, cf. Universal Kriging with improper uniform prior), Z knowing $Z_{\mathbf{X}_n} = \mathbf{z}_n$ is a GP with mean m_n and covariance k_n.

A detour through deterministic function approximation

Approximating f based on evaluations at n points is ill-posed without further assumptions on f. Also in deterministic settings, p.d. kernels play a key role.

Kimeldorf, G. and Wahba, G. (1971)

Some results on Tchebycheffian spline functions

Journal of mathematical analysis and applications 33 (1), 82-95

H. Wendland (2005)

Scattered Data Approximation

Cambridge University Press

Fasshauer, G. E. (2011)

Positive definite kernels: past, present and future

Dolomites Research Notes on Approximation, 4:21-63

Scheuerer, M. and Schaback, R. and Schlather, M. (2013)

Interpolation of spatial data - a stochastic or a deterministic problem?

European Journal of Applied Mathematics, 24, 4, 601-629

Optimal approximation in RKHSs

Theorem (Generalization of Kimeldorf and Wahba's 1971's "representer theorem" by Schölkopf, Herbrich and Smola): Given evaluation results

$$(\mathbf{x}_1, z_1), \ldots, (\mathbf{x}_n, z_n) \in D \times \mathbb{R},$$

an arbitrary cost function $c : (D \times \mathbb{R}^2)^n \longrightarrow \mathbb{R} \cup \{\infty\}$, and a strictly increasing function p on $[0, \infty)$, any $m_n \in \mathcal{H}_k$ (RKHS with kernel k) minimizing

$$g \in \mathcal{H}_k \longrightarrow c\left((\mathbf{x}_1, z_1, g(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, z_n, g(\mathbf{x}_n))\right) + p(||g||_{\mathcal{H}_k})$$

admits a representation of the form

$$m_n(\cdot) = \sum_{i=1}^{n} \alpha_i k(\cdot, \mathbf{x}_i),$$

with $\alpha_1, \ldots, \alpha_n \in \mathbb{R}$ (Notes: noiseless or noisy z_is; real-valued k here.).

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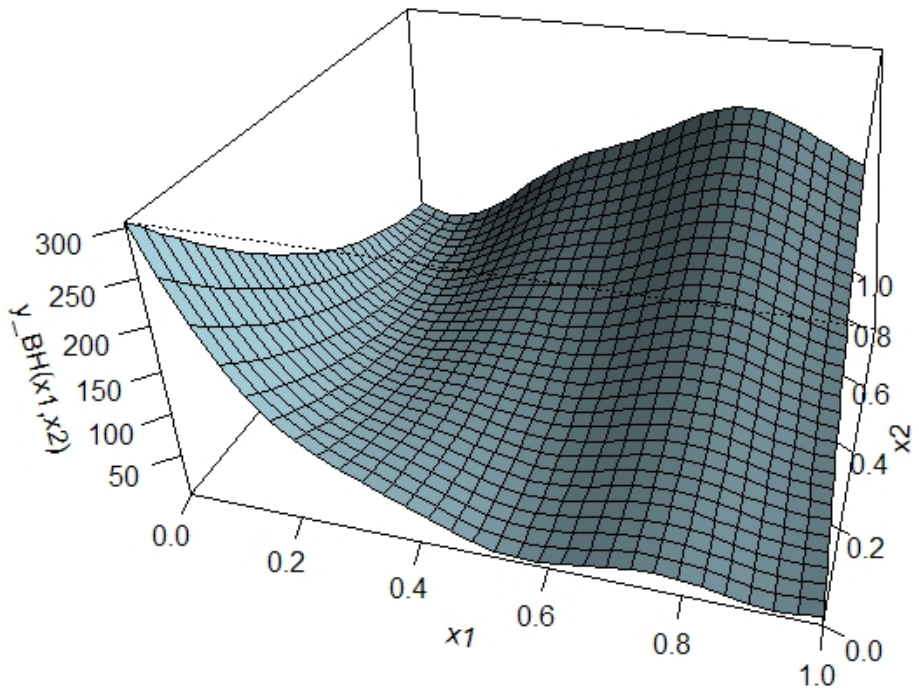
B. Schölkopf, R. Herbrich, A.J. Smola (2001)

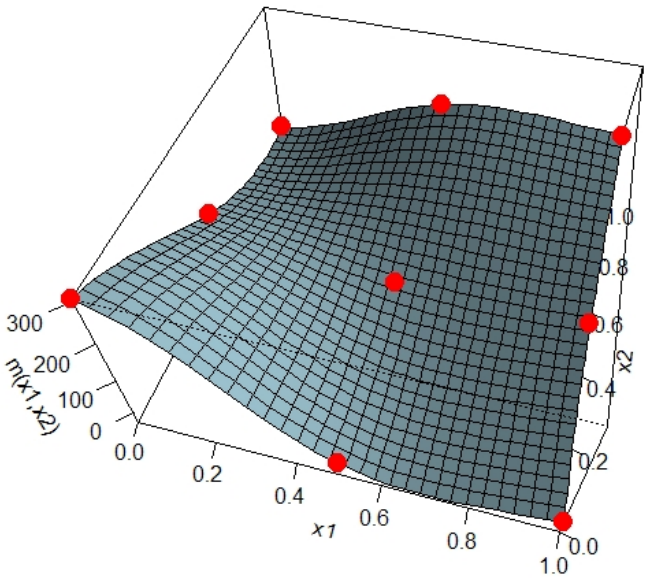
A Generalized Representer Theorem

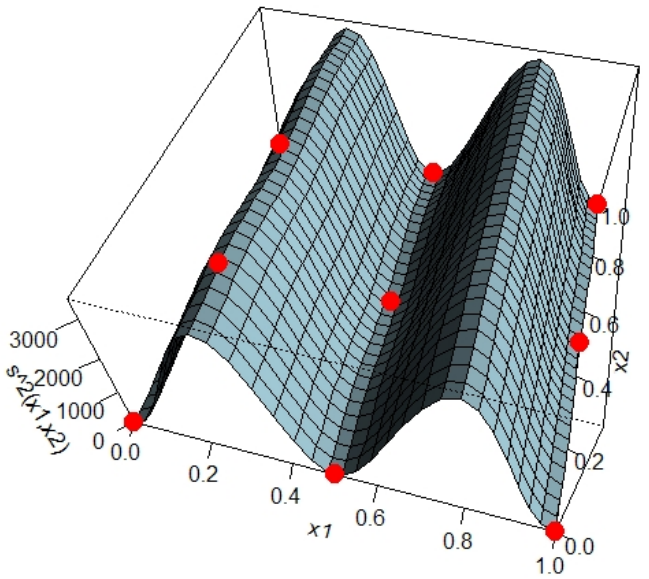
Computational Learning Theory. Lecture Notes in Computer Science 2111:416-426

A classical test function: Branin-Hoo (Eqs)



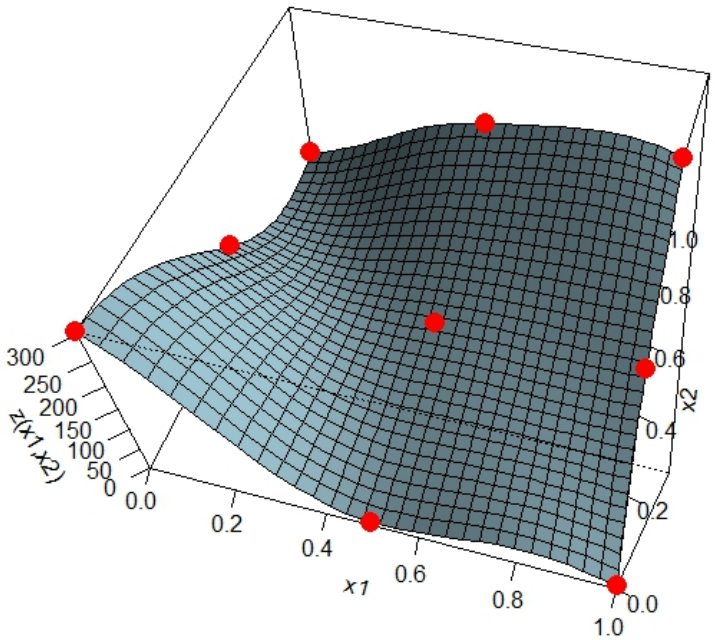
GP Interpolation (Kriging) of the Branin-Hoo function





The covariance is here a **stationary** anisotropic Matérn kernel ($\nu = 5/2$) with scale σ and range parameters (θ_1, θ_2) estimated by Maximum Likelihood.

Conditional simulations of the Branin-Hoo function



About the estimation of covariance parameters

The previous equations were at given $\boldsymbol{\mu}$ and k. In practice, however, trend and/or covariance parameters often have to be estimated. Let us consider the case of known μ and k that depends on a vector of "hyperparameters" ψ.

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Several approaches do exist for dealing with the unknown ψ: Maximum Likelihood Estimation (MLE), Cross-validation (CV), but also Bayesian approaches involving sampling algorithms such as McMC, SMC, etc.

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Let us present a brief overview of the MLE approach, probably the most implemented (although not necessarily the most robust) option.

A brief overview of MLE (back to Branin)

Let us denote by $K(\psi)$ the covariance matrix of responses, say $k(\boldsymbol{X}_n, \boldsymbol{X}_n; \psi)$, under the assumption of covariance hyperparameters with value ψ.

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The principle of MLE is to search for a value of ψ under which it would have been the most likely to observe the responses $\boldsymbol{z}_n$.

Under GP model assumptions, $\boldsymbol{Z}_{\boldsymbol{X}_n} \sim \mathcal{N}(\mu(\boldsymbol{X}_n), K(\psi))$. The likelihood then writes as the probability density of $\boldsymbol{Z}_{\boldsymbol{X}_n}$ at point $\boldsymbol{z}_n$, seen as a function of ψ:

$$L(\psi; \boldsymbol{z}_n) = (2\pi)^{-n/2} \det(K(\psi))^{-1/2} \exp\left(-\frac{1}{2}(\boldsymbol{z}_n - \mu(\boldsymbol{X}_n))' K(\psi)^{-1} (\boldsymbol{z}_n - \mu(\boldsymbol{X}_n))\right)$$

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Solving MLE is typically addressed by equivalently minimizing the function

$$\ell(\psi; \boldsymbol{z}_n) = \log(\det(K(\psi))) + (\boldsymbol{z}_n - \mu(\boldsymbol{X}_n))' K(\psi)^{-1} (\boldsymbol{z}_n - \mu(\boldsymbol{X}_n)).$$

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Writing $K(\psi) = \sigma^2 R(\theta)$ where $\psi = (\sigma^2, \theta)$, one can derive the "optimal" σ^2 as a function of θ. A swift calculation leads indeed to

$$\sigma^{2\star}(\theta) = \frac{1}{n}(\boldsymbol{z}_n - \boldsymbol{\mu}(\boldsymbol{X}_n))' R(\theta)^{-1} (\boldsymbol{z}_n - \boldsymbol{\mu}(\boldsymbol{X}_n)).$$

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Re-injecting the latter equation into ℓ, MLE then boils down to minimizing a function depending solely on θ, the so-called profile (or "concentrated") ℓ:

$$\ell_p(\theta; \boldsymbol{z}_n) = \log(\det(\sigma^{2\star}(\theta) R(\theta)))$$

Towards Universal Kriging

Another situation where an elegant concentration of ℓ is feasible is when k depends on ψ and $\boldsymbol{\mu}$ linearly depends on p basis functions $f_1, \ldots, f_p$:

$$\mu(\mathbf{x}) = \sum_{i=1}^{p} \beta_i f_i(\mathbf{x}),$$

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Plugging-in $\boldsymbol{\beta}^\star(\psi)$ in the predictor and inflating the conditional (co)variance accordingly leads to the "Universal Kriging" equations (See also particular case of "Ordinary Kriging", where $p = 1$ and μ is a constant; Eqs).

NB: In a Bayesian set-up where an improper uniform prior is put on $\boldsymbol{\beta}$, one even recovers a GP posterior distribution.

Some examples of p.d. kernels and GPs

Let us start by a very classical example (for $d = 1$): the Brownian motion $W = (W_t)_{t \in D}$ over $D = [0, +\infty)$. Let us define W (in distribution) as follows:

- $W_0 = 0$,
- for any $t \in D$ and $h > 0$, $W_{t+h} - W_t \sim \mathcal{N}(0, h)$,
- and for any $t_1, t_2, t_3, t_4 \in D$ with $t_1 \leq t_2 \leq t_3 \leq t_4$, the increments $W_{t_4} - W_{t_3}$ and $W_{t_2} - W_{t_1}$ are independent.

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Such conditions define a GP; there remains to work out its expectation and covariance functions. First, for $t \in D$ the two first conditions imply that

$$m(t) = \mathbb{E}[W_t] = \mathbb{E}[W_0 + W_t - W_0] = \mathbb{E}[W_0] + \mathbb{E}[W_t - W_0] = 0 + 0 = 0.$$

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Second, taking two points $t, t' \in D$ (assuming, say, that $t < t'$), the third condition implies that $W_{t'} - W_t$ is independent of $W_t - W_0$. Consequently,

$$\begin{aligned} k_{BM}(t, t') &= \mathbb{E}[W_t W_{t'}] = \mathbb{E}[(W_t - W_0)(W_t - W_0 + W_{t'} - W_t)] \\ &= \mathbb{E}[(W_t - W_0)^2] + \mathbb{E}[(W_t - W_0)(W_{t'} - W_t)] = t + 0 = t = \min(t, t'). \end{aligned}$$

Examples of covariance kernels and GPs (cont'd)

Another famous covariance function stems from the so-called "Brownian Bridge" (ending in 0) $B = (B_t)_{t\in[0,1]}$. Let us first restrict W to $D = [0, 1]$, obtaining a centred process with covariance $k(t, t') = \min(t, t')$ over $[0, 1]^2$.

The distribution of B is then obtained by conditioning W on $W_1 = 0$, thus obtaining the mean $m_B(t) = 0$ and covariance kernel

$$k_{BB}(t, t') = \min(t, t') - tt' = \min(t, t')(1 - \max(t, t')).$$

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Another covariance function of interest can be obtained by integrating W. Defining $(I_t)_{t\in D}$ (with $D = [0, +\infty)$ again) by $I_t = \int_0^t B_u \mathrm{d}u$, we obtain a new centred GP with covariance

$$\begin{aligned} k_{IBM}(t, t') &= \int_0^t \int_0^{t'} \min(u, v)\mathrm{d}u\mathrm{d}v \\ &= \min(t, t')^3/3 + (\max(t, t') - \min(t, t'))\min(t, t')^2/2. \end{aligned}$$

Examples of covariance kernels and GPs (cont'd)

Without entering into much detail, let us list a few further examples of 1-dimensional GPs / associated covariance kernels:

- For $D = [0, 1]$ and $H \in (0, 1)$, $k_{fBM}(t, t') = \frac{1}{2}(|t|^{2H} + |t'|^{2H} - |t - t'|^{2H})$ is the covariance kernel of the *fractional (or "fractal") Brownian Motion* with Hurst coefficient H,
- $k_{\text{triang}}(t, t') = (1 - |t - t'|)^+$ is the "triangular" kernel over $D = \mathbb{R}$,
- Defining $Z_t = \zeta_1 \cos(\omega t) + \zeta_2 \sin(\omega t)$, where $\zeta_1, \zeta_2 \sim \mathcal{N}(0, \sigma^2)$ independently ($\sigma > 0$) and $\omega > 0$, one obtains $k(t, t') = \cos(\omega(t' - t))$,
- $k_{OU}(t, t') = e^{-|t-t'|}$ is called exponential kernel and characterizes the *Ornstein-Uhlenbeck process*.
- $k(t, t') = e^{-|t-t'|^2}$ is the squared-exponential kernel.

Examples of covariance kernels and GPs (cont'd)

Previous k's from real-valued one-dimensional settings can be generalize in a number of ways. Let us review a few simple examples.

- One obtains an admissible k on $[0,+\infty)^d \times [0,+\infty)^d$ by taking $k(\mathbf{x},\mathbf{x}') = \prod_{i=1}^d \min(x_i, x_i')$ where the $x_i^{(')}$'s are the coordinates of $\mathbf{x}^{(')}$. The associated centred GP over $[0,+\infty)^d$ is called "Brownian Sheet".

- The exponential and Gaussian kernels can be generalized to $\mathbb{R}^d \times \mathbb{R}^d$ by taking $k(\mathbf{x},\mathbf{x}') = \exp(-||\mathbf{x}-\mathbf{x}'||)$ and $k(\mathbf{x},\mathbf{x}') = \exp(-||\mathbf{x}-\mathbf{x}'||^2)$, respectively, where $||\cdot||$ refers to the Euclidean norm on $\mathbb{R}^d$.

- From a different perspective, one can define a particular complex-valued GP by taking $Z_{\mathbf{x}} = \zeta \exp^{-\mathrm{i}\langle \mathbf{x},\boldsymbol{\omega}\rangle}$ where $\zeta \sim \mathcal{N}(0,\sigma^2)$ ($\sigma > 0$) and $\boldsymbol{\omega} \in \mathbb{R}^d$. Such Z is centred and has (complex) covariance

$$k(\mathbf{x},\mathbf{x}') = \mathrm{Cov}(Z_x, Z_x') = \mathbb{E}[Z_{\mathbf{x}}\overline{Z_{\mathbf{x}'}}] = \sigma^2 \exp^{-\mathrm{i}\langle \mathbf{x},\boldsymbol{\omega}\rangle} \exp^{\mathrm{i}\langle \mathbf{x}',\boldsymbol{\omega}\rangle} = \exp^{-\mathrm{i}\langle \mathbf{x}-\mathbf{x}',\boldsymbol{\omega}\rangle}.$$

A necessary and sufficient condition of admissibility

A common point about all kernels reviewed so far is that, for ad hoc D, if one takes any $n \geq 1$ and arbitrary points $\mathbf{x}_1, \ldots, \mathbf{x}_n$ and complex numbers $a_1, \ldots, a_n \in \mathbb{C}$, the following holds:

$$0 \leq \text{Var}\left[\sum_{i=1}^{n} a_i Z_{\mathbf{x}_i}\right] = \sum_{i=1}^{n}\sum_{j=1}^{n} a_i \overline{a}_j k(\mathbf{x}_i, \mathbf{x}_j).$$

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This property is indeed necessary for k to be an admissible covariance. Furthermore, it turns out that any k possessing this property is a covariance kernel (there exists some (Gaussian) random process with this k).

RKHS

Reproducing Kernel Hilbert Spaces (RKHS) offer a very convenient framework for function approximation. Here

Definition: A Hilbert space of functions $D \longrightarrow \mathbb{C}$, $(\mathcal{H}, \langle \cdot, \cdot \rangle_{\mathcal{H}})$, is a RKHS if for all $\mathbf{x} \in D$, the evaluation functional $e_{\mathbf{x}} : f \in \mathcal{H} \longrightarrow f(\mathbf{x}) \in \mathbb{C}$ are continuous.

From the so-called *Riesz representation theorem*, for all $\mathbf{x} \in D$ there exists an element of $\mathcal{H}$, denoted here $k_{\mathbf{x}}$, such that $f(\mathbf{x}) = \langle f, k_{\mathbf{x}} \rangle_{\mathcal{H}}$.

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From the so-called *Riesz representation theorem*, for all $\mathbf{x} \in D$ there exists an element of $\mathcal{H}$, denoted here $k_{\mathbf{x}}$, such that $f(\mathbf{x}) = \langle f, k_{\mathbf{x}} \rangle_{\mathcal{H}}$.

From such a RKHS and the collection of Riesz evaluation representers $k_{\mathbf{x}}$, the "kernel" $k : D \times D \longrightarrow \mathbb{C}$ associated with $\mathcal{H}$ can be defined as follows:

$$k : (\mathbf{x}, \mathbf{x}') \in D \times D \longrightarrow k(\mathbf{x}, \mathbf{x}') = \langle k_{\mathbf{x}'}, k_{\mathbf{x}} \rangle_{\mathcal{H}}$$

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Easy to check: k is a p.d. kernel.
Less easy to check: any p.d. kernel defines a unique RKHS
$\rightarrow$ Moore-Aronszajn theorem (Published 1950 :-)

Representing RKHSs based on the Mercer theorem

For simplicity, let us consider here a RKHS $\mathcal{H}_k$ associated with a real-valued Mercer kernel k. $\mathcal{H}_k$ can be represented more concretely as follows.

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with $\langle \sum_{j=1}^{\infty} \alpha_j \sqrt{\lambda_j} \phi_j, \sum_{j=1}^{\infty} \beta_j \sqrt{\lambda_j} \phi_j \rangle_{\mathcal{H}} := \sum_{j=1}^{\infty} \alpha_j \beta_j$.

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Comparing this with the K-L expansion of a GP with kernel k, we find that in the case of an infinite number of non-zero eigenvalues, the paths of Z are **not** in $\mathcal{H}_k$ with probability 1 (Parzen-Kallianpur-LePage theorem, as discussed in Lukić and Beder 2001). However, it can be shown that in general GP paths belong to bigger RKHSs (See, e.g., Steinwart 2017 for more detail).

Some properties of GRFs and kernels

Back to centred Z for simplicity, one can define a (pseudo-)metric d_Z on D by

$$d_Z^2(\mathbf{x}, \mathbf{x}') = \mathbb{E}\left[(Z_{\mathbf{x}} - Z_{\mathbf{x}'})^2)\right] = k(\mathbf{x}, \mathbf{x}) + k(\mathbf{x}', \mathbf{x}') - 2k(\mathbf{x}, \mathbf{x}')$$

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A number of properties of Z are driven by d_Z. For instance,

Theorem (Sufficient condition for the continuity of GRF paths)

Let $(Z_{\mathbf{x}})_{\mathbf{x}\in D}$ be a separable Gaussian random field on a compact index set $D \subset \mathbb{R}^d$. If for some $0 < C < \infty$ and $\delta, \eta > 0$,

$$d_Z^2(\mathbf{x}, \mathbf{x}') \leq \frac{C}{\left|\log ||\mathbf{x} - \mathbf{x}'||\right|^{1+\delta}}$$

for all $\mathbf{x}, \mathbf{x}' \in D$ with $||\mathbf{x} - \mathbf{x}'|| < \eta$, then the paths of Z are almost surely continuous and bounded.

See, e.g., M. Scheuerer's PhD thesis (2009) for details.

Some properties of GRFs and kernels

Starting from p.d. kernels notably obtained via Bochner's theorem, an appealing approach to enrich them is by operations conserving symmetric positive definiteness.

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Starting from p.d. kernels notably obtained via Bochner's theorem, an appealing approach to enrich them is by operations conserving symmetric positive definiteness.

Classical operations of that kind notably encompass:

- Non-negative linear combinations of p.d. kernels
- Products and tensor products of p.d. kernels
- Multiplication by $\sigma(\mathbf{x})\sigma(\mathbf{x}')$ for $\sigma : \mathbf{x} \in D \longrightarrow [0, +\infty)$
- Deformations/warpings: $k(g(\mathbf{x}), g(\mathbf{x}'))$ for $g : D \longrightarrow D$
- Convolutions, etc. . .

See, e.g., Section "making new kernels from old" of the book *Gaussian Processes for Machine Learning* (cited earlier).

The Branin-Hoo function

The rescaled Branin-Hoo function f is defined over $[0,1]^2$ by

$$f(x_1, x_2) = f_{\text{BH}}(15x_1 - 5, 15x_2),$$

where

$$f_{\text{BH}} : (x_1, x_2) \in [-5, 10] \times [0, 15] \longrightarrow a(x_2 - bx_1^2 + cx_1 - r) + s(1-t)\cos(x_1) + s,$$

with $a = 1, b = 5/(4\pi^2), c = 5/\pi, r = 6, s = 10$ and $t = 1/(8\pi)$ back.

Ordinary Kriging Equations –for completeness!–

Assume Z has a covariance kernel k, and constant mean $\mu \in \mathbb{R}$

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$$\begin{cases} m_n(\mathbf{x}) & = k(\mathbf{X}_n, \mathbf{x})^T k(\mathbf{X}_n, \mathbf{X}_n)^{-1} \mathbf{z}_n + \widehat{\mu}_n (1 - k(\mathbf{X}_n, \mathbf{x})^T k(\mathbf{X}_n, \mathbf{X}_n)^{-1} \mathbb{1}_n) \\ k_n(\mathbf{x}, \mathbf{x}') & = k(\mathbf{x}, \mathbf{x}') - k(\mathbf{X}_n, \mathbf{x})^T k(\mathbf{X}_n, \mathbf{X}_n)^{-1} k(\mathbf{X}_n, \mathbf{x}') \\ & \quad + \frac{\left(1 - \mathbb{1}_n^T k(\mathbf{X}_n, \mathbf{X}_n)^{-1} k(\mathbf{X}_n, \mathbf{x})\right)\left(1 - \mathbb{1}_n^T k(\mathbf{X}_n, \mathbf{X}_n)^{-1} k(\mathbf{X}_n, \mathbf{x}')\right)}{\left(\mathbb{1}_n^T k(\mathbf{X}_n, \mathbf{X}_n)^{-1} \mathbb{1}_n\right)} \end{cases}$$

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Under standard conditions, m_n **and** k_n **are** Z**'s conditional mean and covariance** and

$$\boxed{\mathcal{L}(Z | Z_{X_n} = \mathbf{z}_n) = \mathcal{GRF}\left(m_n(\cdot), k_n(\cdot, \cdot')\right)}$$

back

Heterogeneously noisy OK Equations

$$
\begin{cases}
m_n(\mathbf{x}) & = \widehat{\mu}_n + \mathbf{k}_n(\mathbf{x})^T \left(k(\mathbf{X}_n, \mathbf{X}_n) + \Delta_n\right)^{-1} \left(\widetilde{\mathbf{z}}_n - \widehat{\mu}_n \mathbb{1}_n\right) \\
k_n(\mathbf{x}, \mathbf{x}') & = k(\mathbf{x}, \mathbf{x}') - k(\mathbf{X}_n, \mathbf{x})^T \left(k(\mathbf{X}_n, \mathbf{X}_n) + \Delta_n\right)^{-1} k(\mathbf{X}_n, \mathbf{x}') \\
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Under usual assumptions, and if Z and the ε_i's are independent:

$$\boxed{\mathcal{L}(Z|\widetilde{A_n}) = \mathcal{N}\left(m_n(\cdot), k_n(\cdot, \cdot')\right)}$$

back

Proposition (DG et al. 2016)

Let Z be a measurable random field with paths (a.s.) in some function space $\mathcal{F}$ and $T : \mathcal{F} \longrightarrow \mathcal{F}$ be a linear operator such that for all $\mathbf{x} \in D$ there exists a signed measure $\nu_{\mathbf{x}} : \mathcal{D} \longrightarrow \mathbb{R}$ satisfying

$$T(g)(\mathbf{x}) = \int g(\mathbf{u}) \mathrm{d}\nu_{\mathbf{x}}(\mathbf{u}).$$

Assume further that

$$\sup_{\mathbf{x} \in D} \int_D \sqrt{k(\mathbf{u}, \mathbf{u}) + m(\mathbf{u})^2} \mathrm{d}|\nu_{\mathbf{x}}|(\mathbf{u}) < +\infty.$$

Then the following are equivalent:

a) $\forall \mathbf{x} \in D \; \mathbb{P}(T(Z)_{\mathbf{x}} = 0) = 1$ *("$T(Z) = \mathbf{0}$ up to a modification")*

b) $\forall \mathbf{x} \in D \; T(m)(\mathbf{x}) = 0$ *and* $(T \otimes T(k))(\mathbf{x}, \mathbf{x}) = 0$.

Assuming further that $T(Z)$ is separable, ***a)*** *and* ***b)*** *are also equivalent to*

c) $\mathbb{P}(T(Z) = \mathbf{0}) = \mathbb{P}(\forall \mathbf{x} \in D \; T(Z)_{\mathbf{x}} = 0) = 1$ *("$T(Z) = \mathbf{0}$ a.s.") .*

A link with RKHSs in the Gaussian case

In Gaussian case, the Loève isometry Ψ between $\mathcal{L}(Z)$ (The Hilbert space generated by Z) and the RKHS $\mathcal{H}_k$ leads to the following.

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Proposition

Let $T : \mathcal{F} \to \mathbb{R}^D$ be a linear operator such that $T(m) \equiv 0$ and $T(Z)_{\mathbf{x}} \in \mathcal{L}(Z)$ for any $\mathbf{x} \in D$. Then, there exists a unique linear $\mathcal{T} : \mathcal{H}_k \to \mathbb{R}^D$ satisfying

$$\mathrm{cov}(T(Z)_{\mathbf{x}}, Z_{\mathbf{x}'}) = \mathcal{T}(k(\cdot, \mathbf{x}'))(\mathbf{x}) \quad (\mathbf{x}, \mathbf{x}' \in D)$$

and such that $\mathcal{T}(h_n)(\mathbf{x}) \longrightarrow \mathcal{T}(h)(\mathbf{x})$ for any $\mathbf{x} \in D$ and $h_n \xrightarrow{\mathcal{H}} h$.

In addition, we have equivalence between the following:

(i) $\forall \mathbf{x} \in D \; T(Z)_{\mathbf{x}} = 0$ *(almost surely)*

(iii) $\forall \mathbf{x}' \in D \; \mathcal{T}(k(\cdot, \mathbf{x}')) = \mathbf{0}$

(iii) $\mathcal{T}(\mathcal{H}_k) = \{0\}$