A new class of covariance kernels accounting for non-additivity in high-dimensional kriging

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General setting

Point of departure

N. Durrande, D. Ginsbourger and O. Roustant (2012)
Additive covariance kernels for high-dimensional Gaussian process modeling.
Ann. Fac. Sci. Toulouse 21 481-499.

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We consider a GRF $(Z_x)_{x \in D}$ over the domain $D = [0,1]^d$, $d \in \mathbb{N}$. We assume that expectation and covariance kernel exist and call them respectively

$$m(x) = \mathbb{E}[Z_x]$$
$$k(x,y) = \mathrm{Cov}(Z_x, Z_y)$$

Under mild conditions the trajectories of Z are $\mathcal{L}^2$

Considerations in $\mathcal{L}^2$

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$$f = f_{\mathcal{C}} + f_{\mathcal{U}_1} + \ldots + f_{\mathcal{U}_d}$$

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$$\begin{aligned}
f_{\mathcal{C}} &= \int_D f \, d\mu \cdot \mathbf{1}_D \\
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f_{\mathcal{A}} &= f_{\mathcal{C}} + \sum_{i=1}^{d} f_{\mathcal{U}_i} \\
f_{\mathcal{O}} &= f - f_{\mathcal{A}}
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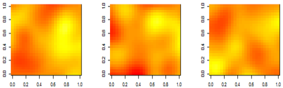
Projecting a random field

Realizations $Z(\omega)$ of a GRF, generated with an isotropic kernel $k(x,y) = \sigma^2 \cdot e^{-(\frac{\|x-y\|}{\theta})^2}$



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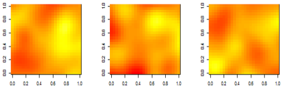

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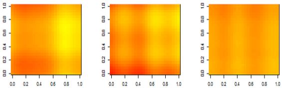

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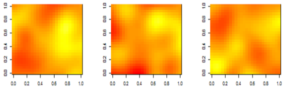

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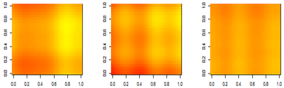

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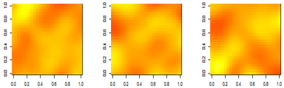

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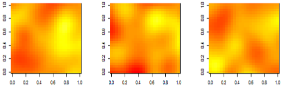

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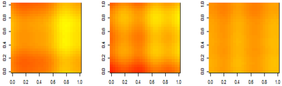

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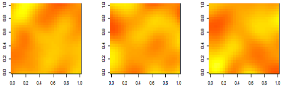
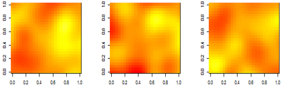


$\pi_{\mathcal{A}} Z(\omega) + \pi_{\mathcal{O}} Z(\omega)$



"Double" decomposition of a kernel

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$$\begin{aligned} k(x,y) = \mathrm{Cov}(Z_x, Z_y) &= \mathrm{Cov}(\sum_{\pi \in \mathcal{P}} \pi\, Z_x, \sum_{\tilde{\pi} \in \mathcal{P}} \tilde{\pi}\, Z_y) \\ &= \sum_{\pi \in \mathcal{P}} \sum_{\tilde{\pi} \in \mathcal{P}} \mathrm{Cov}(\pi\, Z_x, \tilde{\pi}\, Z_y) = \left(\sum_{\pi \in \mathcal{P}} \sum_{\tilde{\pi} \in \mathcal{P}} (\pi \otimes \tilde{\pi}) k \right)(x,y) \end{aligned}$$

Schematic representation of kernels

Applying $\mathcal{P} = \{\pi_{\mathcal{C}}, \pi_{\mathcal{U}_1}, \ldots, \pi_{\mathcal{U}_d}, \pi_{\mathcal{O}}\}$ to a kernel gives us a decomposition into $(d+2)^2$ parts.

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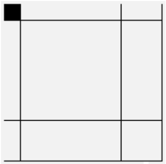

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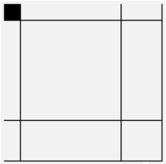

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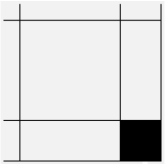

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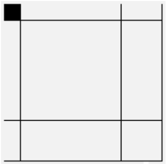

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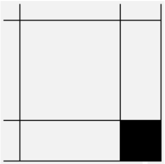

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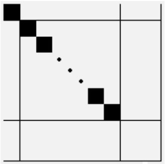

additive

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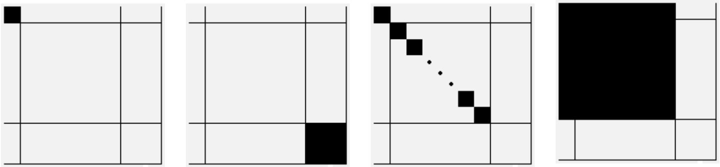

constant | ortho-add. | additive | (full) add.

Decomposition of a product kernel

$$
\begin{aligned}
((\pi_{\mathcal{O}} \otimes \pi_{\mathcal{O}})\, k)(\mathbf{x}, \mathbf{y}) = \mathcal{E} \Bigg[& \frac{k(\mathbf{x}, \mathbf{y})}{\mathcal{E}} + \sum_{i=1}^{d} \left(\frac{k_i(x_i, y_i)}{\mathcal{E}_i} - \frac{E_i(x_i) E_i(y_i)}{\mathcal{E}_i^2} \right) \\
& - \frac{E(\mathbf{x})}{\mathcal{E}} \left(1 + \sum_{i=1}^{d} \left(\frac{k_i(x_i, y_i)}{E_i(x_i)} - 1 \right) \right) \\
& - \frac{E(\mathbf{y})}{\mathcal{E}} \left(1 + \sum_{i=1}^{d} \left(\frac{k_i(x_i, y_i)}{E_i(y_i)} - 1 \right) \right) \\
& + \left(1 + \sum_{i=1}^{d} \left(\frac{E_i(x_i)}{\mathcal{E}_i} - 1 \right) \right) \cdot \left(1 + \sum_{i=1}^{d} \left(\frac{E_i(y_i)}{\mathcal{E}_i} - 1 \right) \right) \Bigg]
\end{aligned}
$$

where

- $E_i(x_i) := E_i(x_i, a_i, b_i) = \int_{a_i}^{b_i} k_i(x_i, y_i)\, dy_i$
- $E(\mathbf{x}) := E(\mathbf{x}, \mathbf{a}, \mathbf{b}) = \prod_{i=1}^{d} E_i(x_i, a_i, b_i)$
- $\mathcal{E}_i := \mathcal{E}_i(a_i, b_i) = \int_{a_i}^{b_i} E(x_i, a_i, b_i)\, dx_i$
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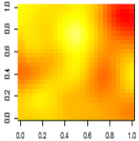
Controlled experiment:

- generate a realization of a random field using some kernel
- Split the data into a learning set and a test set
- Based on the learning set predict the other values using a misspecified kernel!
- Assess the quality of the predictions

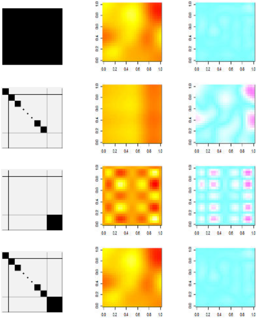
Concrete Experiment

Realization of a GRF generated with a Gaussian kernel



Z

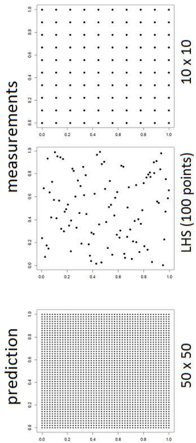
Predictions



!

$\hat{Z}$ error

Concrete Experiment



- Define learning and test set on a domain $D = [0, 1]^2$

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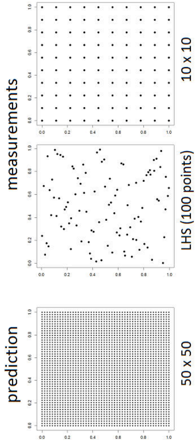

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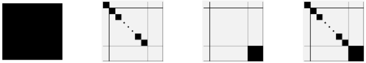

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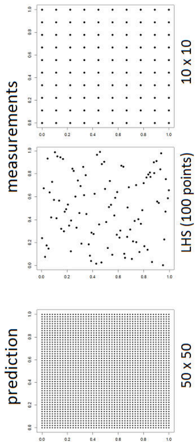

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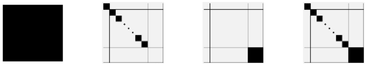

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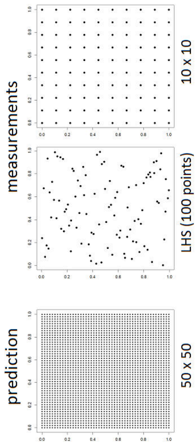

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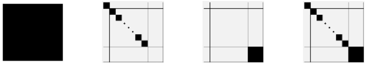

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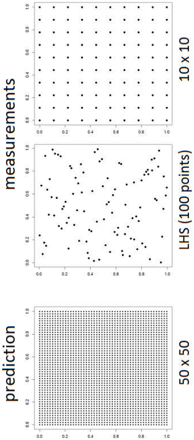

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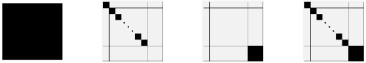

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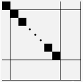
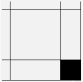
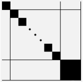
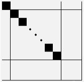
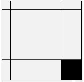
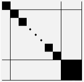
- Estimate $\int_D \left(\hat{Z}(x) - Z(x)\right)^2 d\mu$
- Repeat the procedure 200 times and take the mean over all results

Results

				
	(0.086) 1	(0.033) 3	(0.055) 3	(0.088) 2
	(0.456) 3	(0.032) 1	(0.429) 4	(0.457) 3
	(6.472) 4	(5.927) 4	(0.043) 1	(5.579) 4
	(0.087) 2	(0.032) 2	(0.055) 2	(0.087) 1

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		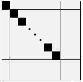	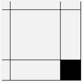	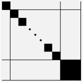
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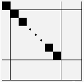
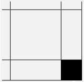
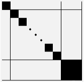
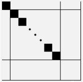
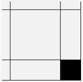
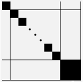
	(0.456) 3	(0.032) 1	(0.429) 4	(0.457) 3
	(6.472) 4	(5.927) 4	(0.043) 1	(5.579) 4
	(0.087) 2	(0.032) 2	(0.055) 2	(0.087) 1

Results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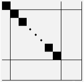
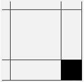
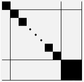
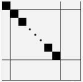
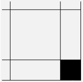
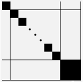
	(0.456) 3	(0.032) 1	(0.429) 4	(0.457) 3
	(6.472) 4	(5.927) 4	(0.043) 1	(5.579) 4
	(0.087) 2	(0.032) 2	(0.055) 2	(0.087) 1

Results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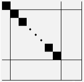
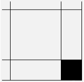
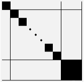
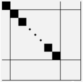
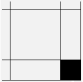
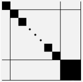
	(0.456) 3	(0.032) 1	(0.429) 4	(0.457) 3
	(6.472) 4	(5.927) 4	(0.043) 1	(5.579) 4
	(0.087) 2	(0.032) 2	(0.055) 2	(0.087) 1

Results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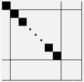
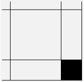
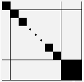
	(0.456) 3	(0.032) 1	(0.429) 4	(0.457) 3
	(6.472) 4	(5.927) 4	(0.043) 1	(5.579) 4
	(0.087) 2	(0.032) 2	(0.055) 2	(0.087) 1

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		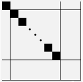	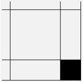	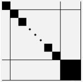
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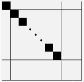
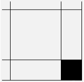
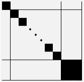
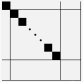
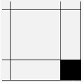
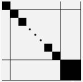
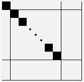
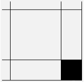
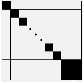
	(0.456) 3	(0.032) 1	(0.429) 4	(0.457) 3
	(6.472) 4	(5.927) 4	(0.043) 1	(5.579) 4
	(0.087) 2	(0.032) 2	(0.055) 2	(0.087) 1

Results

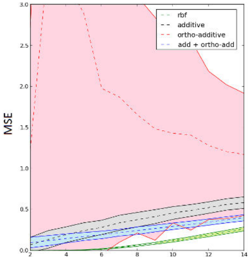
				
	**(0.086)** **1**	**(0.033)** **3**	**(0.055)** **3**	**(0.088)** **2**
	(0.456) 3	(0.032) 1	(0.429) 4	(0.457) 3
	(6.472) 4	(5.927) 4	(0.043) 1	(5.579) 4
	**(0.087)** **2**	**(0.032)** **2**	**(0.055)** **2**	**(0.087)** **1**

Some first Conclusions

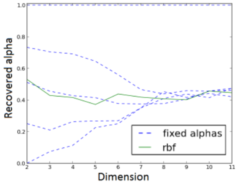
Summary of the presented work

- The kernel used for simulating the data always did the best predictions
- The additive kernel was less stable under the chosen circumstances
- The ortho-additive kernel much worse
- The combined additive and ortho-additive kernel performed as reliable as the full kernel
- A sparse kernel can carry almost the same information as a full one

Work in progress: Considerations in high dimensions



Development of the mean squared error with respect to the dimension



Simulation of GRFs with a kernel of the form

$$\alpha(\pi_{\mathcal{A}} \otimes \pi_{\mathcal{A}})k + (1-\alpha)(\pi_{\mathcal{O}} \otimes \pi_{\mathcal{O}})k, \ \alpha \in [0,1]$$

Recover the value of α by MLE

Summary of the presented work

- Ortho-additivity was introduced along with according projections of functions
- A kernel "double" decomposition was presented, and explicitly derived in the case of product kernels over $\mathbb{R}^d$
- Experiments suggested that neglecting cross-correlations between additive and ortho-additive parts have little influence on prediction for data generated with a Gaussian kernel

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Selected perspectives

- Analyse which term is negligible by calculating relevant norms
- Define classes of kernels enabling to further exploit synergies between Kriging and Global Sensitivity Analysis
- Investigate further estimation procedures for high dimensions

References

Thank you for your attention!

This presentation is based on...

N. Durrande and D. Ginsbourger and O. Roustant and L. Carraro (2013)
ANOVA kernels and RKHS of zero mean functions for model-based sensitivity analysis. Journal of Multivariate Analysis 115 57 - 67

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J.E. Oakley and A. O'Hagan (2004)
Probabilistic Sensitivity Analysis of Complex Models: A Bayesian Approach. J. Roy. Statist. Soc. 66 751–769

F. Y. Kuo, I. H. Sloan, G. W. Wasilkowski and H. Wozniakowski (2010)
On decompositions of multivariate functions. Mathematics of Computation 79 953-966.