MASCOT-NUM annual meeting

Non-stationary Gaussian process modelling and sequential design of experiments for exploration of high variation regions

22nd March 2017 Institut Henri Poincaré

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based on joined work with
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Gaussian process model for design of experiments

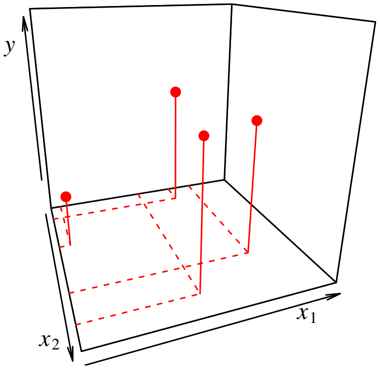
→ Framework

How to approximate $f : D \subset \mathbb{R}^d \to \mathbb{R}$ expensive to evaluate?

Bayesian approach:

- f assumed to be a realization of a Gaussian Process (GP) $Y \sim \mathcal{GP}\left(\mu(\cdot), C(\cdot,\cdot)\right)$.
- n points evaluated $\mathcal{A}_n = (\boldsymbol{y}_{1:n}, X_{1:n})$.
- Model given by the posterior distribution $\mathcal{GP}\left(\mu_n(\cdot), C_n(\cdot,\cdot)\right)$.

Initial design



How to choose the next evaluations $X_{n+1:n+q}$?

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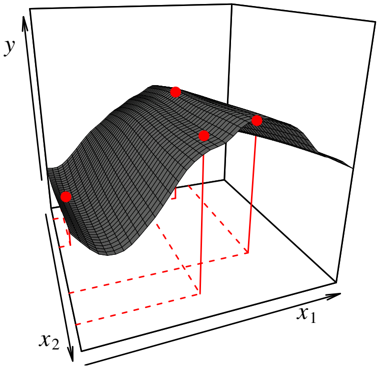
Sample path of posterior GP



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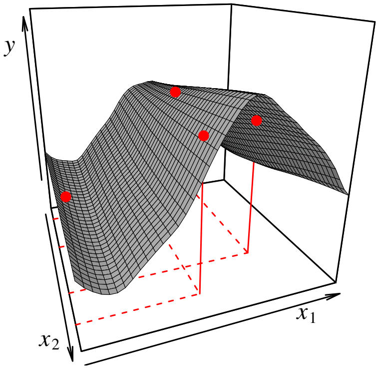

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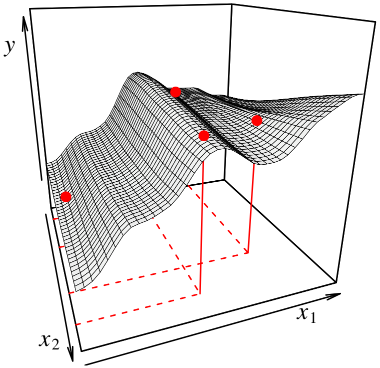

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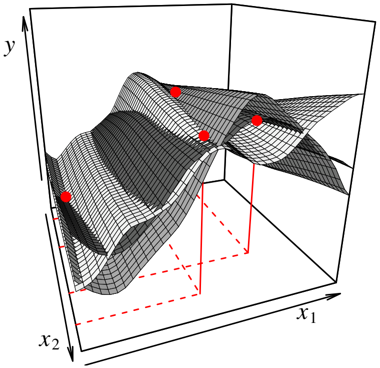

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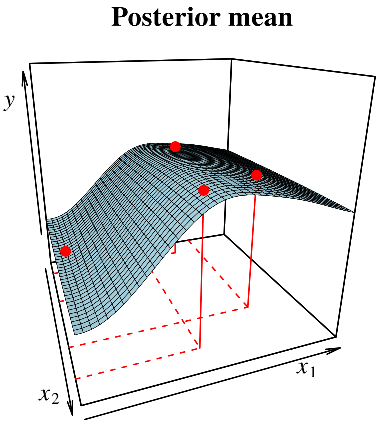

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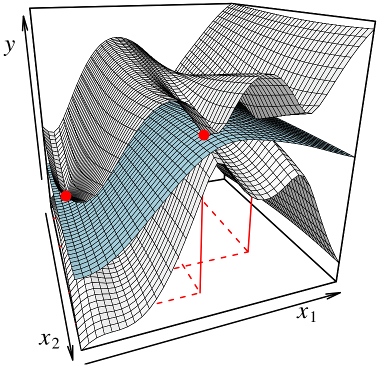
Posterior 5%, 50%, 95% quantiles



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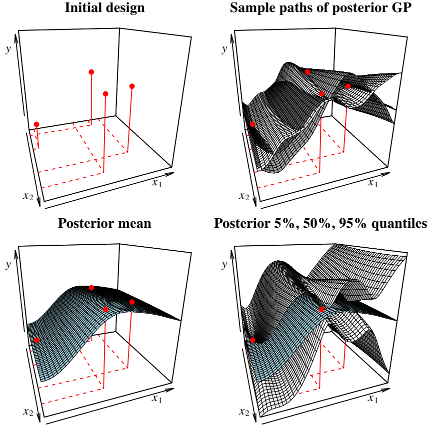


How to choose the next evaluations $X_{n+1:n+q}$?

Gaussian process model for design of experiments

→ Variance-based criteria for sequential design

Next evaluations maximize a criterion function:

$$J_n^{\mathrm{MSE}}(\boldsymbol{x}) = C_n\left(\boldsymbol{x}, \boldsymbol{x}\right),$$

$$J_n^{\mathrm{IMSE}}(\boldsymbol{x}) = -\int_{\boldsymbol{u} \in D} C_{n,\boldsymbol{x}}\left(\boldsymbol{u}, \boldsymbol{u}\right) \mathbf{d}\boldsymbol{u},$$

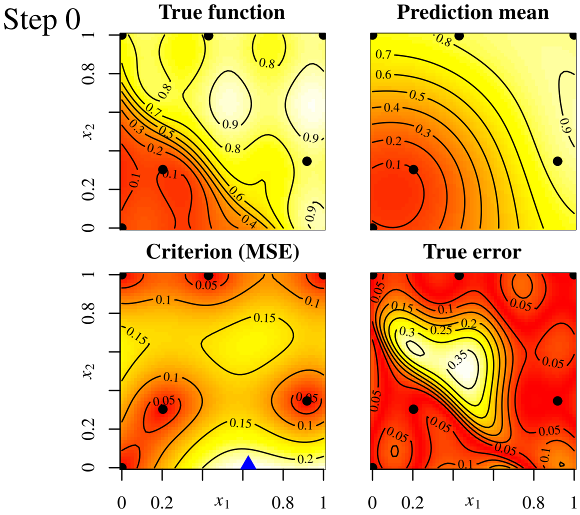
$$J_n^{q\text{-IMSE}}(\underset{\mathbb{R}^{d \times q}}{\underset{\cap}{X}}) = -\int_{\boldsymbol{u} \in D} C_{n,X}\left(\boldsymbol{u}, \boldsymbol{u}\right) \mathbf{d}\boldsymbol{u}.$$

with $C_{n,X}(\boldsymbol{u}, \boldsymbol{v}) = \mathbb{E}\left(\mathrm{cov}\left(Y_{\boldsymbol{u}}, Y_{\boldsymbol{v}} \middle| \boldsymbol{Y}_X\right)\right) = \mathrm{cov}\left(Y_{\boldsymbol{u}}, Y_{\boldsymbol{v}} \middle| \boldsymbol{Y}_X\right).$

→ $\mathrm{cov}\left(Y_{\boldsymbol{u}}, Y_{\boldsymbol{v}} \middle| \boldsymbol{Y}_{\boldsymbol{X}}\right)$ is deterministic : it depends only on X (not on $\boldsymbol{Y}_X$).

Gaussian process model for design of experiments

→ Sequential design of experiments with the MSE criterion



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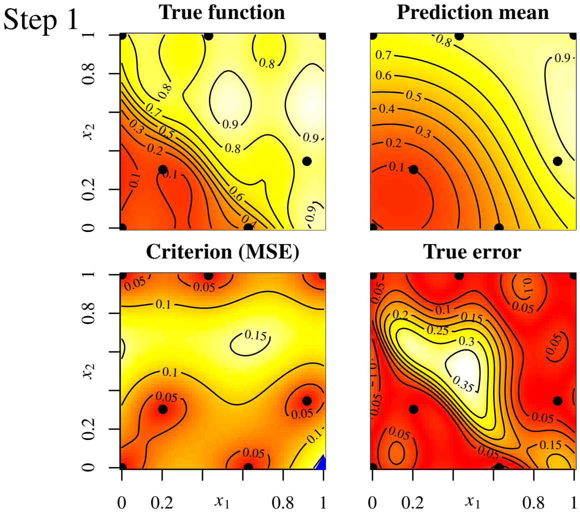

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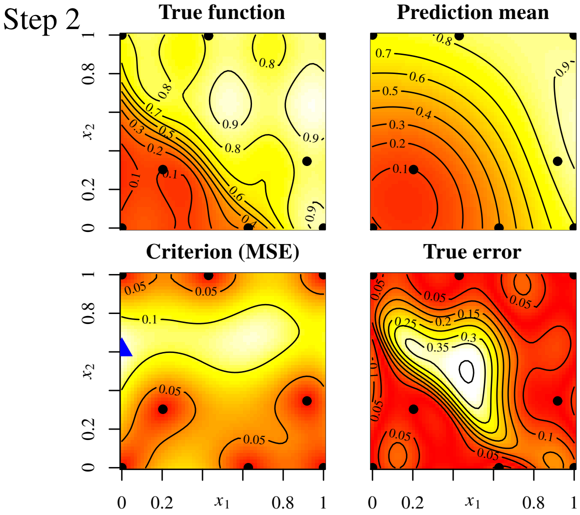

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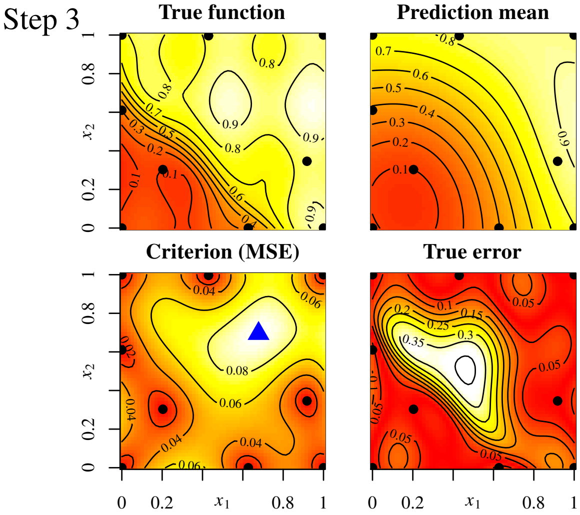

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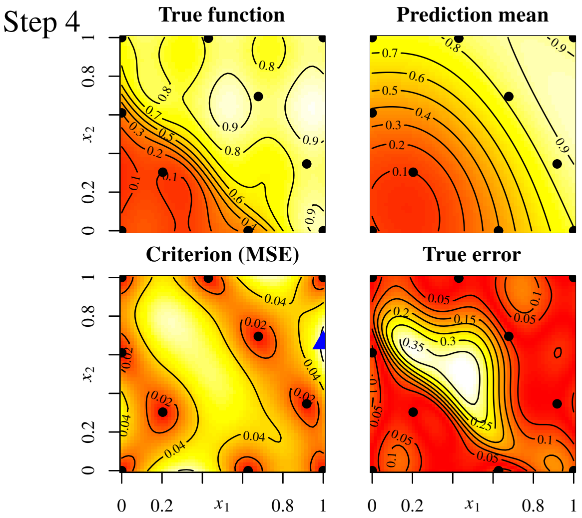

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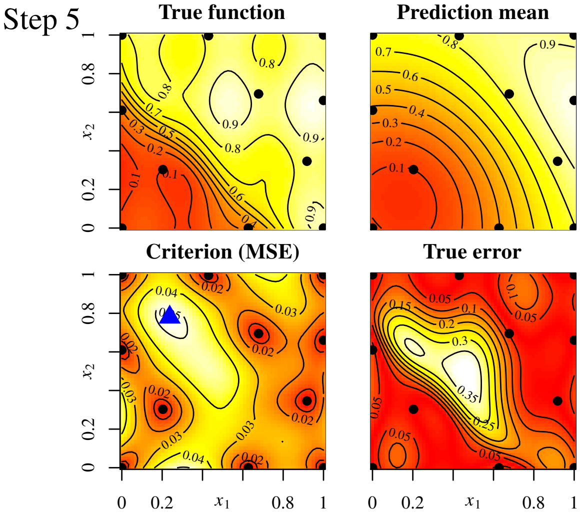

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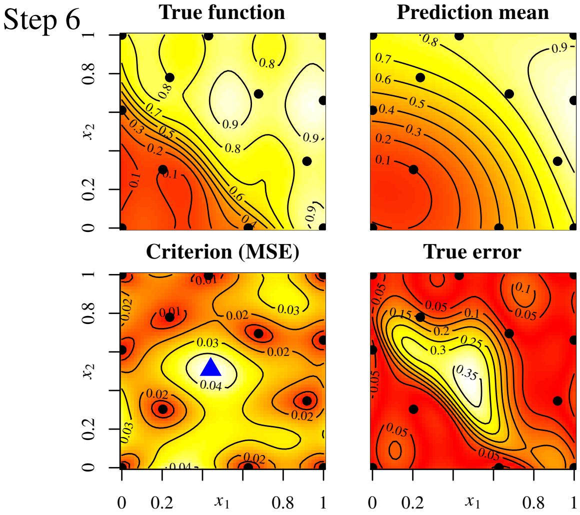

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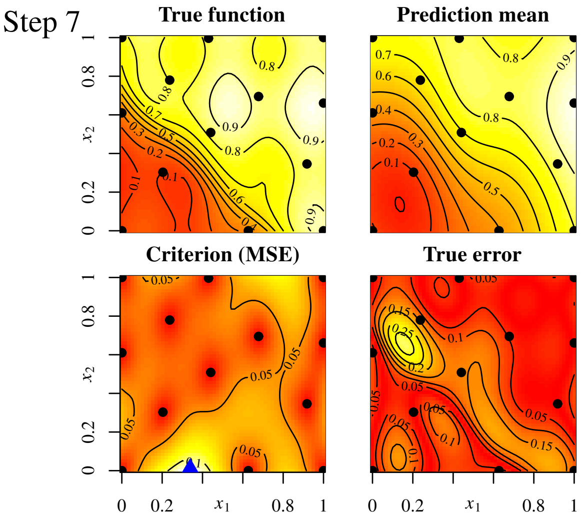


Variance-based criteria fill the space but do not focus on a specific region...
→ How to deal with functions exhibiting heterogeneous variations?

- Take a non-stationary model,
- define a criterion that intensifies exploration in high variation regions.

Non-stationary Gaussian process models

Input space warping:

- Non-linear input space warping $T : D \to T(D) \subset \mathbb{R}^d$ creates non-stationary GP [Sampson and Guttorp, 1992].

$$C(\boldsymbol{x}, \boldsymbol{x}') = k(T(\boldsymbol{x}), T(\boldsymbol{x}')).$$

- T can be decomposed with basis functions [Gibbs, 1997].
  $\rightarrow$ Many parameters to estimate.
- T can be simplified as a tensor product $T(\boldsymbol{x}) = (T_i(x_i))_{i=1,\dots,d}$ [Xiong et al., 2007].
  $\rightarrow$ irrelevant when high variations occur along unknown non-canonical directions.

Treed Gaussian Process (TGP):

- different GPs are independently build on several partitions of the input space [Gramacy, 2005].
  $\rightarrow$ not a GP model.

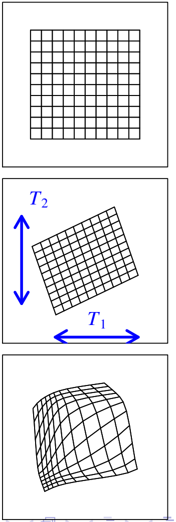
Warped Multiple Index Gaussian Process (WaMI-GP)

Definition

$$C(\boldsymbol{x}, \boldsymbol{x}') = k(T(\boldsymbol{x}), T(\boldsymbol{x}')), \text{ with } T(\boldsymbol{x}) = \left(T_i \left(\boldsymbol{a}_i^\top \boldsymbol{x}; \boldsymbol{\tau}_i \right) \right)_{i=1,\ldots,p}. \tag{1}$$

Composition of warping T

1. Linear transformation of input space,
   $\boldsymbol{x} \to A\boldsymbol{x}$, $A \in \mathbb{R}^{p \times d}$;
   $\to$ reduces dimension ($p \leq d$),
   $\to$ changes canonical axis.
2. Axial warping, $A\boldsymbol{x} \to (T_i((A\boldsymbol{x})_i; \boldsymbol{\tau}_i))_{i=1,\ldots,d}$
   $\to$ produces non-stationarity.



Parameters

$A = (\boldsymbol{a}_i)_{i=1,\ldots,p}$ and $(\boldsymbol{\tau}_i)_{i=1,\ldots,p}$.

Proposed covariance kernel family

→ Example

- Stationary isotropic

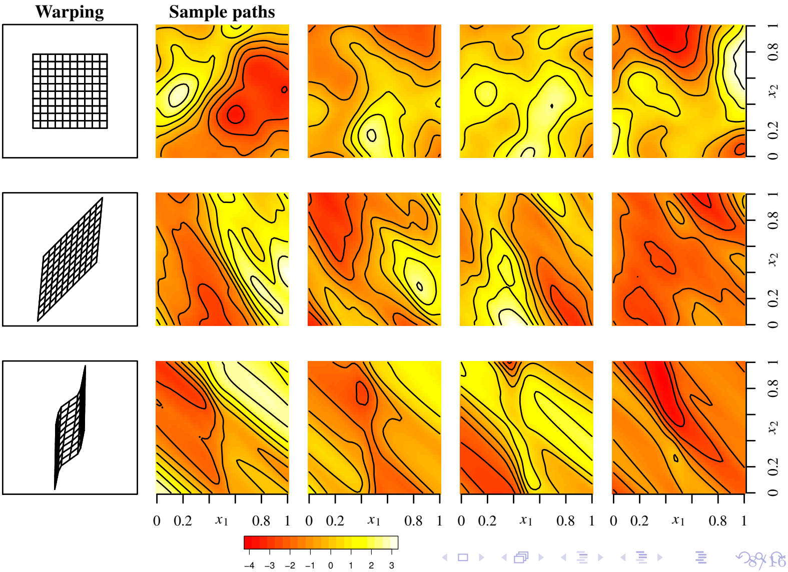
  $k(\boldsymbol{x}, \boldsymbol{x}')$.

- Stationary anisotropic

  $k(A\boldsymbol{x}, A\boldsymbol{x}')$.

- WaMI

  $k(T(\boldsymbol{x}), T(\boldsymbol{x}'))$.

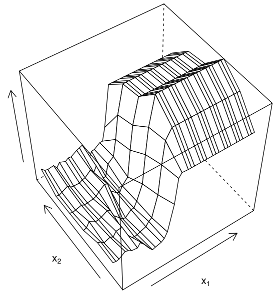


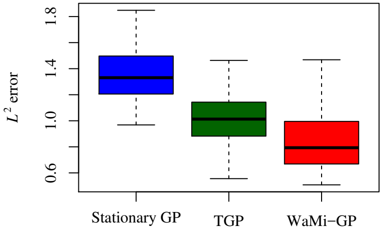
Proposed covariance kernel family

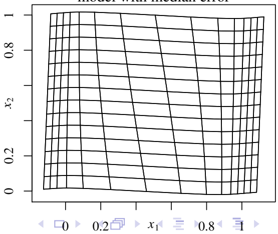
→ Results on a mechanical test case

- test case in dimension $d = 2$,
- $n = 20$ initial evaluations (optimized Latin hypercube design),
- comparison between stationary GP, TGP, WaMI-GP,
- 100 repetitions of the calculation from different maximin LHS designs optimized,
- parameter estimations by maximum likelihood (R package `kergp`).

Response studied (IRSN XPER platform)







Proposed covariance kernel family

→ Properties

- Strict positive definiteness, Appendix 1
- mean-squared differentiability, Appendix 2
- sample path differentiability. Appendix 3

Sampling criteria

→ Gradient random field

- ∇Y is a vector-valued GP with $\forall \boldsymbol{x}, \boldsymbol{x}' \in D$

$$\mathbb{E}\left(\nabla Y(\boldsymbol{x}) \middle| \mathcal{A}_n\right) = \nabla \mu_n(\boldsymbol{x}), \text{ and}$$

$$\operatorname{cov}\left(\frac{\partial}{\partial x_i} Y(\boldsymbol{x}), \frac{\partial}{\partial x_j} Y(\boldsymbol{x}') \middle| \mathcal{A}_n\right) = \left.\frac{\partial^2}{\partial t_i \partial t_j'} C_n(\boldsymbol{t}, \boldsymbol{t}')\right|_{\boldsymbol{t}=\boldsymbol{x}, \boldsymbol{t}'=\boldsymbol{x}'}.$$

→ Proposed criteria

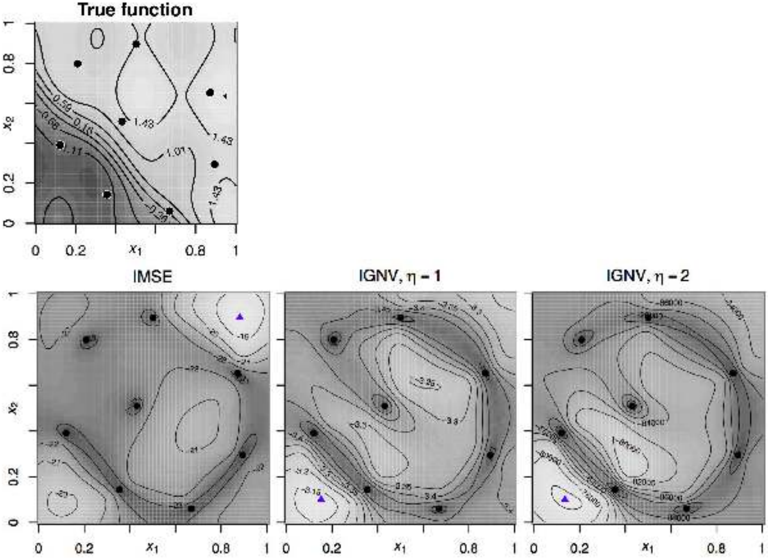
- Gradient Norm (power η) Variance (GNV):

$$J_n^{\mathrm{GNV},\eta}(\boldsymbol{x}) = \operatorname{var}\left(||\nabla Y_{\boldsymbol{x}}||^{\eta} \middle| \mathcal{A}_n\right).$$

- The corresponding integrated form:

$$J_n^{\mathrm{IGNV},\eta}(\underset{\mathbb{R}^{d\times q}}{\underset{\cap}{X}}) = -\int_{\boldsymbol{u}\in D} \mathbb{E}\left(\operatorname{var}\left(||\nabla Y_{\boldsymbol{u}}||^{\eta} \middle| \mathcal{A}_n, \boldsymbol{Y}_X\right)\right) \mathbf{d}\boldsymbol{u}.$$

Sampling criteria



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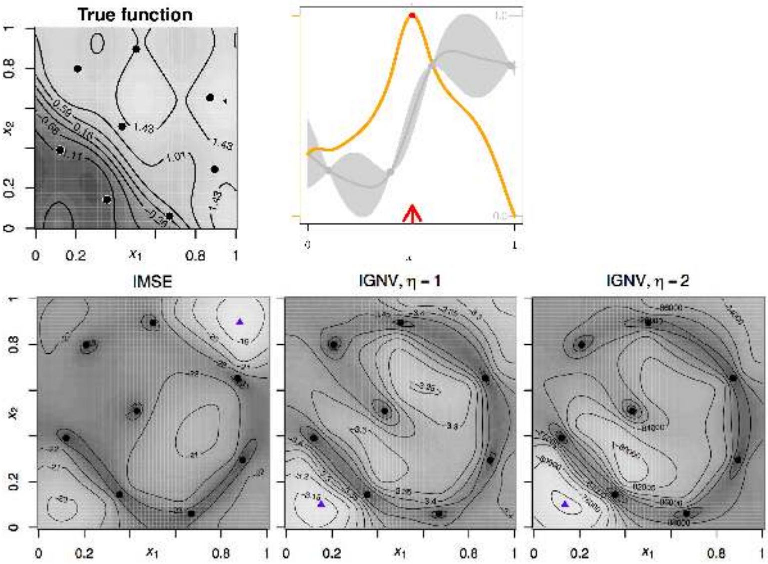


Sampling criteria

→ Calculation of $J_n^{\mathrm{GNV},\eta}(\boldsymbol{x})$ and $\mathbb{E}\left(\mathrm{var}\left(||\nabla Y_{\boldsymbol{u}}||^{\eta} | \mathcal{A}_n, \boldsymbol{Y}_X\right)\right)$:

- $\eta = 1$, semi-analytic (requires an reduced integral quadrature),
- $\eta = 2$, analytic.

Proposition

Let $\boldsymbol{x} \in D$ and denote by $(\lambda_i(\boldsymbol{x}))_{1 \leq i \leq d}$ the eigenvalues of $\nabla^2 c_n(\boldsymbol{x}, \boldsymbol{x})$. Then, the GNV(2) *criterion can be written as follows:*

$$J_n^{\mathrm{GNV},\eta=2}(\boldsymbol{x}) = 4\ \nabla m_n(\boldsymbol{x})^{\top} \nabla^2 c_n(\boldsymbol{x}, \boldsymbol{x}) \nabla m_n(\boldsymbol{x}) + 2 \sum_{i=1}^{d} \lambda_i(\boldsymbol{x})^2,$$

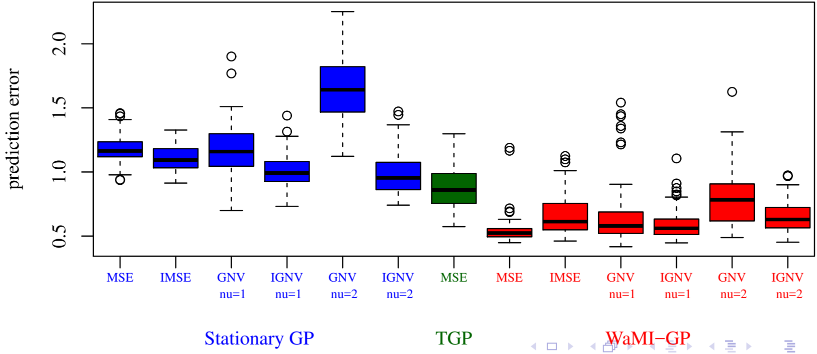
where $\lambda_{i,\boldsymbol{x}}(\boldsymbol{u})$ are the eigenvalues of $\nabla^2 c_{n,\boldsymbol{x}}(\boldsymbol{u}, \boldsymbol{u})$.
Furthermore, the GNV(1) *criterion can be expanded as follows:*

$$J_n^{\mathrm{GNV},\eta=1}(\boldsymbol{x}) = ||\nabla m_n(\boldsymbol{x})||^2 + \mathrm{tr}\left(\nabla^2 c_n(\boldsymbol{x}, \boldsymbol{x})\right) - \mathbb{E}\left(||Y_{\boldsymbol{x}}||\ |\mathcal{A}_n\right)^2.$$

Application

→ IRSN test case

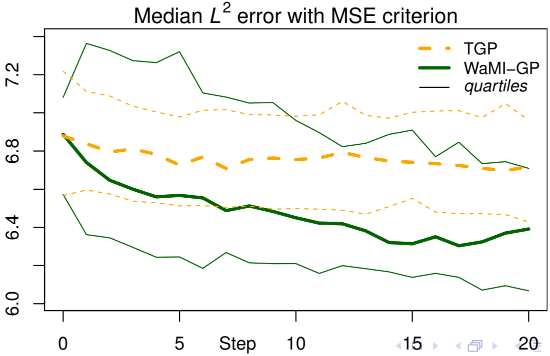
- test case in dimension $d = 2$,
- $n = 20$ initial evaluations (optimized Latin hypercube design),
- comparison between several sequential design strategies under stationary GP, TGP, WaMI-GP,
- 100 repetitions of the calculation from different initial designs,
- parameter estimation by maximum likelihood (R package `kergp`).
- sequential sampling of $r = 10$ points with the different criteria.



Application

→ NASA fuild mechanics test case

- test case in dimension $d = 3$,
- $n = 50$ initial evaluations (optimized Latin hypercube design),
- comparison between several sequential design strategies under stationary GP, TGP, WaMI-GP,
- 50 repetitions of the calculation from different initial designs,
- parameter estimation by maximum likelihood (R package **kergp**).
- sequential sampling of $r = 20$ points with the different criteria.



Conclusion

For sampling functions with heterogeneous variations:

- We propose a new class of non-stationary GP models (WaMI-GP).
- In a generic GP framework (notably with stationary kernels), we define and provide analytical formulas for gradient-based criteria, GNV and IGNV.

Numerical applications:

- On a first test case, WaMI-GP reduces prediction errors compared to stationary GP and TGP. With a stationary model, we observe better performance of the IGNV criterion compared to classical variance-based criteria. Overall best performance is obtained with WaMI-GP combined with MSE.
- On a second test-case in higher dimension, TGP offers better performances at the initial design stage but is outperformed by WaMI-GP along sequential design based on the MSE criterion.

Currently under development:

- Definition and derivation of new criteria,
- open source R implementation,
- parameter estimation procedures for higher dimension cases.

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Thank you

Appendix

Proposition

Positive definiteness: *Assume that k is strictly positive definite, that the $T_i(\cdot; \boldsymbol{\tau}_i)$ are injective and that the rank of A is equal to d. Then the WaMI kernel of equation (1) is strictly positive definite.*

Appendix

Proposition

Mean-squared differentiability. *The centred Gaussian process with the covariance c defined in (1) is mean-squared differentiable in all canonical direction under the following conditions:*

- $T_i(\cdot;\boldsymbol{\tau}_i)$, $i = 1, \dots, q$, *have regularity* C^1 *on* $\mathbb{R}$. *We write* $T_i'(\cdot;\boldsymbol{\tau}_i)$ *the univariate and continuous derivatives.*
- $\forall j, j' \in \{1, \dots, q\}, \forall \boldsymbol{u} \in \mathbb{R}^q$, $\left.\frac{\partial^2 k(\boldsymbol{v},\boldsymbol{v}')}{\partial v_j \partial v'_{j'}}\right|_{(\boldsymbol{u},\boldsymbol{u})}$ *exists and is finite.*

Appendix

Proposition

Sample path differentiability. *With the same assumptions on* $T_i(\cdot;\boldsymbol{\tau}_i)$*'s and* k *as in the previous proposition, and assuming in addition that*

- D *is compact,*
- *there exist* $C_0, \eta_0, \varepsilon_0 > 0$ *such that* $\forall j, j' \in \{1, \ldots, q\}$*, and* $\forall \boldsymbol{u}, \boldsymbol{u}' \in \mathbb{R}^q$, $||\boldsymbol{u} - \boldsymbol{u}'|| < \varepsilon_0$*, we have*
  $$\left.\frac{\partial^2 k(\boldsymbol{v},\boldsymbol{v}')}{\partial v_j \partial v'_{j'}}\right|_{(\boldsymbol{u},\boldsymbol{u})} + \left.\frac{\partial^2 k(\boldsymbol{v},\boldsymbol{v}')}{\partial v_j \partial v'_{j'}}\right|_{(\boldsymbol{u}',\boldsymbol{u}')} - 2\left.\frac{\partial^2 k(\boldsymbol{v},\boldsymbol{v}')}{\partial v_j \partial v'_{j'}}\right|_{(\boldsymbol{u},\boldsymbol{u}')} \leq \frac{C_0}{|\ln ||\boldsymbol{u}-\boldsymbol{u}'|||^{1+\eta_0}},$$

then the covariance c *gives rise to a centred Gaussian Process possessing a version with differentiable sample paths.*