Learning of multi-fidelity data with a mixture of Gaussian processes

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Discussion on multi-fidelity simulators, GdR MASCOT-NUM
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Surrogate modelling with multi-fidelity data I

The goal

Predict the output of a **high fidelity but time-consuming** input-output system $z(\mathbf{x})$.

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The way

Statistical learning of inputs-output observations coming from sources with **different levels of fidelity**:

- fine models ;
- degraded versions of the fine models;
- physical reduced models;
- experimental measurements; ...

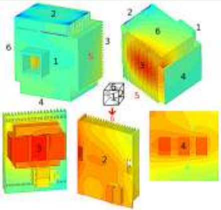
$\Rightarrow$ **one of them is the reference model $z(\mathbf{x})$ to replace.**

Surrogate modelling with multi-fidelity data II

Industrial application (EPSILON - ALCEN)

A **switchgear cubicle** with:

- electrical and electronic components warming up;
- a cooling system ⇒ **2 main types of behavior**: forced and free convections.



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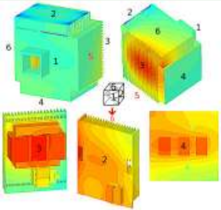

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4 inputs = Pression + Ambient temperature + Intensity + Airflow

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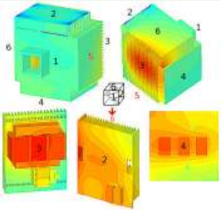

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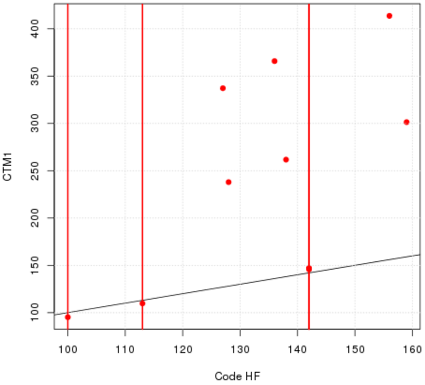
1 High-Fidelity Model = 3D numerical model based upon physical equations
2 Low-Fidelity Models = compact thermal models based upon a thermal-electrical analogy

Surrogate modelling with multi-fidelity data III

	I	Tamb	P	Q	T
1	300	70	1013	40	156
2	300	45	812	32	136
3	265	45	812	16	138
4	175	55	812	0	142
5	155	70	1013	0	142
6	300	30	1013	25	127
7	265	70	1013	20	159
8	265	30	1013	12.5	128
9	150	40	812	0	113
10	85	55	812	0	100



2 Compact Thermal Models:

1. free convection (CTM1)
2. forced convection (CTM2)

Model	1	2	3	4	5	6	7	8	9	10
CTM1	-165.21	-169.05	-89.67	**-2.68**	**-3.66**	-165.53	-89.55	-85.92	**2.86**	**4.74**
CTM2	**-0.88**	**-4.14**	**-9.28**	-563.39	-330.23	**-0.69**	**-3.45**	**-9.03**	-374.56	-334.69

Relative errors in % of the Compact Thermal Models (CTM)

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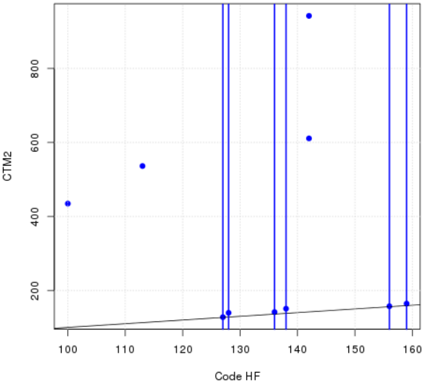

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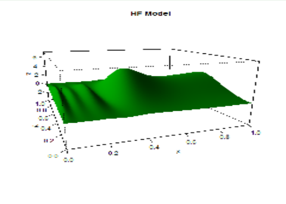
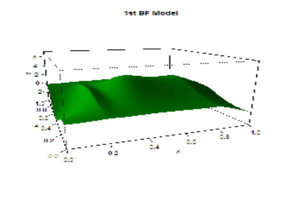
Relative errors in % of the Compact Thermal Models (CTM)

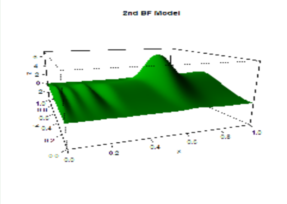
Toy example: $z(\mathbf{x}) : [0,1]^2 \mapsto \mathbb{R}$

1 high-fidelity function $z(\mathbf{x}) \rightarrow$ function visualization



2 low-fidelity functions $z_1(\mathbf{x})$ and $z_2(\mathbf{x}) \rightarrow$ functions visualization





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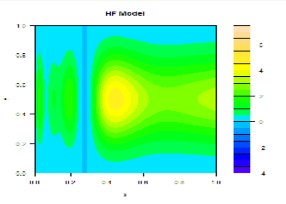

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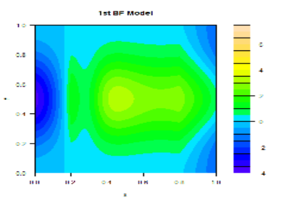

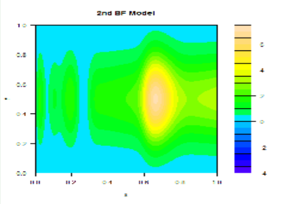

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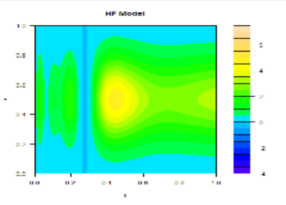
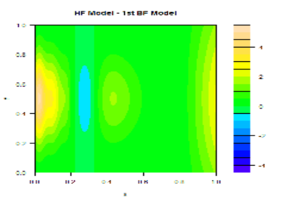
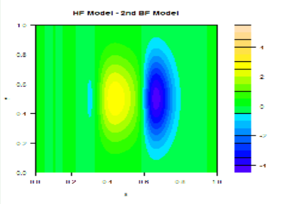


2 low-fidelity functions $z_1(\mathbf{x})$ and $z_2(\mathbf{x}) \rightarrow$ errors visualization





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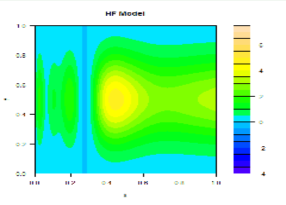
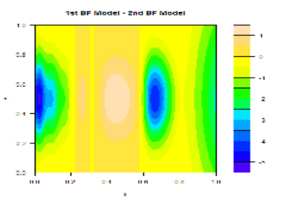
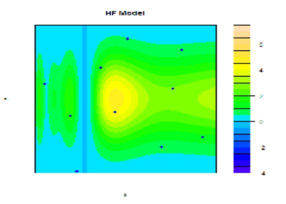


2 low-fidelity functions $z_1(\mathbf{x})$ and $z_2(\mathbf{x}) \rightarrow$ difference visualization

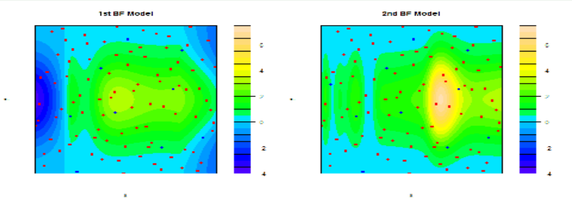


Toy example: two LHS such that $\mathcal{D}_{HF} \subset \mathcal{D}_{BF}$

1 high-fidelity function $z(\mathbf{x})$ with $n_{HF} = 10$ runs



2 low-fidelity functions $z_1(\mathbf{x})$ and $z_2(\mathbf{x})$ with $n_{LF,\{1,2\}} = 100$ runs



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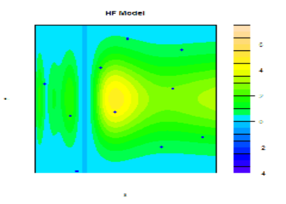

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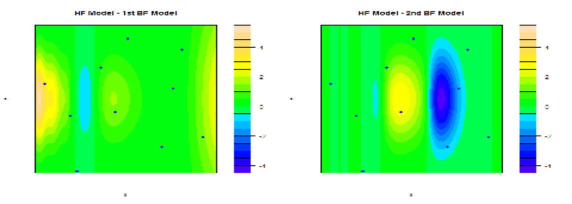

Kriging model fo $z(\mathbf{x})$ [Rasmussen & Williams, 2006]

Design of experiments: $\mathbf{D}_{HF} = (\mathbf{x}_1, ..., \mathbf{x}_{n_{HF}})$
Responses of $z(\mathbf{x})$: $\mathbf{z}^{n_{HF}} := z(\mathbf{D}_{HF}) := (z(\mathbf{x}_1), ..., z(\mathbf{x}_{n_{HF}}))^T$

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Prior

$$Z(\mathbf{x}) \sim \mathcal{GP}\left(\mathbf{f}^T(\mathbf{x})\beta, \sigma^2 r(\mathbf{x}, \tilde{\mathbf{x}})\right)$$

with $r(\mathbf{x}, \tilde{\mathbf{x}})$ the Mátern 5.2 kernel parametrized by $\boldsymbol{\theta} \in \mathbb{R}^d$ and $\mathbf{f}^T(\mathbf{x}) = 1$ by default.

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Posterior

$$\hat{Z}(\mathbf{x}) = [Z(\mathbf{x}) | \mathbf{Z}^{n_{HF}} = \mathbf{z}^{n_{HF}}] \sim \mathcal{GP}\left(\hat{\mu}(\mathbf{x}), \hat{s}^2(\mathbf{x}, \tilde{\mathbf{x}})\right) \text{ where:}$$

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Posterior with $\hat{\mu}(\mathbf{x})$ the predictor

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$\hat{\mu}(\mathbf{x}) = \mathbf{f}^T(\mathbf{x})\hat{\beta} + r(\mathbf{x}, \mathbf{D}_{HF})\mathbf{R}^{-1}(\mathbf{z}^{n_{HF}} - \mathbf{F}\hat{\beta})$ with $\hat{\beta}$ the m.l.e.

$r(\mathbf{x}, \mathbf{D}_{HF})_i = r(\mathbf{x}, \mathbf{x}_i)$, $\mathbf{R}_{i,j} = r(\mathbf{x}_i, \mathbf{x}_j)$ and $\mathbf{F}_{i,:} = \mathbf{f}^T(\mathbf{x}_i)$.

Kriging model fo $z(\mathbf{x})$ [Rasmussen & Williams, 2006]

Design of experiments: $\mathbf{D}_{HF} = (\mathbf{x}_1, \dots, \mathbf{x}_{n_{HF}})$
Responses of $z(\mathbf{x})$: $\mathbf{z}^{n_{HF}} := z(\mathbf{D}_{HF}) := (z(\mathbf{x}_1), \dots, z(\mathbf{x}_{n_{HF}}))^T$

Prior

$$Z(\mathbf{x}) \sim \mathcal{GP}\left(\mathbf{f}^T(\mathbf{x})\beta, \sigma^2 r(\mathbf{x}, \tilde{\mathbf{x}})\right)$$

with $r(\mathbf{x}, \tilde{\mathbf{x}})$ the Mátern 5.2 kernel parametrized by $\boldsymbol{\theta} \in \mathbb{R}^d$ and $\mathbf{f}^T(\mathbf{x}) = 1$ by default.

Posterior with $\hat{\mu}(\mathbf{x})$ the predictor and $\hat{s}^2(\mathbf{x}, \mathbf{x})$ a confidence measure

$$\hat{Z}(\mathbf{x}) = [Z(\mathbf{x}) | \mathbf{Z}^{n_{HF}} = \mathbf{z}^{n_{HF}}] \sim \mathcal{GP}\left(\hat{\mu}(\mathbf{x}), \hat{s}^2(\mathbf{x}, \tilde{\mathbf{x}})\right) \text{ where:}$$

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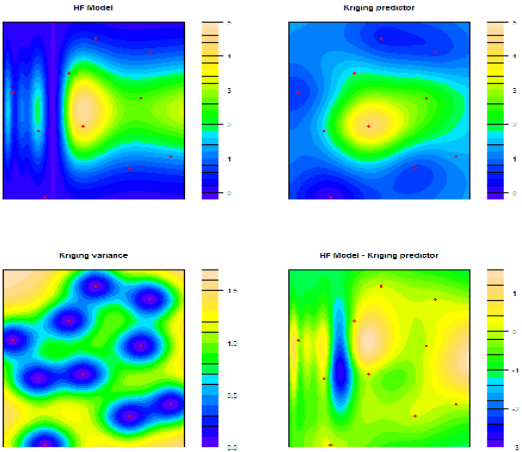
$$\hat{s}^2(\mathbf{x}, \tilde{\mathbf{x}}) = \hat{\sigma}^2 \left(r(\mathbf{x}, \tilde{\mathbf{x}}) - \left(\mathbf{f}^T(\mathbf{x}) \; r(\mathbf{x}, \mathbf{D}_{HF})\right) \begin{pmatrix} 0 & \mathbf{F}^T \\ \mathbf{F} & \mathbf{R} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{f}(\tilde{\mathbf{x}}) \\ r(\mathbf{D}_{HF}, \tilde{\mathbf{x}}) \end{pmatrix} \right)$$

Toy example: Kriging model with $\mathbf{f}(\mathbf{x})^T = 1$



Kriging model : an alternative formulation (K')

$\mathbf{D}_{HF} = (\mathbf{x}_1, ..., \mathbf{x}_{n_{HF}})$ and $\mathbf{z}^{n_{HF}} := z(\mathbf{D}_{HF}) := (z(\mathbf{x}_1), ..., z(\mathbf{x}_{n_{HF}}))^T$.

New kriging model [Le Gratiet *et al.*, 2013]

$$Z^{n_{HF}}(\mathbf{x}) = \hat{\mu}(\mathbf{x}) - \tilde{\mu}(\mathbf{x}) + \tilde{Z}(\mathbf{x}) \sim \mathcal{GP}\left(\hat{\mu}(\mathbf{x}), \hat{s}^2(\mathbf{x}, \tilde{\mathbf{x}})\right)$$

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$$\tilde{\mu}(\mathbf{x}) = \mathbf{f}^T(\mathbf{x})\tilde{\beta} + \mathbf{r}^T(\mathbf{x}, \mathbf{D_{HF}})\mathbf{R}^{-1}(\tilde{\mathbf{Z}}^{n_{HF}} - \mathbf{F}\tilde{\beta})$$

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$$\hat{\beta} = (\mathbf{F}^T\mathbf{R}^{-1}\mathbf{F})^{-1}\mathbf{F}^T\mathbf{R}^{-1}\mathbf{z}^{n_{HF}}$$
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Co-Kriging (CK) I

Low-fidelity level = Kriging model (K')

$$Z_{LF}^{n_{LF}}(\mathbf{x}) = \hat{\mu}_{LF}(\mathbf{x}) - \tilde{\mu}_{LF}(\mathbf{x}) + \tilde{Z}_{LF}(\mathbf{x}) \sim \mathcal{GP}\left(\hat{\mu}_{LF}(\mathbf{x}), \hat{s_{LF}}^2(\mathbf{x}, \tilde{\mathbf{x}})\right)$$

where $\tilde{Z}_{LF}(\mathbf{x})$ is a $\mathcal{GP}(0, \sigma_{LF}^2 r_{LF}(\mathbf{x}, \tilde{\mathbf{x}}))$ and:

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$$\tilde{\mu}_{LF}(\mathbf{x}) = \mathbf{f}_{LF}^T(\mathbf{x})\tilde{\beta}_{LF} + \mathbf{r}_{LF}^T(\mathbf{x}, \mathbf{D}_{LF})\mathbf{R}_{LF}^{-1}\left(\tilde{\mathbf{Z}}_{LF}^{n_{LF}} - \mathbf{F}_{LF}\tilde{\beta}_{LF}\right)$$

with:

$$\hat{\beta}_{LF} = (\mathbf{F}_{LF}^T\mathbf{R}_{LF}^{-1}\mathbf{F}_{LF})^{-1}\mathbf{F}_{LF}^T\mathbf{R}_{LF}^{-1}\mathbf{z}_{LF}^{n_{LF}}$$

$$\tilde{\beta}_{LF} = (\mathbf{F}_{LF}^T\mathbf{R}_{LF}^{-1}\mathbf{F}_{LF})^{-1}\mathbf{F}_{LF}^T\mathbf{R}_{LF}^{-1}\tilde{\mathbf{Z}}_{LF}^{n_{LF}}$$

Co-Kriging (CK) II

High-fidelity level = Kriging model (K') for the residuals

$$Z_{HF}^{n_{HF}}(\mathbf{x}) = \rho Z_{LF}^{n_{LF}}(\mathbf{x}) + \mu_\delta(\mathbf{x}) - \tilde{\mu}_\delta(\mathbf{x}) + \tilde{\delta}(\mathbf{x}) \sim \mathcal{GP}\left(\hat{\mu}_{HF}(\mathbf{X}), \hat{s}_{HF}^2(\mathbf{x}, \tilde{\mathbf{x}})\right)$$

where $\tilde{\delta}(\mathbf{x})$ is a $\mathcal{GP}(0, \sigma_\delta^2 r_\delta(\mathbf{x}, \tilde{\mathbf{x}}))$.

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$$\mu_\delta(\mathbf{x}) = \mathbf{f}_\delta^T(\mathbf{x})\boldsymbol{\beta}_\delta + \mathbf{r}_\delta^T(\mathbf{x}, \mathbf{D}_{HF})\mathbf{R}_\delta^{-1}(\mathbf{z}_{HF}^{n_{HF}} - \mathbf{F}_\delta\boldsymbol{\beta}_\delta - \rho\mathbf{z}_{LF}^{n_{HF}})$$

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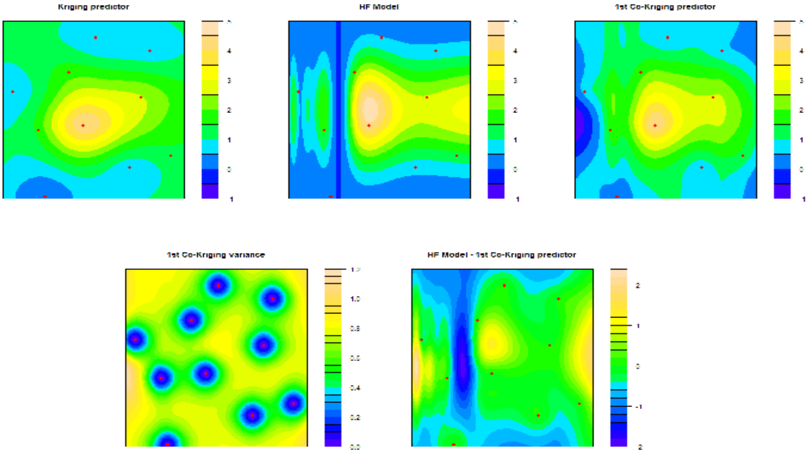
$$\tilde{\mu}_\delta(\mathbf{x}) = \mathbf{r}_\delta^T(\mathbf{x}, \mathbf{D}_{HF})\mathbf{R}_\delta^{-1}\tilde{\boldsymbol{\delta}}^{n_{HF}}$$

with:

$$(\rho, \boldsymbol{\beta}_\delta^T)^T \sim \mathcal{N}\left(\boldsymbol{\Sigma}_{\rho,\boldsymbol{\beta}_\delta}\mathbf{H}^T\mathbf{R}_\delta^{-1}\mathbf{z}^{n_{HF}}, \sigma_\delta^2\boldsymbol{\Sigma}_{\rho,\boldsymbol{\beta}_\delta}\right) \text{ and } (\rho, \boldsymbol{\beta}_\delta)^T \perp Z_{LF}^{n_{LF}}(\mathbf{x}), \tilde{\delta}(\mathbf{x})$$

$$\boldsymbol{\Sigma}_{\rho,\boldsymbol{\beta}_\delta} = (\mathbf{H}^T\mathbf{R}_\delta^{-1}\mathbf{H})^{-1}, \ \mathbf{H} = [\mathbf{z}_{LF}^{n_{LF}} \ \mathbf{F}_\delta]$$

Toy example: Co-Kriging model with $\mathbf{f}_\delta(\mathbf{x})^T = 1$



Leave-One-Out Co-Kriging (LOOCK) I

High-fidelity model when n_{HF} is very small

Leave-one-out aggregation (e.g. [Lecué, 2012])

$$\bar{Z}_{HF}^{n_{HF}}(\mathbf{x}) = \rho Z_{LF}^{n_{LF}}(\mathbf{x}) + \frac{1}{n_{HF}} \sum_{i=1}^{n_{HF}} \delta_{-i}^{n_{HF}}(\mathbf{x}) \sim \mathcal{GP}\left(\hat{\bar{\mu}}_{HF}(\mathbf{x}), \hat{\bar{s}}_{HF}^2(\mathbf{x}, \tilde{\mathbf{x}})\right)$$

where:

$$\delta_{-i}^{n_{HF}}(\mathbf{x}) = \mu_{\delta,-i}(\mathbf{x}) - \tilde{\mu}_{\delta,-i}(\mathbf{x}) + \tilde{\delta}(\mathbf{x})$$

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with:

$$\mu_{\delta,-i}(\mathbf{x}) = \mathbf{f}_{\delta}^{T}(\mathbf{x})\boldsymbol{\beta}_{\delta} + \mathbf{r}_{\delta,-i}^{T}(\mathbf{x}, \mathbf{D}_{HF})\mathbf{R}_{\delta,-i,-i}^{-1}(\mathbf{z}_{HF,-i}^{n_{HF}} - \mathbf{F}_{\delta,-i}\boldsymbol{\beta}_{\delta} - \rho z_{LF,-i}^{n_{HF}})$$

$$\tilde{\mu}_{\delta,-i}(\mathbf{x}) = \mathbf{r}_{\delta,-i}^{T}(\mathbf{x}, \mathbf{D}_{HF})\mathbf{R}_{\delta,-i,-i}^{-1}\tilde{\boldsymbol{\delta}}_{-i}^{n_{HF}}$$

Leave-One-Out Co-Kriging (LOOCK) II

CK predictor [Kennedy & O'Hagan, 2000]

$$\begin{aligned}\hat{\mu}_{HF}(\mathbf{x}) &= \hat{\rho}\hat{\mu}_{LF}(\mathbf{x}) + \mathbf{f}'_\delta(\mathbf{x})\hat{\boldsymbol{\beta}}_\delta \\ &+ \mathbf{r}'_\delta(\mathbf{x}, \mathbf{D}_{HF})\mathbf{R}_\delta^{-1}\left(\mathbf{z}_{HF}^{n_{HF}} - \mathbf{F}_\delta\hat{\boldsymbol{\beta}}_\delta - \hat{\rho}\mathbf{z}_{LF}^{n_{HF}}\right)\end{aligned}$$

where $(\hat{\rho}\ \hat{\boldsymbol{\beta}}_\delta^T)^T = \boldsymbol{\Sigma}_{\rho,\boldsymbol{\beta}_\delta}\mathbf{H}^T\mathbf{R}_\delta^{-1}\mathbf{z}^{n_{HF}}$ with $\boldsymbol{\Sigma}_{\rho,\boldsymbol{\beta}_\delta} = (\mathbf{H}^T\mathbf{R}_\delta^{-1}\mathbf{H})^{-1}$ and $\mathbf{H} = [\mathbf{z}_{LF}^{n_{LF}}\ \mathbf{F}_\delta]$.

Leave-One-Out Co-Kriging (LOOCK) II

CK predictor [Kennedy & O'Hagan, 2000]

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LOOCK predictor when n_{HF} is very small

$$\begin{aligned}\hat{\hat{\mu}}_{HF}(\mathbf{x}) &= \hat{\rho}\hat{\mu}_{LF}(\mathbf{x}) + \mathbf{f}'_\delta(\mathbf{x})\hat{\boldsymbol{\beta}}_\delta \\ &+ \frac{1}{n_{HF}}\sum_{i=1}^{n_{HF}}\left(\mathbf{r}'_{\delta,-i}(\mathbf{x}, \mathbf{D}_{HF})\mathbf{R}_{\delta,-i,-i}^{-1}(\mathbf{z}_{HF,-i}^{n_{HF}} - \mathbf{F}_{\delta,-i}\hat{\boldsymbol{\beta}}_\delta - \hat{\rho}\mathbf{z}_{LF,-i}^{n_{LF}})\right)\end{aligned}$$

LOO Co-Kriging (LOOCK) III

$$\bar{Z}_{HF}^{n_{HF}}(\mathbf{x}) = \rho Z_{LF}^{n_{LF}}(\mathbf{x}) + \frac{1}{n_{HF}} \sum_{i=1}^{n_{HF}} \delta_{-i}^{n_{HF}}(\mathbf{x})$$

Properties

- $\bar{Z}_{HF}^{n_{HF}}(\mathbf{x})$ is a Gaussian process, consequently:

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Properties

- $\bar{Z}_{HF}^{n_{HF}}(\mathbf{x})$ is a Gaussian process, consequently:
  - $\hat{\bar{\mu}}_{HF}(\mathbf{x})$ is an **estimator** of $z(\mathbf{x})$;
  - $\hat{\bar{s}}_{HF}^{2}(\mathbf{x}, \mathbf{x})$ is a **confidence measure** for $\hat{\bar{\mu}}_{HF}(\mathbf{x})$.

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- The estimator $\hat{\mu}_{HF}(\mathbf{x})$ is a regressive function $\rightarrow$ **an alternative to the nugget effect when n_{HF} is very small**.
- The learning mean squared error is equal to the leave-one-out error of the co-kriging model obtained with the n_{HF} observations.

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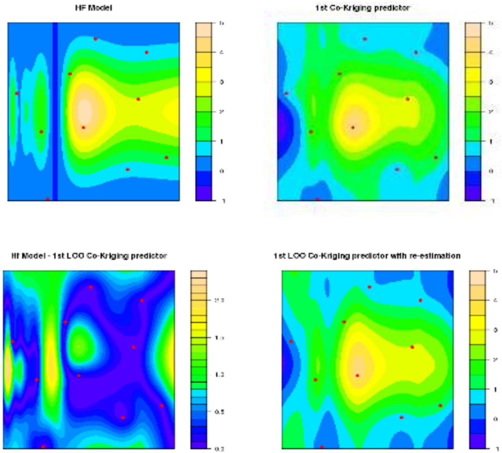
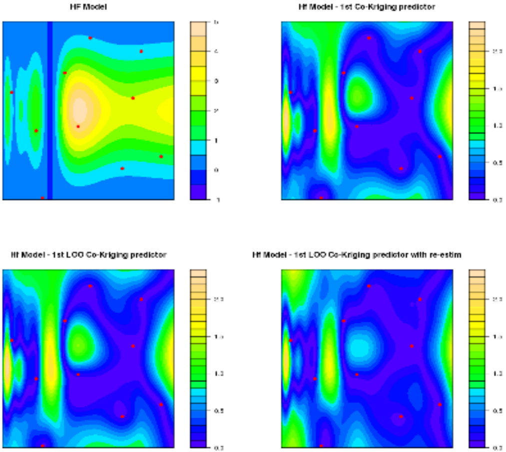
- The learning mean squared error is equal to the leave-one-out error of the co-kriging model obtained with the n_{HF} observations.

Possibility to extend these results to the case where some parameters are re-estimated for the n_{HF} sub-co-kriging models.

Toy example: LOO Co-Kriging Model



Toy example: LOO Co-Kriging Model



Industrial application: results

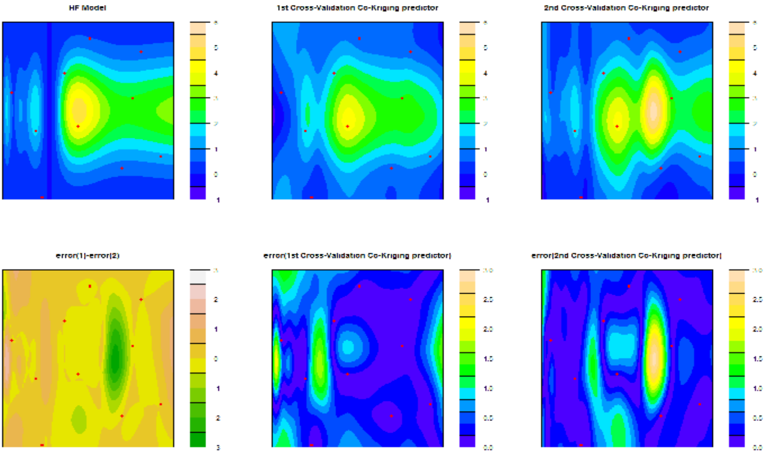
	I	Tamb	P	Q	T
1	300	70	1013	40	156
2	300	45	812	32	136
3	265	45	812	16	138
4	175	55	812	0	142
5	155	70	1013	0	142
6	300	30	1013	25	127
7	265	70	1013	20	159
8	265	30	1013	12.5	128
9	150	40	812	0	113
10	85	55	812	0	100

$$\mathbf{f}_\delta(\mathbf{x}) = (1 \text{ I Tamb Q}) \text{ and } \mathbf{f}(\mathbf{x}) = (1 \text{ I Tamb Q})$$

Model	1	2	3	4	5	6	7	8	9	10
CTM1	-165.21	-169.05	-89.67	-2.68	-3.66	-165.53	-89.55	-85.92	2.86	4.74
CTM2	**-0.88**	-4.14	-9.28	-563.39	-330.23	-0.69	-3.45	-9.03	-374.56	-334.69
K-LOO	5.44	0.31	-2.22	6.14	**-2.21**	-0.93	-3.58	-0.80	2.38	-10.36
CK1-LOO	3.77	**-0.20**	-1.65	6.00	-2.98	**0.23**	-2.25	**0.16**	-10.58	-18.04
CK2-LOO	2.79	-1.42	**-0.10**	**1.77**	-2.35	-2.41	**0.75**	2.16	**1.43**	**-0.96**

Relative errors in % of the Compact Thermal Models (CTM), Kriging model (K) and Co-Kriging models (CK)

Two LOO co-kriging models and now ?



Soft or "randomly hard" mixture of LOOCK models ? I

Soft mixture

$$\bar{Z}(\mathbf{x}) = \frac{w_1(\mathbf{x})\bar{Z}_{HF,1}^{n_{HF}}(\mathbf{x}) + w_2(\mathbf{x})\bar{Z}_{HF,2}^{n_{HF}}(\mathbf{x})}{w_1(\mathbf{x}) + w_2(\mathbf{x})}$$

where $w_1(\mathbf{x})$ and $w_2(\mathbf{x})$ are positive weights.
But the confidence measure $\mathrm{Var}\left(\bar{Z}(\mathbf{x})\right)$ is undefined.

Soft or "randomly hard" mixture of LOOCK models ? I

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where $w_1(\mathbf{x})$ and $w_2(\mathbf{x})$ are positive weights.
But the confidence measure $\text{Var}\left(\bar{Z}(\mathbf{x})\right)$ is undefined.

A solution...

Hard mixture

$$\bar{Z}(\mathbf{x}) = \bar{Z}^{n_{HF}}_{HF,1}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in C_1} + \bar{Z}^{n_{HF}}_{HF,2}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in C_2}$$

where (C_1, C_2) is a partition of $\mathcal{D}_x$, $[0,1]^2$ in our case.
$\text{Var}\left[\bar{Z}(\mathbf{x})\right] = \text{Var}\left[\bar{Z}^{n_{HF}}_{HF,1}(\mathbf{x})\right]\mathbb{I}_{\mathbf{x}\in C_1} + \text{Var}\left[\bar{Z}^{n_{HF}}_{HF,2}(\mathbf{x})\right]\mathbb{I}_{\mathbf{x}\in C_2}$

Soft or "randomly hard" mixture of LOOCK models ? II

Hard mixture

$$\bar{Z}(\mathbf{x}) = \bar{Z}_{HF,1}^{n_{HF}}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in C_1} + \bar{Z}_{HF,2}^{n_{HF}}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in C_2}$$

where (C_1, C_2) is a partition of $\mathcal{D}_x$, $[0,1]^2$ in our case.
But the estimator of $z(\mathbf{x})$ which is equal to:

$$\mathbb{E}\left[\bar{Z}(\mathbf{x})\right] = \hat{\bar{\mu}}_{HF,1}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in C_1} + \hat{\bar{\mu}}_{HF,2}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in C_2}$$

is clearly discontinuous.

Soft or "randomly hard" mixture of LOOCK models ? II

Hard mixture

$$\bar{Z}(\mathbf{x}) = \bar{Z}^{n_{HF}}_{HF,1}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in C_1} + \bar{Z}^{n_{HF}}_{HF,2}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in C_2}$$

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is clearly discontinuous.

A solution...

"Randomly hard" mixture

$$\bar{Z}(\mathbf{x};\omega) = \bar{Z}^{n_{HF}}_{HF,1}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in \tilde{C}_1(\omega)} + \bar{Z}^{n_{HF}}_{HF,2}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in \tilde{C}_2(\omega)}$$

where $(\tilde{C}_1(\omega), \tilde{C}_2(\omega))$ is a realization of the partition (C_1, C_2).

Soft or "randomly hard" mixture of LOOCK models ? III

"Randomly hard" mixture

$$\bar{Z}(\mathbf{x};\omega) = \bar{Z}^{n_{HF}}_{HF,1}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in\tilde{C}_1(\omega)} + \bar{Z}^{n_{HF}}_{HF,2}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in\tilde{C}_2(\omega)}$$

where $(\tilde{C}_1(\omega), \tilde{C}_2(\omega))$ is a realization of the partition (C_1, C_2).
In this case, the estimator of $z(\mathbf{x})$ is:

$$\begin{aligned}\mathbb{E}\left[\bar{Z}(x)\right] &= \mathbb{E}\left[\mathbb{E}\left[\bar{Z}(x)|(C_1,C_2)\right]\right] \\ &= \mathbb{P}\left[C_1 \ni \mathbf{x}\right]\hat{\hat{\mu}}_{HF,1}(\mathbf{x}) + \mathbb{P}\left[C_2 \ni \mathbf{x}\right]\hat{\hat{\mu}}_{HF,2}(\mathbf{x})\end{aligned}$$

with $\mathbb{P}\left[C_2 \ni \mathbf{x}\right] = 1 - \mathbb{P}\left[C_1 \ni \mathbf{x}\right]$. Moreover:

$$\begin{aligned}\mathrm{Var}\left[\bar{Z}(x)\right] &= \mathbb{E}\left[\mathrm{Var}\left[\bar{Z}(x)|(C_1,C_2)\right]\right] + \mathrm{Var}\left[\mathbb{E}\left[\bar{Z}(x)|(C_1,C_2)\right]\right] \\ &= \mathbb{P}\left[C_1 \ni \mathbf{x}\right]\hat{\hat{s}}^2_{HF,1}(\mathbf{x}) + (1 - \mathbb{P}\left[C_1 \ni \mathbf{x}\right])\hat{\hat{s}}^2_{HF,2}(\mathbf{x}) \\ &+ \mathbb{P}\left[C_1 \ni \mathbf{x}\right]\hat{\hat{\mu}}^2_{HF,1}(\mathbf{x}) + (1 - \mathbb{P}\left[C_1 \ni \mathbf{x}\right])\hat{\hat{\mu}}^2_{HF,2}(\mathbf{x}) \\ &- \left(\mathbb{P}\left[C_1 \ni \mathbf{x}\right]\hat{\hat{\mu}}_{HF,1}(\mathbf{x}) + (1 - \mathbb{P}\left[C_1 \ni \mathbf{x}\right])\hat{\hat{\mu}}_{HF,2}(\mathbf{x})\right)^2\end{aligned}$$

Soft or "randomly hard" mixture of LOOCK models ? IV

"Randomly hard" mixture

$$\bar{Z}(\mathbf{x};\omega) = \bar{Z}^{n_{HF}}_{HF,1}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in\tilde{C}_1(\omega)} + \bar{Z}^{n_{HF}}_{HF,2}(\mathbf{x})\mathbb{I}_{\mathbf{x}\in\tilde{C}_2(\omega)}$$

where $(\tilde{C}_1(\omega), \tilde{C}_2(\omega))$ is a realization of the partition (C_1, C_2).

$$\mathbb{E}\left[\bar{Z}(x)\right] = \mathbb{P}\left[x \in C_1\right]\hat{\bar{\mu}}_{HF,1}(\mathbf{x}) + (1 - \mathbb{P}\left[x \in C_1\right])\hat{\bar{\mu}}_{HF,2}(\mathbf{x})$$

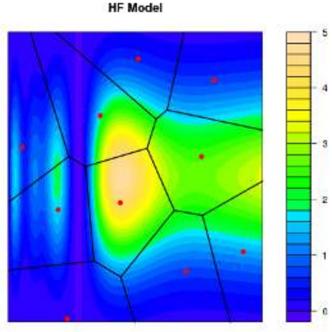
$$\begin{aligned}
\mathrm{Var}\left[\bar{Z}(x)\right] \;=\; & \mathbb{P}\left[x \in C_1\right]\hat{\bar{s}}^2_{HF,1}(\mathbf{x}) + (1 - \mathbb{P}\left[x \in C_1\right])\hat{\bar{s}}^2_{HF,2}(\mathbf{x}) \\
+ \; & \mathbb{P}\left[x \in C_1\right]\hat{\bar{\mu}}^2_{HF,1}(\mathbf{x}) + (1 - \mathbb{P}\left[x \in C_1\right])\hat{\bar{\mu}}^2_{HF,2}(\mathbf{x}) \\
- \; & \left(\mathbb{P}\left[x \in C_1\right]\hat{\bar{\mu}}_{HF,1}(\mathbf{x}) + (1 - \mathbb{P}\left[x \in C_1\right])\hat{\bar{\mu}}_{HF,2}(\mathbf{x})\right)^2
\end{aligned}$$

Possibility to extend this method to the situation where the number of low fidelity models is greather than 2 ($\rightarrow$ multinomial law).

Creation of a hard classification

Recipe

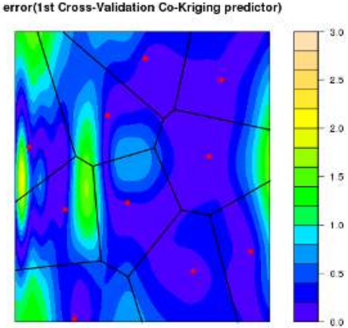
Voronoi diagram + "Robustness estimation"

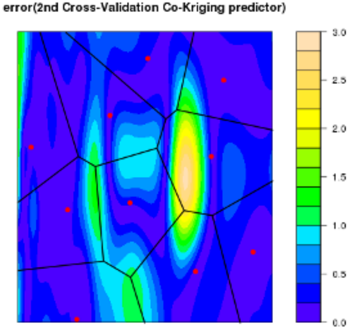


Creation of a hard classification

Recipe

Voronoi diagram + "Robustness estimation"

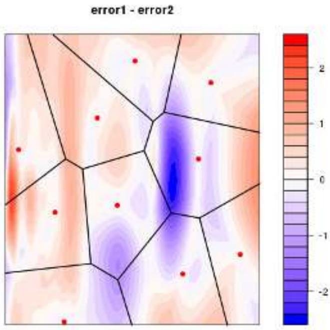


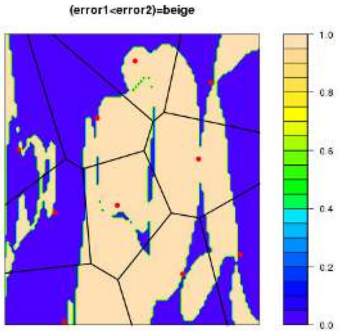


Creation of a hard classification

Recipe

Voronoi diagram + "Robustness estimation"

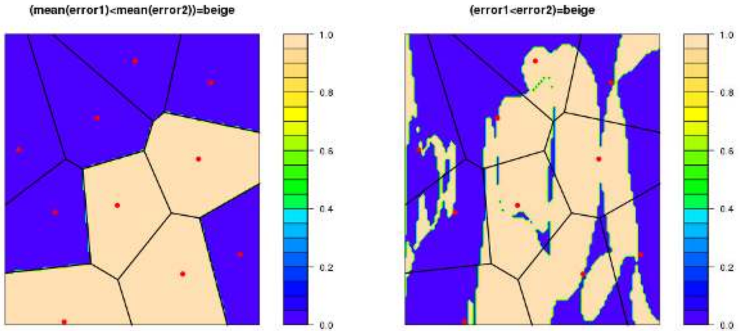




Creation of a hard classification

Recipe

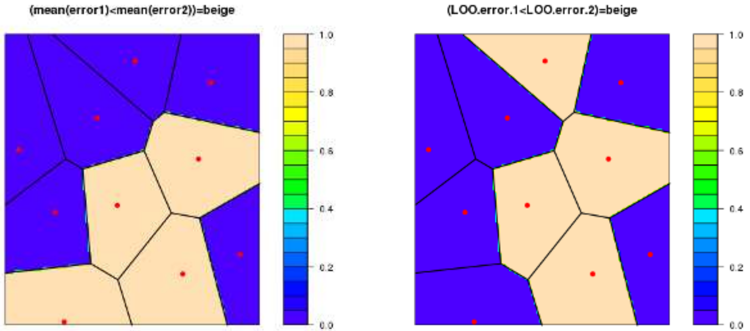
Voronoi diagram + "Robustness estimation"



Creation of a hard classification

Recipe

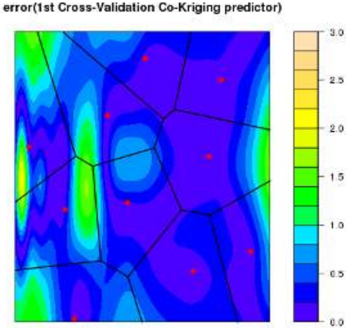
Voronoi diagram + LOO errors

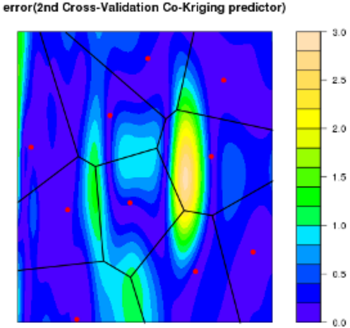


Creation of a hard classification

Recipe

Voronoi diagram + "Error estimation"

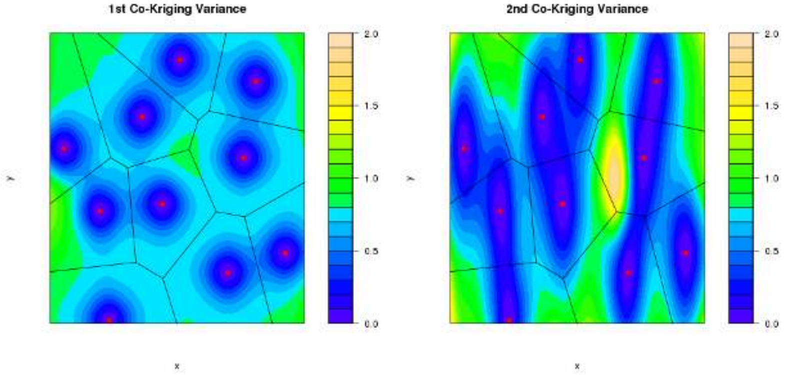




Creation of a hard classification

Recipe

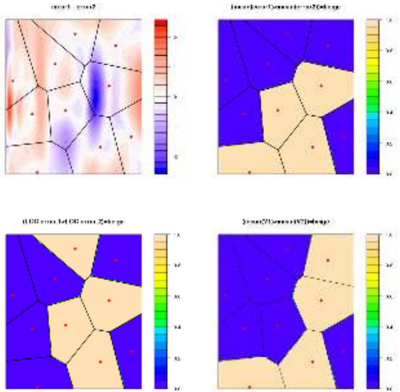
Voronoi diagram + Co-Kriging Variances



Creation of a hard classification

Recipe

Voronoi diagram + Co-Kriging Variances



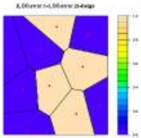
Creation of a "randomly" hard classification

Recipe

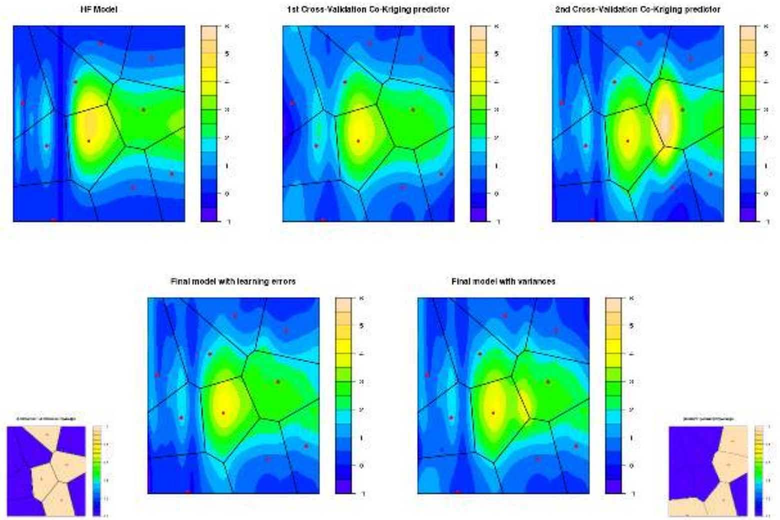
Repeat K times:

1. Add a Gaussian noise to the boundary between the beige and the blue classes.
   or in an equivalent way
   Add **the same** Gaussian noise to the points of interest.
2. Update the labels of each point of interest, according to the label of its Voronoi cell, *i.e.* $\mathbf{x} \in C_1^{(k)}$ or $\mathbf{x} \in C_2^{(k)}$

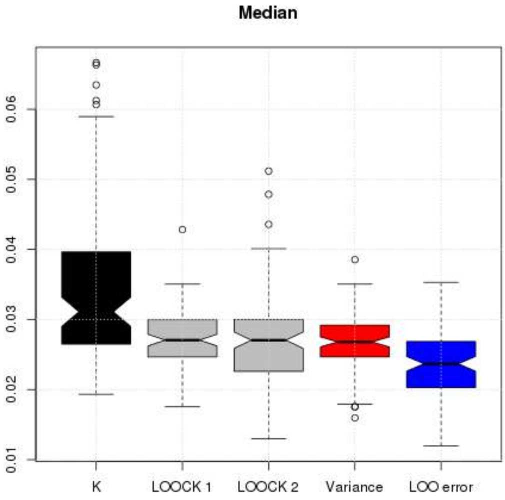
$\rightarrow \mathbb{P}[C_1 \ni \mathbf{x}] \approx \frac{1}{K} \sum_{k=1}^{K} \mathbb{I}(\mathbf{x} \in C_1^{(k)})$



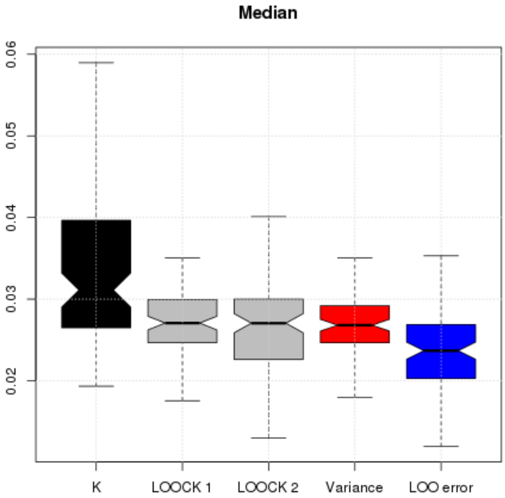
Toy example: randomly hard mixture of LOOCK models I



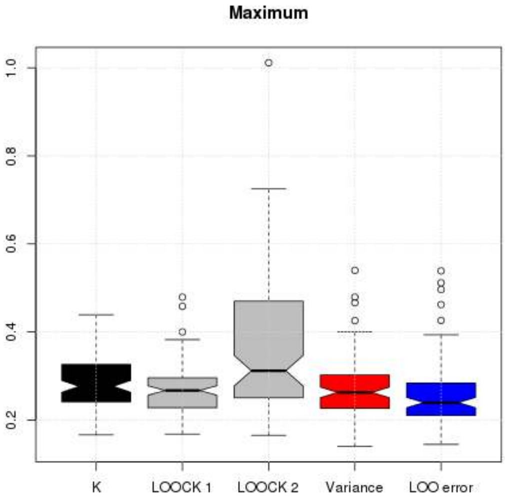
Toy example: randomly hard mixture of LOOCK models II



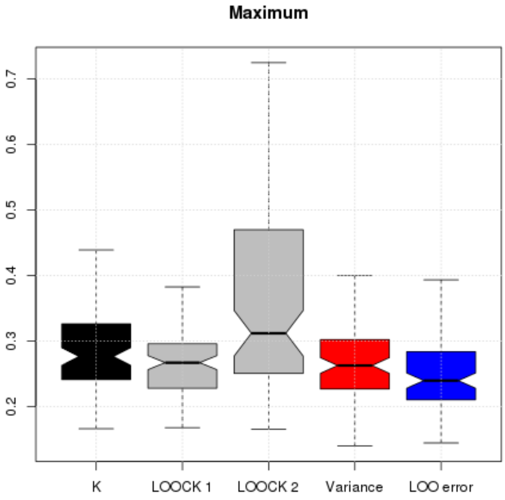
Toy example: randomly hard mixture of LOOCK models II



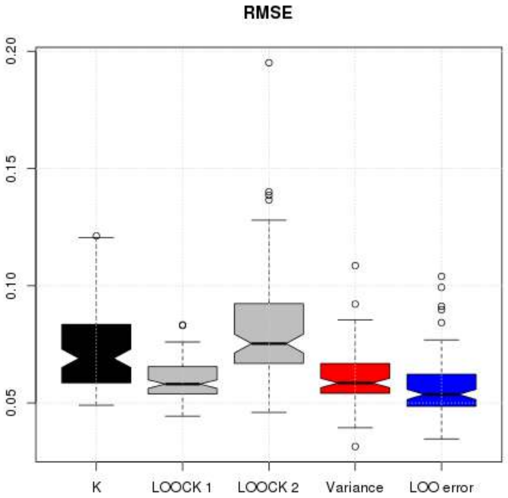
Toy example: randomly hard mixture of LOOCK models II



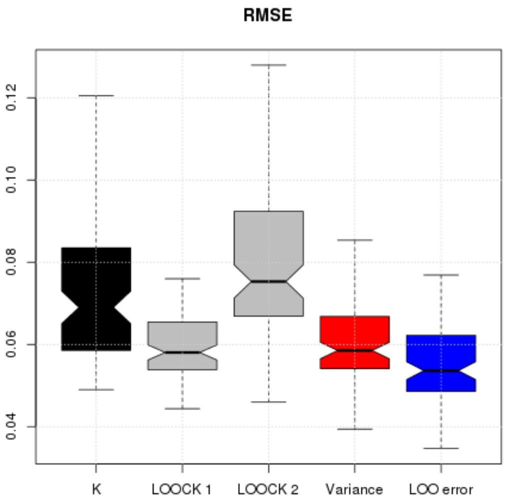
Toy example: randomly hard mixture of LOOCK models II



Toy example: randomly hard mixture of LOOCK models II



Toy example: randomly hard mixture of LOOCK models II



Perspectives

- Criterion based on the boostrap estimator of the kriging variance [Hertog et al., 2005] for a soft, hard or "randomly" hard mixture
- Choice of another distance for the Voronoï cells
- Validation of the selected method on the industrial application

Learning of multi-fidelity data with a mixture of Gaussian processes

Matthias De Lozzo & Loïc Le Gratiet

Thank you for your attention.

Discussion on multi-fidelity simulators, GdR MASCOT-NUM
May 17th, 2013, Institut Henri Poincaré, Paris