Multi-fidelity co-kriging models

Application to Sequential design

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ANR CHORUS
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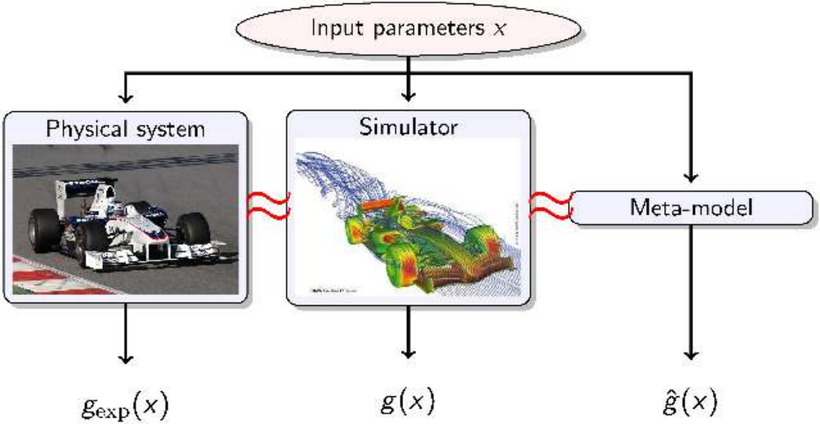
Context

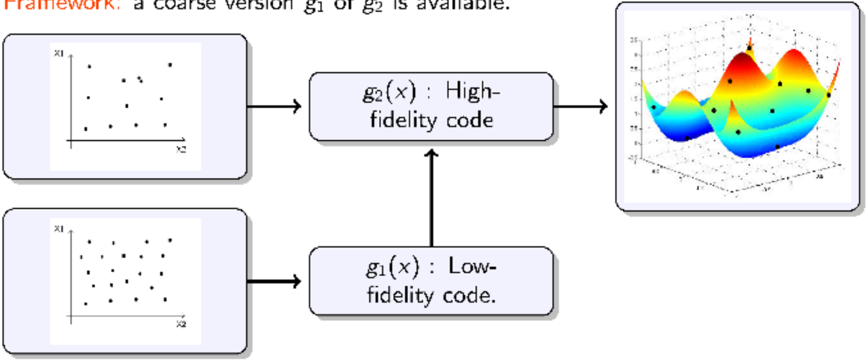

Input parameters x
Physical system
Simulator
Meta-model
$g_{\mathrm{exp}}(x)$
$g(x)$
$\hat{g}(x)$

Motivations

- Objective: replace the output of a code, called $g_2(x)$, by a metamodel.

$$g_2(x) : x \in Q \subset \mathbb{R}^d \mapsto \mathbb{R}$$

- Framework: a coarse version g_1 of g_2 is available.



Principle: build a metamodel of $g_2(x)$ which integrates as well observations of the coarse code output. $\longrightarrow$ Multi-fidelity co-kriging model

Recursive formulation of the model

- Multi-fidelity co-kriging model: [Kennedy & O'Hagan (2000), Le Gratiet (2013), Le Gratiet (2014)]

$$\begin{cases} Z_2(x) = \rho Z_1^*(x) + \delta(x) \\ Z_1^*(x) \perp \delta(x) \end{cases}$$

where $Z_1^*(x) \sim [Z_1(x) | \mathbf{Z}_1 = \mathbf{g}_1 , \boldsymbol{\beta}_1 , \sigma_1^2 , \boldsymbol{\theta}_1]$, with $\mathbf{g}_1 = g_1(x), x \in \mathbf{D}_1$

and $Z_1(x) \sim \mathrm{GP}\left(\mathbf{f}_1^t(x)\boldsymbol{\beta}_1, \sigma_1^2 r_1(x, \tilde{x}; \boldsymbol{\theta}_1)\right)$, $\delta(x) \sim \mathrm{GP}\left(\mathbf{f}_\delta^t(x)\boldsymbol{\beta}_\delta, \sigma_\delta^2 r_\delta(x, \tilde{x}; \boldsymbol{\theta}_\delta)\right)$

- Parameters estimation:
  - $\boldsymbol{\theta}_1$, $\boldsymbol{\theta}_\delta$, σ_1^2, σ_δ^2 : maximum likelihood method
  - $\boldsymbol{\beta}_1$, $\begin{pmatrix} \boldsymbol{\beta}_\delta \\ \rho \end{pmatrix}$: analytical posterior distribution (Bayesian inference)

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- Finally, $Z_2^*(x) \sim [Z_2(x) | \mathbf{Z}_2 = \mathbf{g}_2, \mathbf{Z}_1 = \mathbf{g}_1]$ with $\mathbf{g}_2 = g_2(x), x \in \mathbf{D}_2$

We suppose that $\mathbf{D}_2 \subset \mathbf{D}_1$ and $\boldsymbol{\theta}_1, \boldsymbol{\theta}_\delta, \sigma_1^2, \sigma_\delta^2$ are known.

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Predictive distribution

- In Universal Cokriging, the predictive distribution of $Z_2^*(x)$ is not Gaussian.

  The predictive mean and variance can be decomposed as:

$$\begin{aligned}\mu_{Z_2}(x) &= \mathbb{E}\left[Z_2(x)|\mathbf{Z}_2 = \mathbf{g}_2, \mathbf{Z}_1 = \mathbf{g}_1\right] \\ &= \hat{\rho}\mu_{Z_1}(x) + \mu_\delta(x)\end{aligned}$$

$$\begin{aligned}\sigma^2_{Z_2}(x) &= \mathrm{var}\left(Z_2(x)|\mathbf{Z}_2 = \mathbf{g}_2, \mathbf{Z}_1 = \mathbf{g}_1]\right) \\ &= \hat{\sigma}^2_\rho \sigma^2_{Z_1}(x) + \sigma^2_\delta(x)\end{aligned}$$

- Remarks:
  - in $\mu_{Z_2}(x)$: $\boldsymbol{\beta}$ and ρ are replaced by their posterior means.
  - in $\sigma^2_{Z_2}(x)$: we infer from the posterior distributions of $\boldsymbol{\beta}$ and ρ.

Generalizations

- Generalizations for the AR(1) model:
  - $s > 2$ levels of code.
  - $\rho(x) = f'_\rho(x)\beta_\rho$.
  - Bayesian formulation.
  - Non-nested experimental design sets (see L. Le Gratiet thesis 2013).
- Extend the AR(1) approach (see F. Zertuche):

$$Z_2(x) = \psi(Z_1(x)) + \delta(x)$$

- Other Bayesian formulation with (see Qian and Wu 2008):
  - $\rho(x)$ a Gaussian process.
  - $z_1(x)$ is supposed as known.

Sequential design

- Objective: we want to minimize the following generalization error:

$$\mathrm{IMSE} = \int_Q \sigma^2_{Z_2}(x)dx = \hat{\sigma}^2_\rho \int_Q \sigma^2_{Z_1}(x)dx + \int_Q \sigma^2_\delta(x)dx$$

- Sequential strategy: we select a new point x_{n+1} such that :

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  - What is the contribution of each code level to the model error?

$$\sigma^2_{Z_2}(x_{n+1}) = \hat{\sigma}^2_\rho \sigma^2_{Z_1}(x_{n+1}) + \sigma^2_\delta(x_{n+1})$$

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Code level selection

- What is computational cost of each code ?
  - C : CPU time ration between $g_2(x)$ and $g_1(x)$.
  - 1 run of $g_1(x)$ and $g_2(x) \Leftrightarrow C+1$ runs of $g_1(x)$ (i.e. $\mathbf{D}_2 \subset \mathbf{D}_1$)
- What is the expected reduction of the error?
  - Reduction of the generalization error for $Z_1(x)$:

$$\hat{\sigma}_\rho^2 \sigma_{Z_1}^2(x_{n+1}) \prod_{i=1}^{d} \boldsymbol{\theta}_1^i$$

  - Reduction of the generalization error for the bias $\delta(x)$:

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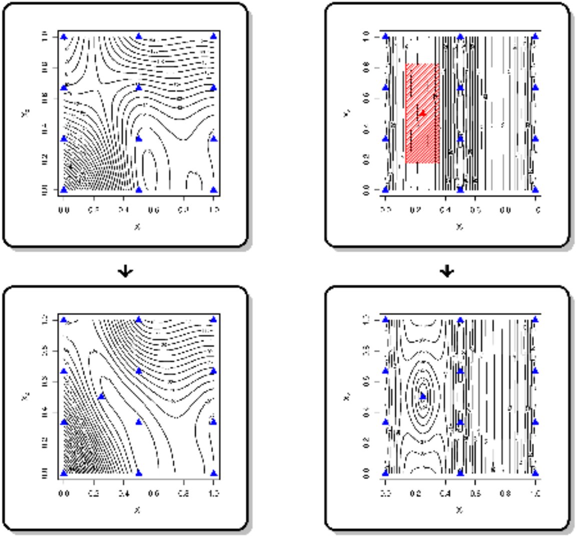
Illustration of the design criterion



Code level selection

- Expected error reduction for the code level 2 :

$$\hat{\sigma}_{\rho}^{2}\sigma_{Z_1}^{2}(x_{n+1})\prod_{i=1}^{d}\boldsymbol{\theta}_{1}^{i}+\sigma_{\delta}^{2}(x_{n+1})\prod_{i=1}^{d}\boldsymbol{\theta}_{\delta}^{i}$$

- Expected error reduction for the code level 1 :

$$(C+1)\,\hat{\sigma}_{\rho}^{2}\sigma_{Z_1}^{2}(x_{n+1})\prod_{i=1}^{d}\boldsymbol{\theta}_{1}^{i}$$

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- Expected error reduction for the code level 1 :

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- It is worth simulating $g_2(x)$ if :

$$(C+1)\,\hat{\sigma}_{\rho}^{2}\sigma_{Z_1}^{2}(x_{n+1})\prod_{i=1}^{d}\boldsymbol{\theta}_{1}^{i}<\hat{\sigma}_{\rho}^{2}\sigma_{Z_1}^{2}(x_{n+1})\prod_{i=1}^{d}\boldsymbol{\theta}_{1}^{i}+\sigma_{\delta}^{2}(x_{n+1})\prod_{i=1}^{d}\boldsymbol{\theta}_{\delta}^{i}$$

i.e.

Code level selection

- Expected error reduction for the code level 2 :

$$\hat{\sigma}_\rho^2 \sigma_{Z_1}^2(x_{n-1}) \prod_{i=1}^{d} \theta_1^i + \sigma_\delta^2(x_{n+1}) \prod_{i=1}^{d} \theta_\delta^i$$

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New strategy

- Problem: the following criterion does not take into account the real prediction error

$$x_{n+1} = \arg\max_{x} \sigma^2_{Z_2}(x)$$

- New strategy: to take into account the true prediction error we consider the following criterion (adjusted variance) :

$$x_{n+1} = \arg\max_{x} \quad \hat{\sigma}^2_{\rho}\sigma^2_{Z_1,UK}(x)\left(1 + \sum_{i=1}^{n_1} \frac{\varepsilon^2_{LOO,1}(x_i^{(1)})}{\sigma^2_{LOO,1}(x_i^{(1)})}\mathbf{1}_{x\in V_{i,1}}\right)$$
$$+\sigma^2_{\delta,UK}(x)\left(1 + \sum_{i=1}^{n_2} \frac{\varepsilon^2_{LOO,\delta}(x_i^{(2)})}{\sigma^2_{LOO,\delta}(x_i^{(2)})}\mathbf{1}_{x\in V_{i,2}}\right)$$

where $V_{i,j}$ is the Voronoi cell associated to $x_i^{(j)}$, $j = 1, 2$, $i = 1, \ldots, n_j$.

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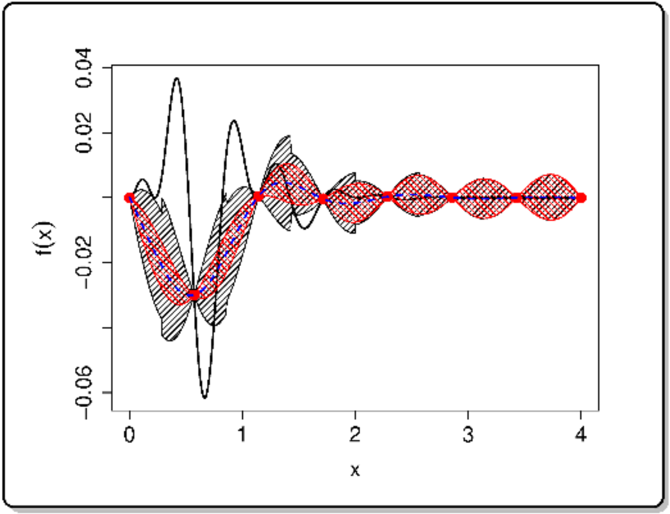
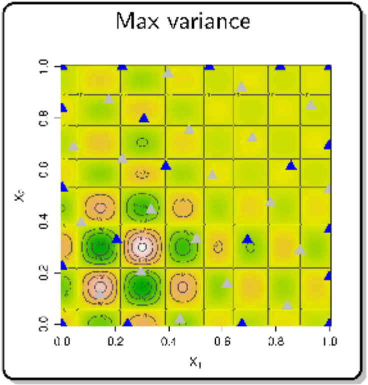
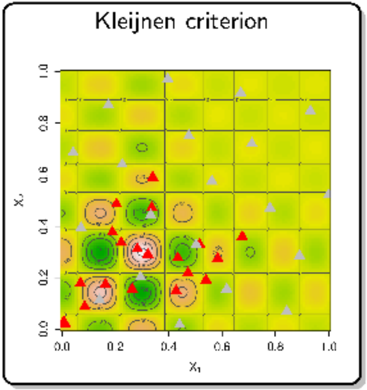


Academic example: the Schubert's function

$$g(x) = \left(\sum_{i=1}^{5} i\cos\left((i+1)x^1 + i\right)\right)\left(\sum_{i=1}^{5} i\cos\left((i+1)x^2 + i\right)\right)$$





Kleijnen, JPC and van Beers, WCM (2004), Application-driven sequential designs for simulation experiments : Kriging metamodelling. *Journal of the Operational Research*

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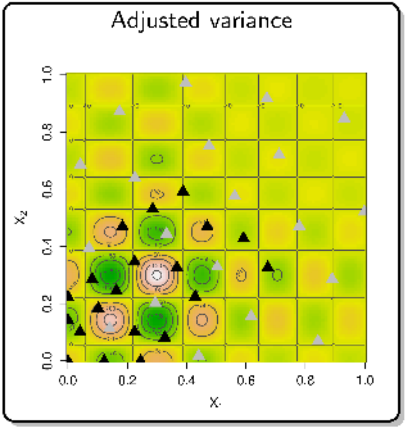

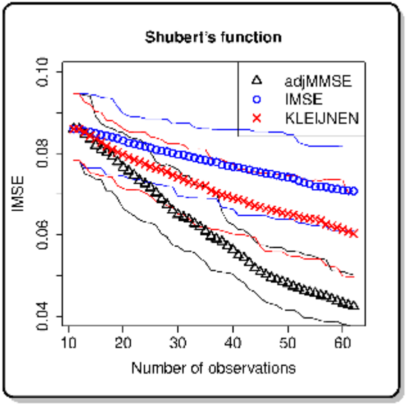

Application : spherical tank under internal pressure

- **High-fidelity code:** $g_2(x)$ is the von Mises stress at point 1, 2 or 3 provided by a finit elements code. $x = (P, R_{\text{int}}, T_{\text{shell}}, T_{\text{cap}}, E_{\text{shell}}, E_{\text{cap}}, \sigma_{\text{y,shell}}, \sigma_{\text{y,cap}})$ $\quad (d = 8)$

  P : internal pression.
  R_{int}: tank internal radius.
  T_{shell}: tank thickness.
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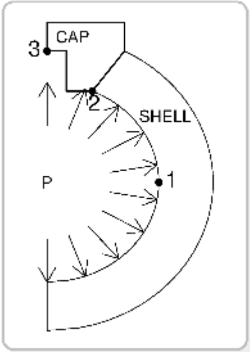

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  g_1 is the 1D approximation of g_2 (perfectly spherical tank).

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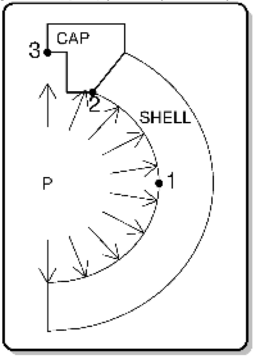

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  The model efficiency Q_2 is estimated from a test set of 7000 points. $Q_2 \approx 86\%$.

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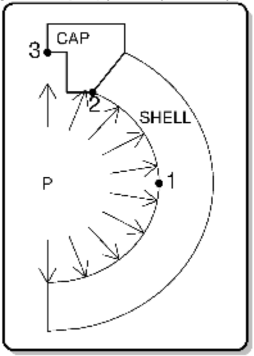

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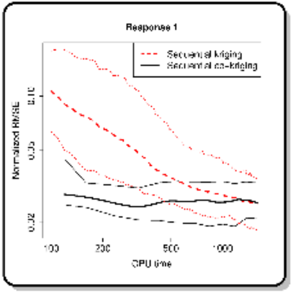
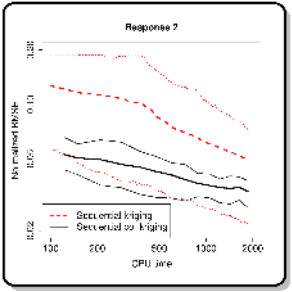
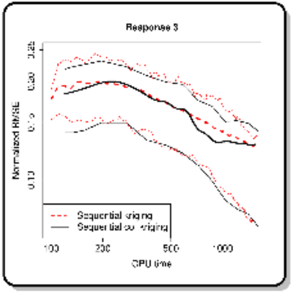
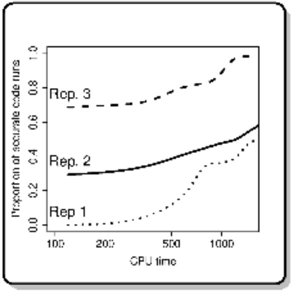
Results


Response 1
Sequential kriging
Sequential co-kriging
Normalized RMSE
0.10
0.05
0.02
100
200
500
1000
CPU time


Response 2
Sequential kriging
Sequential co-kriging
Normalized RMSE
0.10
0.05
0.02
100
200
500
1000
2000
CPU time


Response 3
Sequential kriging
Sequential co-kriging
Normalized RMSE
0.25
0.20
0.15
0.10
100
200
500
1000
CPU time


Rep. 3
Rep. 2
Rep 1
Proportion of accurate code runs
0.0
0.2
0.4
0.6
0.8
1.0
100
200
500
1000
CPU time

Kennedy, M. C. & O'Hagan, A. (2000) , Predicting the output from a complex computer code when fast approximations are available. *Biometrika* **87**, 1–13.

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