Robust Estimation of bottom friction

Parameter control in the presence of uncertainties

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s151431

Master Thesis Defence

DTU Aqua

National Institute of Aquatic Resources

The AIRSEA team, Grenoble, FRANCE

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- Modelling Oceanic and Atmospheric flows: parametrization and coupling of the equations
- Model reduction, multiscale algorithms
- High-performance computing
- Dealing with uncertainties

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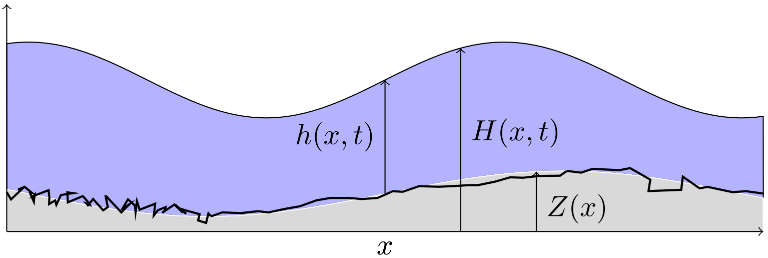
$h(x,t)$
$H(x,t)$
$Z(x)$
x

Outline

Deterministic Framework

- Introduction
- Deterministic Framework
  - The 1D Shallow Water Equations
  - Adjoint-based optimization
- Global sensitivity analysis
- Robust Optimization
- Conclusion

The 1D Shallow Water Equations

1D-SWE

$$\partial_t h + \partial_x q = 0 \qquad \text{(Conservation)}$$

$$\partial_t q + \partial_x \left(\frac{q^2}{h} + \frac{1}{2} g h^2 \right) = -g h \partial_x Z - S \qquad \text{(Momentum)}$$

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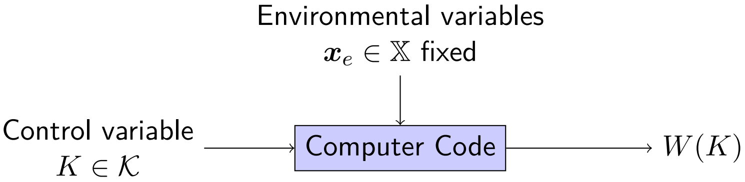
Quadratic Friction

$$S = -K|q|qh^{-\eta}, \quad \eta = 7/3$$

K: control parameter. Either a scalar value or a vector

Computer code

- 1D Shallow water equations
  - K: Bottom friction
  - Boundary conditions (considered fixed and known)
- Output $W(K)$:
  $W_i^n(K) = [h_i^n(K) \quad q_i^n(K)]^T$, for $0 \leq i \leq N_x$ and $0 \leq n \leq N_t$



Data assimilation

K_{ref} and $\mathcal{H}$ observation operator
We have $Y = \mathcal{H}W(K_{\text{ref}}) = \{h_i^n(K_{\text{ref}})\}_{i,n}$

$$j(K) = \frac{1}{2}\|\mathcal{H}W(K) - Y\|^2$$

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$$\arg\min_{K \in \mathcal{K}} j(K)?$$

- Gradient-free: Simulated annealing, Nelder-mead,... $\rightarrow$ High number of runs. Very expensive in practice

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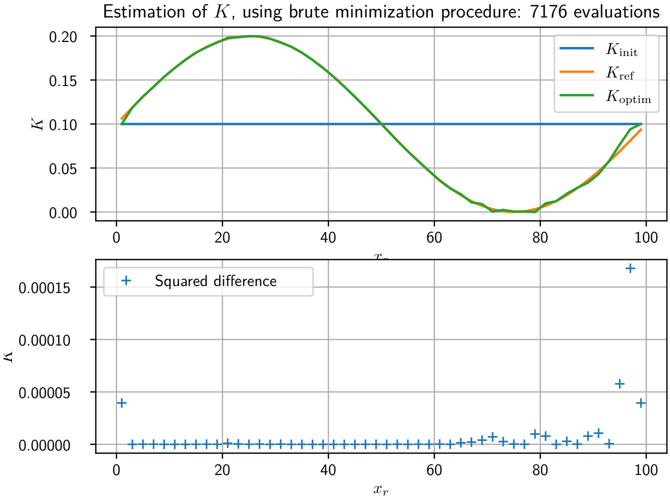
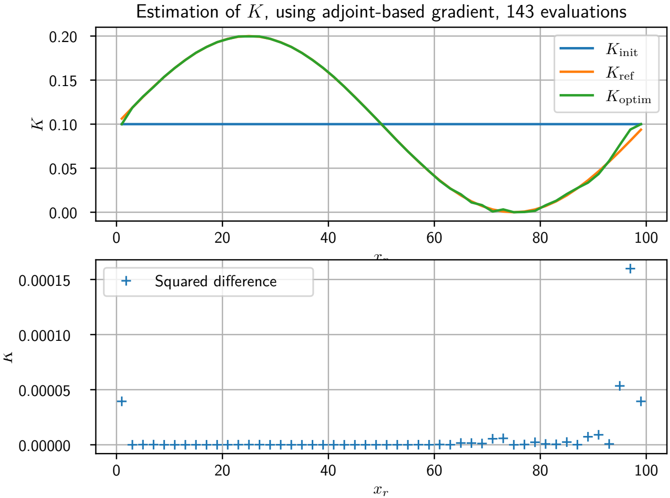
$$\underset{K\in\mathcal{K}}{\arg\min}\, j(K)?$$

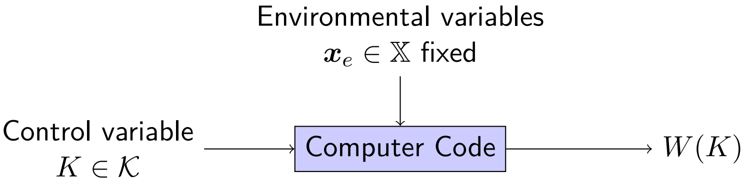
- Gradient-free: Simulated annealing, Nelder-mead,... $\rightarrow$ High number of runs. Very expensive in practice
- Gradient-based: gradient-descent, (quasi-) Newton method ... $\rightarrow$ Less number of runs, but need to derive adjoint code

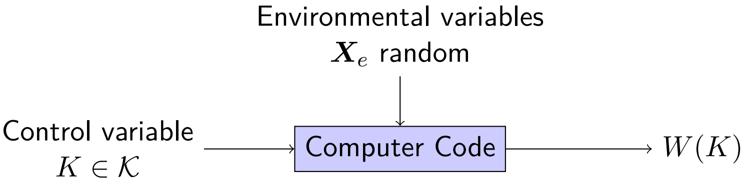
Estimation procedure no gradient



Estimation procedure adjoint-based gradient




Environmental variables
$\boldsymbol{x}_e \in \mathbb{X}$ fixed
Control variable
$K \in \mathcal{K}$
Computer Code
$W(K)$


Environmental variables
$\boldsymbol{X}_e$ random
Control variable
$K \in \mathcal{K}$
Computer Code
$W(K)$

Introducing uncertainties

$\boldsymbol{X}_e$ random vector with realizations $\boldsymbol{x}_e \in \mathbb{X}$

Variable	`mean.h`	`ampli`	`period`	`phase`
$\boldsymbol{X}_e$	$\mathcal{U}([19.5, 20.5])$	$\mathcal{U}([4.9, 5.1])$	$\mathcal{U}([49.9, 50.1])$	$\mathcal{U}([-0.001, 0.001])$
$\boldsymbol{x}_{e,\mathrm{ref}}$	20.0	5.0	50.0	0.000

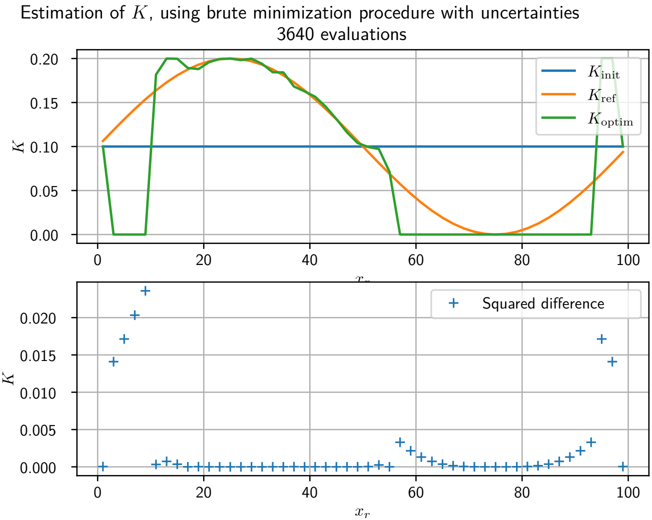
$$W(K) \quad \text{becomes} \quad W(\boldsymbol{x}_e, K)$$

We have $Y = \mathcal{H}W(\boldsymbol{x}_{e,\mathrm{ref}}, K_{\mathrm{ref}})$
The (deterministic) quadratic error is now

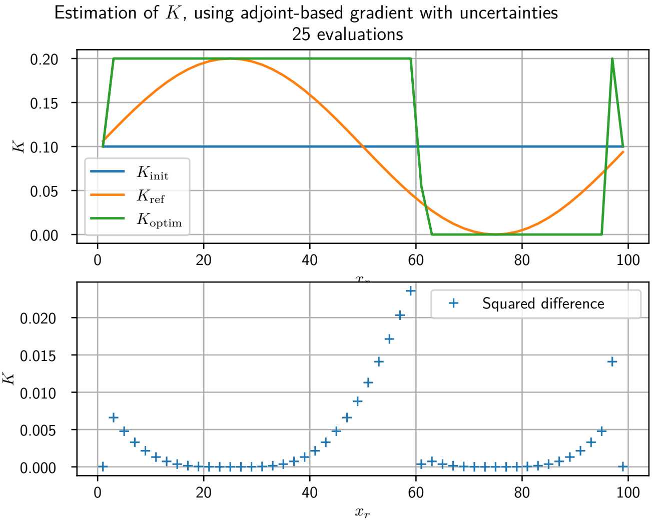
$$j(\boldsymbol{x}_e, K) = \frac{1}{2}\|\mathcal{H}W(\boldsymbol{x}_e, K) - Y\|^2$$

$\longrightarrow$ sample one $\boldsymbol{x}_e$ and min w.r.t. K ?

Estimation procedure with uncertainties no gradient



Estimation procedure with uncertainties adjoint-based gradient



Influence of $\boldsymbol{X}_e$?
Minimizing $j(\boldsymbol{x}_e, K)$ wrt K ?
Computational cost ?

Influence of $\boldsymbol{X}_e$?	$\longrightarrow$ Sensitivity analysis
Minimizing $j(\boldsymbol{x}_e, K)$ wrt K ?	$\longrightarrow$ Robust optimization
Computational cost ?	$\longrightarrow$ Use of surrogate

Sensitivity Analysis

Sobol Indices [Sobol, 2001]

Let $\mathcal{J} = J(\boldsymbol{X})$ a rv, with $\boldsymbol{X} = (X_1, \dots X_p)$ uniformly distributed on $[0;1]^p$ and components independent.

$$\mathbb{E}[\mathcal{J}|X_i = \alpha]$$

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$$S_i = \frac{\mathbb{V}\mathrm{ar}[\mathbb{E}[\mathcal{J}|X_i]]}{\mathbb{V}\mathrm{ar}[\mathcal{J}]}$$

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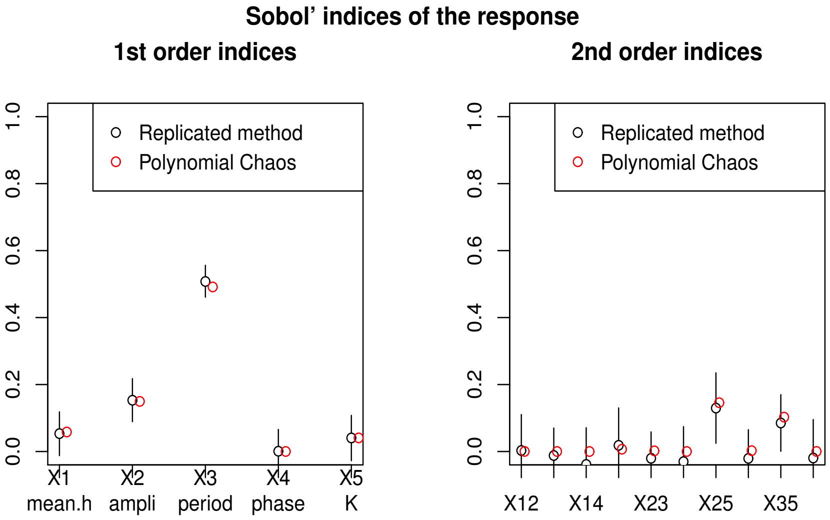
Variance of the ANOVA decomposition

$$1 = \underbrace{\sum_{i=1}^{p} S_i}_{\text{Single variable influence}} + \underbrace{\sum_{1\leq i<j\leq p} S_{ij}}_{\text{Interactions order 2}} + \cdots + \underbrace{S_{1\dots p}}_{\text{Interaction order } p}$$

[Gilquin et al., 2017, Sudret, 2015]

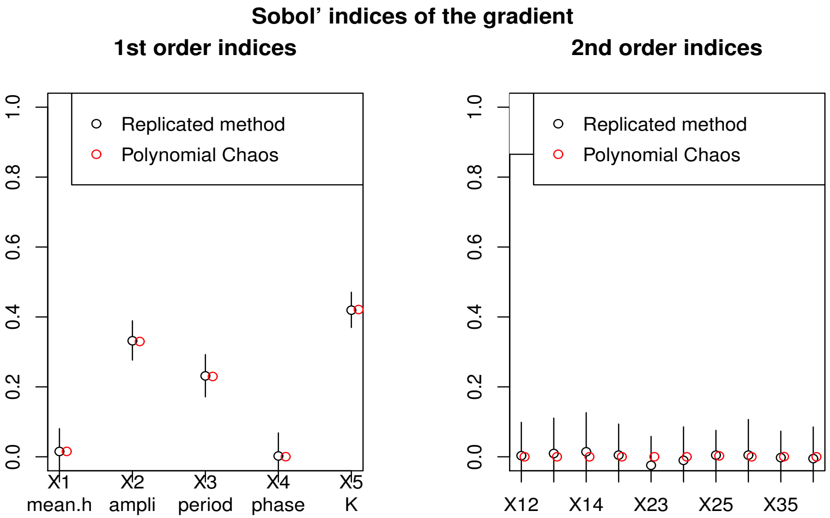
Sobol' indices of the cost function

$j(\boldsymbol{X}_e, K)$



Sobol' indices of the gradient of cost function

$\frac{\mathrm{d}j}{\mathrm{d}K}(\boldsymbol{X}_e, K)$

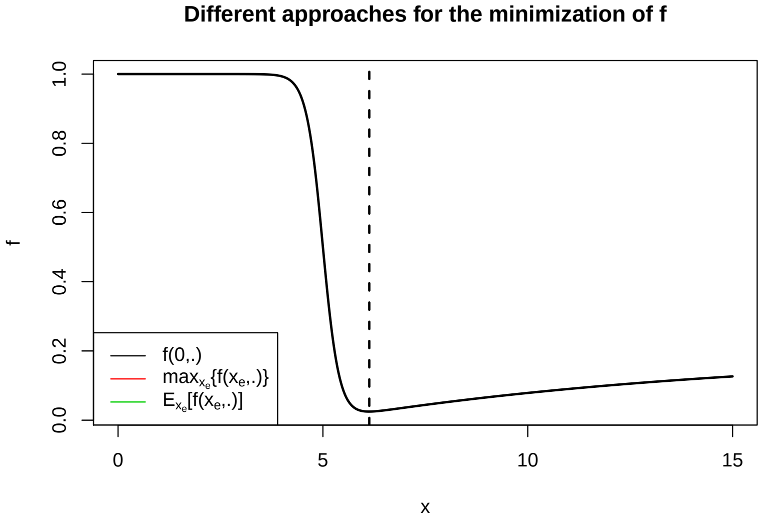


Robust Optimization

- Introduction
- Deterministic Framework
- Global sensitivity analysis
- Robust Optimization
  - Concepts of robustness
  - Metamodeling
  - Adaptative sampling
- Conclusion

A first example

$(x_e, K) \mapsto f(x_e, K) = \tilde{f}(x_e + K)$ and $X_e \sim \mathcal{N}(0, s^2)$ truncated on $[-3; 3]$



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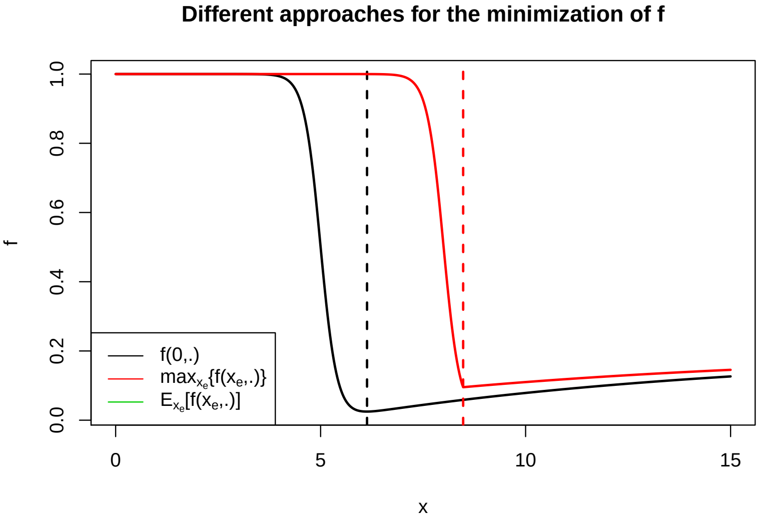

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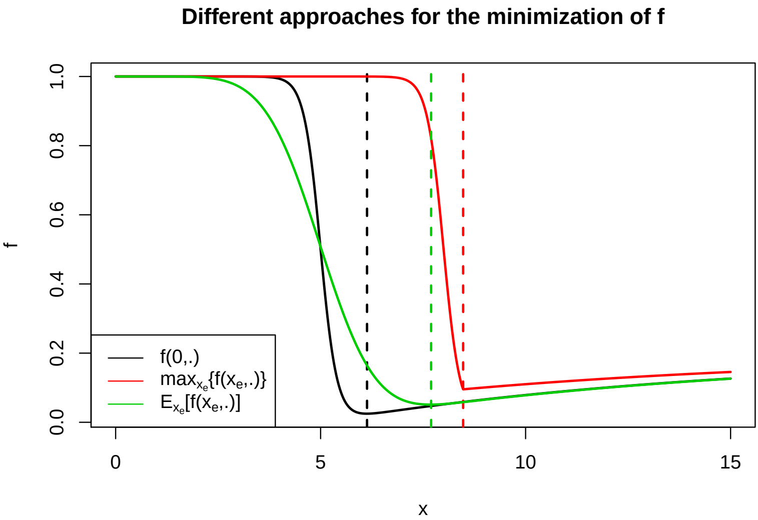

Different Notions of robustness

- Global Optimum: $\min j(\boldsymbol{x}_e, K) \longrightarrow$ EGO

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- Multiobjective: choice within Pareto frontier $\longrightarrow$ 1L/2L kriging

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Why surrogates ?

- Model $\longrightarrow$ expensive to run
- High dimensional problem + taking into account uncertainties ?

Environmental variables

$\boldsymbol{X}_e$ random

Control variable

$K \in \mathcal{K}$

Computer Code

$W(\boldsymbol{x}_e, K) \longrightarrow j(\boldsymbol{x}_e, K)$

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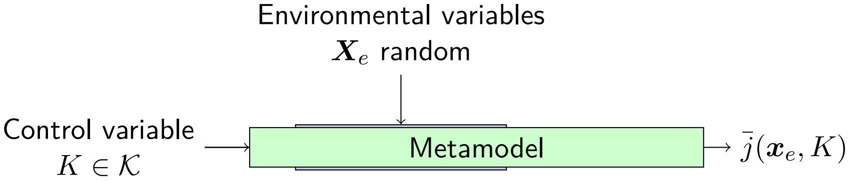

Comparison between PCE and Kriging

	Polynomial Chaos	Kriging
Surrogate	$J(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \hat{J}_{\boldsymbol{\alpha}} \boldsymbol{\Phi}_{\boldsymbol{\alpha}}(\boldsymbol{X})$	$\bar{J}(\boldsymbol{x}) \sim \mathcal{N}(\hat{m}(\boldsymbol{x}), \hat{s}^2(\boldsymbol{x}))$
Estim.	Numerical quadrature/Regression	Regression
Quantity	Statistical moments	estimate + CI
Ref.	[Wiener, 1938, Sudret, 2015]	[Krige, 1951, Matheron, 1969]

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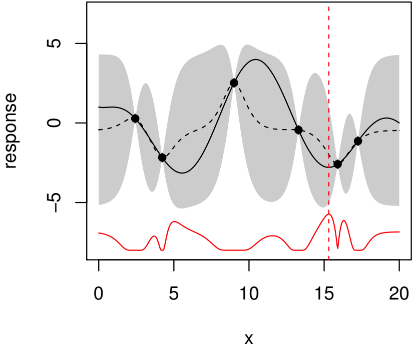
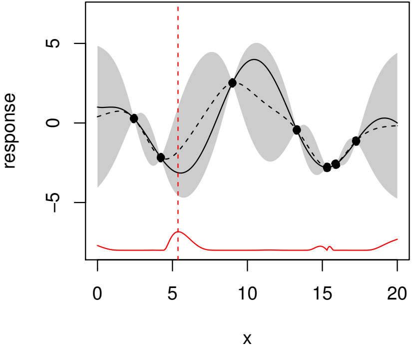
Principle of adaptative sampling

Based on kriging model $\longrightarrow$ mean and variance
How to choose a new point to evaluate ? Criterion $\kappa(\boldsymbol{x}) \longrightarrow$ "potential" of the point

$$\boldsymbol{x}_{\text{new}} = \arg\max \kappa(\boldsymbol{x})$$





EGO [Jones et al., 1998]

Global Optimum

$\mathcal{P}_N$ experimental design on $\mathbb{X} \times \mathcal{K}$, $\mathcal{Y}_N = j(\mathcal{P}_N)$.

$$\bar{J}_N(\boldsymbol{x}_e, K) \sim \mathcal{N}\left(\hat{m}_N(\boldsymbol{x}_e, K), \hat{s}_N^2(\boldsymbol{x}_e, K)\right)$$

EGO [Jones et al., 1998]

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$$j_{\min}^N = \min \mathcal{Y}_N$$

Expected improvement

$$j_{\min}^N - \bar{J}_N(\boldsymbol{x}_e, K)$$

EGO [Jones et al., 1998]

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Expected improvement

$$\max\{0, j_{\min}^N - \bar{J}_N(\boldsymbol{x}_e, K)\}$$

EGO [Jones et al., 1998]
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Expected improvement

$$EI(\boldsymbol{x}_e, K) = \mathbb{E}[\max\{0, j_{\min}^N - \bar{J}_N(\boldsymbol{x}_e, K)\}]$$

EGO [Jones et al., 1998]

Global Optimum

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Expected improvement

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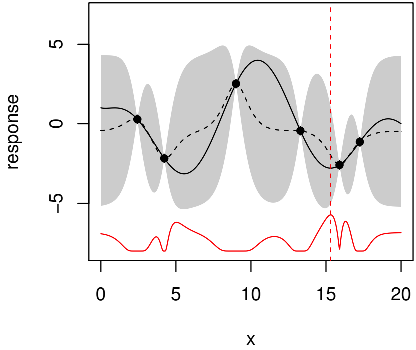
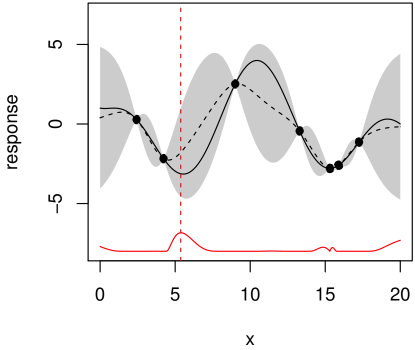
EGO iteration

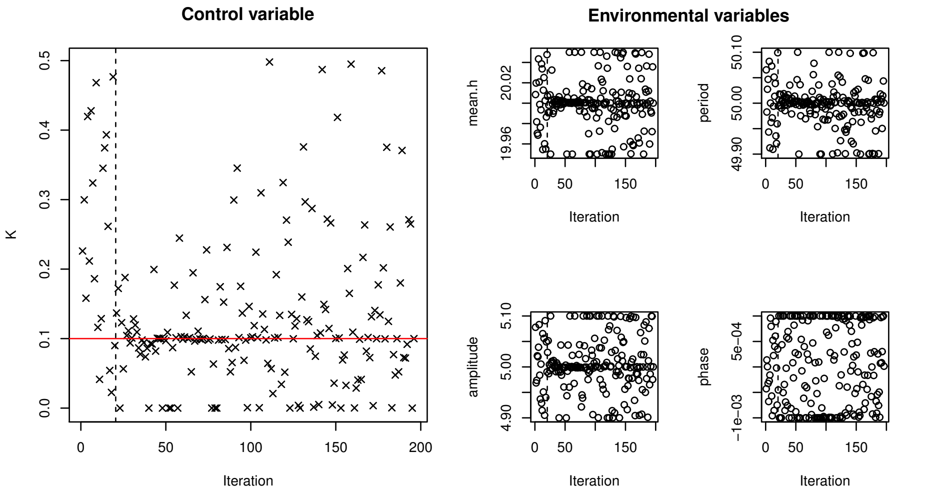
$$\begin{aligned} (\tilde{\boldsymbol{x}}_e, \tilde{K}) &= \arg\max EI(\boldsymbol{x}_e, K) \\ \mathcal{P}_{N+1} &= \mathcal{P}_N \cup (\tilde{\boldsymbol{x}}_e, \tilde{K}) \\ \bar{J}_{N+1}(\boldsymbol{x}_e, K) &\sim \mathcal{N}\left(\hat{m}_{N+1}(\boldsymbol{x}_e, K), \hat{s}_{N+1}^2(\boldsymbol{x}_e, K)\right) \end{aligned}$$

Example of an EGO iteration





EGO


Control variable
Environmental variables
K
0.0
0.1
0.2
0.3
0.4
0.5
0
50
100
150
200
Iteration
mean.h
19.96
20.02
period
49.90
50.00
50.10
amplitude
4.90
5.00
5.10
phase
−1e−03
5e−04
0
50
150
Iteration

Explorative EGO [Lehman et al., 2004]

Worst-case scenario

$\mathcal{P}_N$ experimental design on $\mathbb{X} \times \mathcal{K}$, $\mathcal{Y}_N = j(\mathcal{P}_N)$.

$$\bar{J}_N(\boldsymbol{x}_e, K) \sim \mathcal{N}\left(\hat{m}_N(\boldsymbol{x}_e, K), \hat{s}_N^2(\boldsymbol{x}_e, K)\right)$$

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Expected improvement

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Explorative EGO iteration

$$\begin{aligned}
(\tilde{\boldsymbol{x}}_e, \tilde{K}) &= \arg\max EI(\boldsymbol{x}_e, K) \\
\boldsymbol{x}_e^* &= \arg\max_{\boldsymbol{x}_e} d\left((\boldsymbol{x}_e, \tilde{K}), \mathcal{P}_N\right) \\
\mathcal{P}_{N+1} &= \mathcal{P}_N \cup (\boldsymbol{x}_e^*, \tilde{K}) \\
\bar{J}_{N+1}(\boldsymbol{x}_e, K) &\sim \mathcal{N}\left(\hat{m}_{N+1}(\boldsymbol{x}_e, K), \hat{s}_{N+1}^2(\boldsymbol{x}_e, K)\right)
\end{aligned}$$

Explorative EGO [Lehman et al., 2004]

Worst-case scenario

$\mathcal{P}_N$ experimental design on $\mathbb{X} \times \mathcal{K}$, $\mathcal{Y}_N = j(\mathcal{P}_N)$.

$$\bar{J}_N(\boldsymbol{x}_e, K) \sim \mathcal{N}\left(\hat{m}_N(\boldsymbol{x}_e, K), \hat{s}^2_N(\boldsymbol{x}_e, K)\right)$$

$j^N_{\min} = \min \mathcal{Y}_N$

Expected improvement

$$EI(\boldsymbol{x}_e, K) = \mathbb{E}[\max\{0, j^N_{\min} - \bar{J}_N(\boldsymbol{x}_e, K)\}]$$

Explorative EGO iteration

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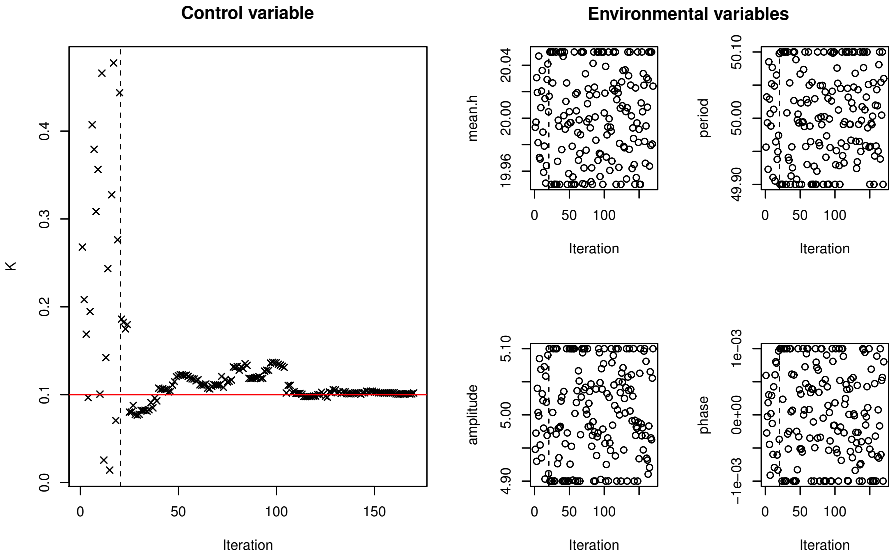
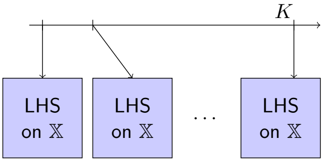
$$\boldsymbol{x}^*_e = \arg\max_{\boldsymbol{x}_e} d\left((\boldsymbol{x}_e, \tilde{K}), \mathcal{P}_N\right)$$
$$\mathcal{P}_{N+1} = \mathcal{P}_N \cup (\boldsymbol{x}^*_e, \tilde{K})$$
$$\bar{J}_{N+1}(\boldsymbol{x}_e, K) \sim \mathcal{N}\left(\hat{m}_{N+1}(\boldsymbol{x}_e, K), \hat{s}^2_{N+1}(\boldsymbol{x}_e, K)\right)$$

Explorative EGO iterations [Lehman et al., 2004]



Iterated LHS

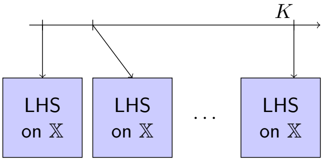
M-robustness



to build $\hat{\mu}(K)$ and $\hat{\sigma}^2(K)$

Iterated LHS

M-robustness



to build $\hat{\mu}(K)$ and $\hat{\sigma}^2(K)$

Estimate of the mean

$$\mathbb{E}[J(\boldsymbol{X}_e, K)|K] \xrightarrow{\text{estimator}} \hat{\mu}(K) = n_e^{-1} \sum_{i=1}^{n_e} J(\boldsymbol{X}_e^i, K) \text{ (r.v.)}$$

$$\mathbb{V}\mathrm{ar}[J(\boldsymbol{X}_e, K)|K] \xrightarrow{\text{estimator}} \hat{\sigma}^2(K) = (n_e - 1)^{-1} \sum_{i=1}^{n_e} (J(\boldsymbol{X}_e^i, K) - \hat{\mu}(K))^2 \text{ (r.v.)}$$

$$\mathbb{E}[\hat{\mu}(K)] = \mathbb{E}[J(\boldsymbol{X}_e, K)|K] \quad \text{and} \quad \mathbb{V}\mathrm{ar}[\hat{\mu}(K)] = \frac{\mathbb{V}\mathrm{ar}[J(\boldsymbol{X}_e, K)|K]}{n_e} \approx \frac{\hat{\sigma}^2(K)}{n_e}$$

Estimated mean as a random variable

$$\hat{\mu}(K) \sim \mathcal{N}\left(\mathbb{E}[J(\boldsymbol{X}_e, K)|K], \frac{\hat{\sigma}^2(K)}{n_e}\right) \qquad \text{(CLT approximation)}$$

Idea [Rullière et al., 2013] :

- Add a new point K_{new} and estimate $\mathbb{E}[J(\boldsymbol{X}_e, K)|K = K_{\mathrm{new}}]$
- OR Reduce the variance by increasing n_e

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- OR Reduce the variance by increasing n_e

In an adaptative sampling strategy: $K^* = \arg\max_{K \in \mathcal{K}} \kappa(K)$

- if K^* "close" to an existing point $\longrightarrow$ increase n_e
- if not $\longrightarrow$ add K^* to the design

Knowledge-gradient criterion

Metamodel of the *estimated* mean:

Based on $\mathcal{P}_N$, an experimental design of N points on $\mathcal{K}$.

$$\bar{\mu}_N(K) \sim \mathcal{N}\left(\hat{m}_N(K), \hat{s}_N^2(K)\right)$$

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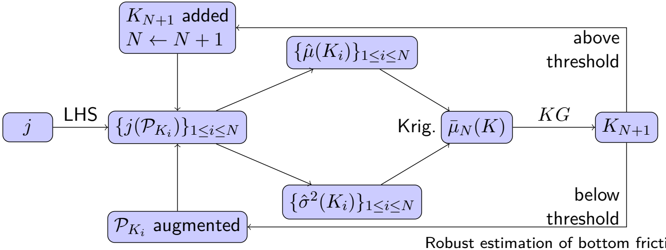
In the presence of noise in the kriging model:

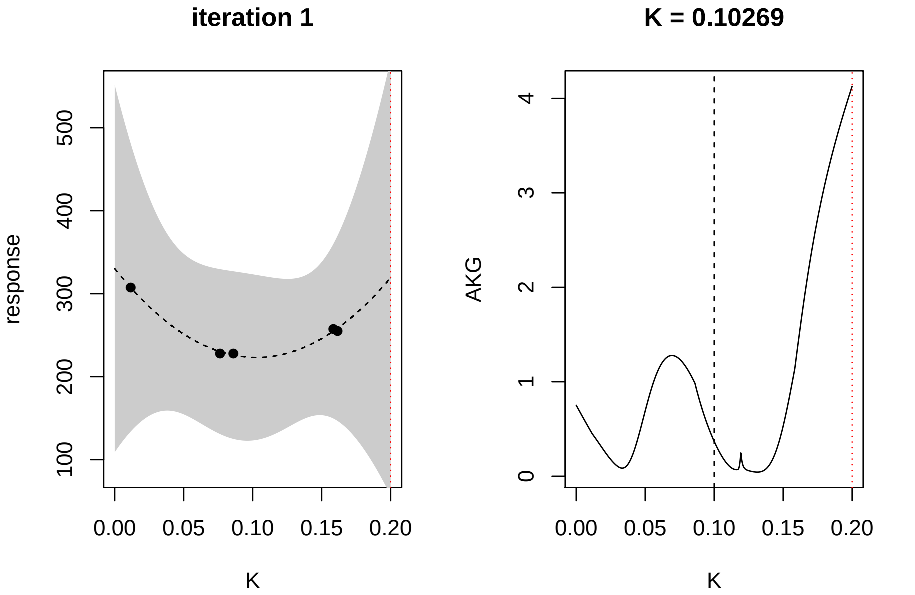
Definition of the KG [Frazier et al., 2008]

$$KG(\tilde{K}) = \min_{K' \in \mathcal{K}} \hat{m}_N(K') - \mathbb{E}\left[\min_{K' \in \mathcal{K}} \hat{m}_{N+1}(K') \middle| \tilde{K}\right]$$

where $\hat{m}_{N+1}$ is the kriging mean computed based on $\mathcal{P}_N \cup \{\tilde{K}\}$



Iterated LHS



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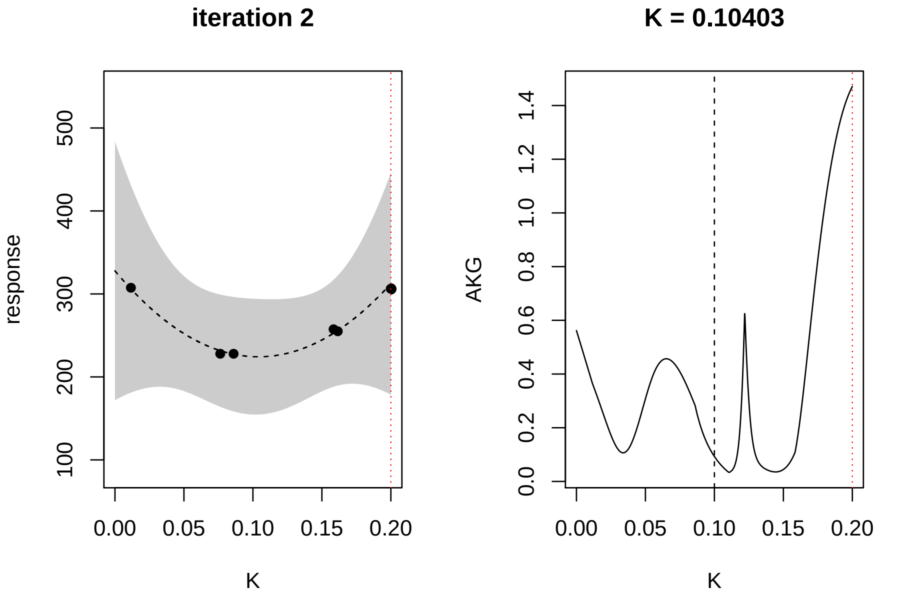

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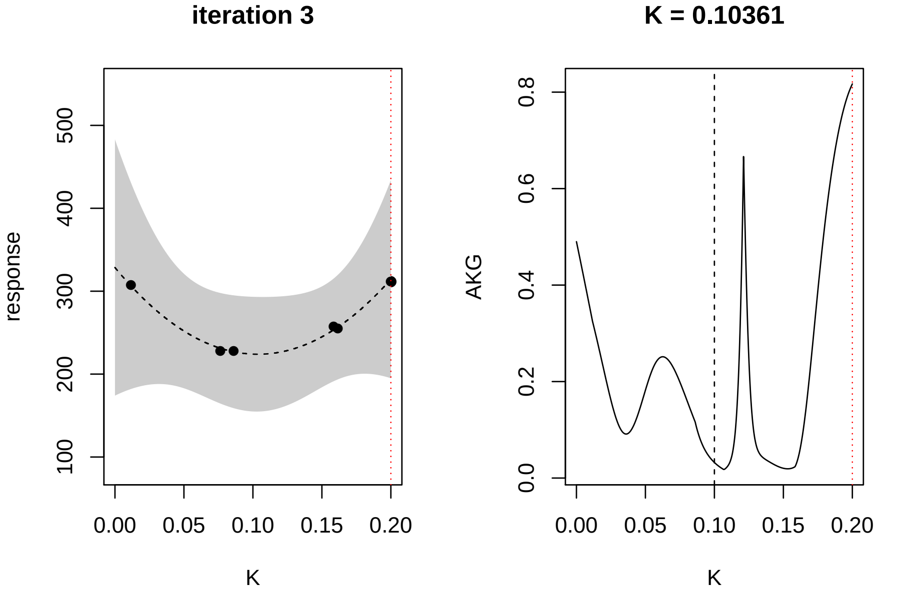

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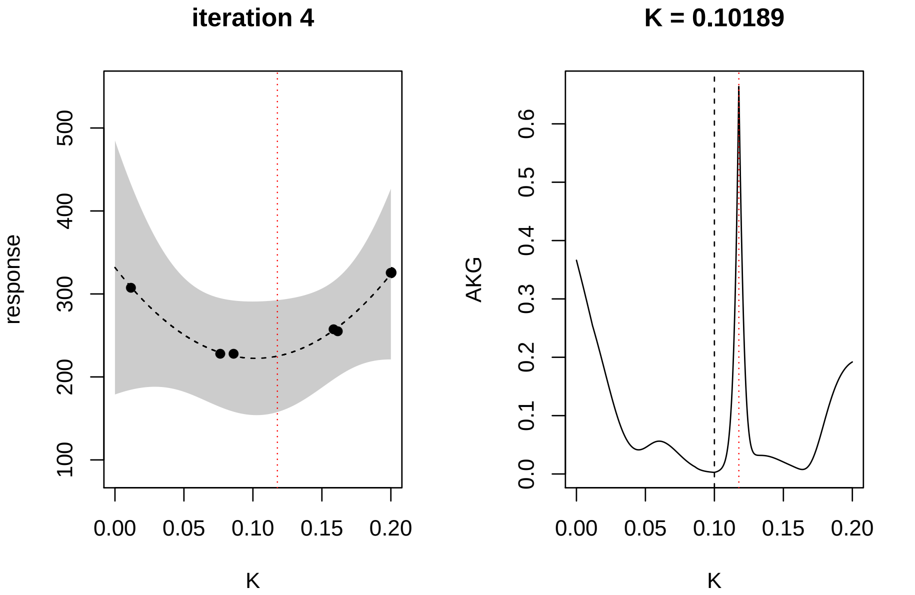
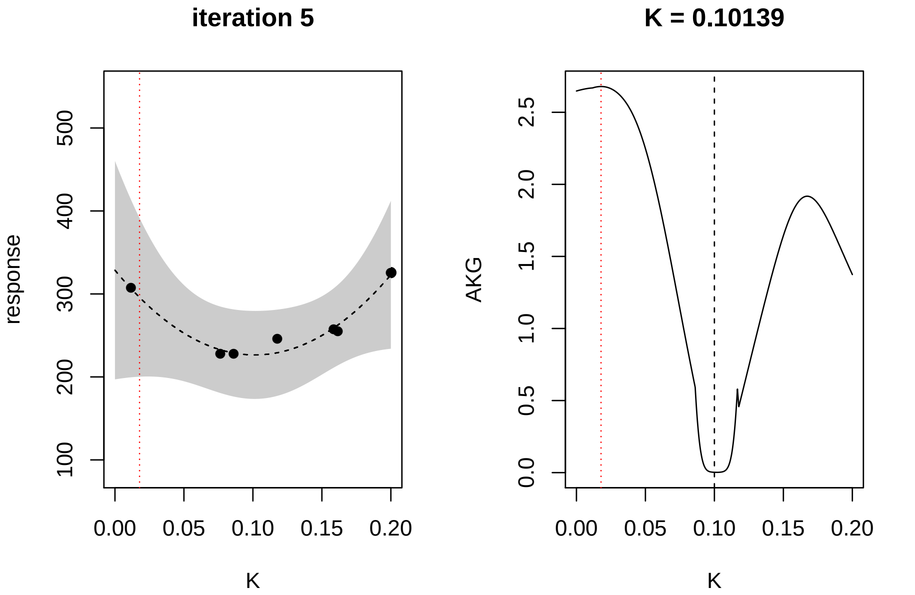
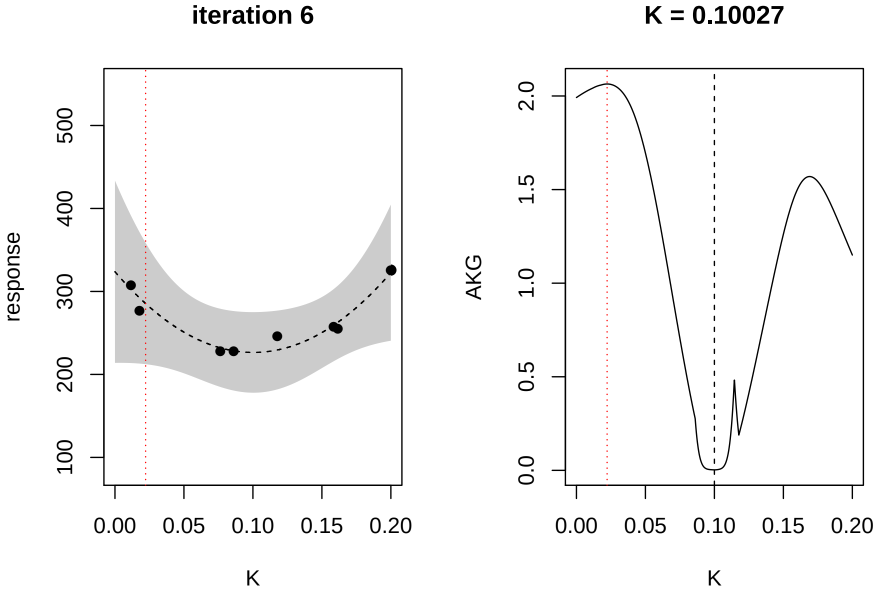


Iterated LHS



Iterated LHS



Wrapping up

- Notion of robustness
- Metamodelling techniques $\rightarrow$ include uncertainties
- Balance between precision and number of runs

Perspective and future work

- Better numerical model
  - 2D
  - Better numerical scheme
- Influence of observation operator $\mathcal{H}$
  - Y as real measurements
- Extension to K multidimensional
- Choice of metamodel:
  - Kriging
    - not adapted to high-dimensional input space
    - Adaptative sampling in multidimensional case?
  - PC
    - adapted to K multidimensional
    - "Fixed" grid to evaluate
    - May need more evaluation in some cases + adjoint

Thank you for your attention

- Introduction
  - AIRSEA team
  - Context and scope of the project
- Deterministic Framework
  - The 1D Shallow Water Equations
  - Adjoint-based optimization
- Global sensitivity analysis
  - Definition
  - SA of different outputs of the model
- Robust Optimization
  - Concepts of robustness
  - Metamodeling
  - Adaptative sampling
- Conclusion

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Principle of the adjoint method

Let us assume that we have the (formal) model

$$J(W(K), K) \qquad \text{(Cost function)}$$

$$\text{s.t. } R(W(K), K) = 0 \qquad \text{(Model equation (SWE))}$$

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$$\frac{\mathrm{d}J}{\mathrm{d}K} = \frac{\partial J}{\partial W}\frac{\partial W}{\partial K} + \frac{\partial J}{\partial K} \tag{2}$$

$$\frac{\mathrm{d}R}{\mathrm{d}K} = \frac{\partial R}{\partial W}\frac{\partial W}{\partial K} + \frac{\partial R}{\partial K} = 0 \tag{3}$$

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And by introducing a Lagrange multiplier λ

Principle of the adjoint method

$$\frac{\mathrm{d}J}{\mathrm{d}K} = \frac{\partial J}{\partial W}\frac{\partial W}{\partial K} + \frac{\partial J}{\partial K} - \lambda^T \left(\frac{\partial R}{\partial W}\frac{\partial W}{\partial K} + \frac{\partial R}{\partial K} \right) \tag{4}$$

$$= \underbrace{\left(\frac{\partial J}{\partial W} - \lambda^T \frac{\partial R}{\partial W} \right)}_{=0 \text{ if } \lambda \text{ is choosen wisely}} \frac{\partial W}{\partial K} + \left(\frac{\partial J}{\partial K} - \lambda^T \frac{\partial R}{\partial K} \right) \tag{5}$$

Adjoint model

$$\left(\frac{\partial R}{\partial W} \right)^T \lambda = \left(\frac{\partial J}{\partial W} \right)^T \tag{6}$$

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For a value K:

- solve $R(W(K), K) = 0$ for W
- solve $\left(\frac{\partial R}{\partial W}\right)^T \lambda = \left(\frac{\partial J}{\partial W}\right)^T$ for λ
- compute $\frac{\mathrm{d}J}{\mathrm{d}K}$

Orthogonal Polynomials in a Hilbert space

X, $J(X)$ r.v., such that $\mathbb{E}[X^2], \mathbb{E}[J(X)^2] < +\infty$
$\rightarrow$ Expand J on a basis of orthogonal polynomials with respect to a specific inner product [Wiener, 1938, Sudret, 2015].

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$\rightarrow$ Expand J on a basis of orthogonal polynomials with respect to a specific inner product [Wiener, 1938, Sudret, 2015].
Functional inner product:

$$\langle f, g \rangle = \int_{D_X} f(\xi) g(\xi) p_X(\xi) \, \mathrm{d}\xi$$

Family of orthogonal polynomials

$$\langle \varphi_i, \varphi_j \rangle = \|\varphi_i\|^2 \delta_{ij}$$

Family	D_X	p.d.f.	Distribution
Legendre	$[-1;1]$	$p_X(\xi) = {}^1\!/_2$	$\mathcal{U}([-1;1])$
Hermite	$\mathbb{R}$	$p_X(\xi) = e^{-\xi^2/2}$	$\mathcal{N}(0,1)$
Laguerre	$[0, +\infty[$	$p_X(\xi) = e^{-\xi}$	Exp

The expansion as a surrogate model

Polynomial Chaos Expansion, 1D

$$\mathcal{J} = J(X) = \sum_{i=0}^{+\infty} \hat{J}_i \varphi_i(X) \approx \sum_{i=0}^{P} \hat{J}_i \varphi_i(X)$$

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$$\boldsymbol{\alpha} = (\alpha_1, \dots \alpha_p), \quad |\boldsymbol{\alpha}| = \sum_i \alpha_i$$

$$\Phi_{\boldsymbol{\alpha}}(\boldsymbol{X}) = \prod_i \varphi_{\alpha_i}(X_i)$$

Polynomial Chaos Expansion, multidimensional

$$\mathcal{J} = J(\boldsymbol{X}) = \sum_{|\boldsymbol{\alpha}|=0}^{+\infty} \hat{J}_{\boldsymbol{\alpha}} \Phi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \approx \sum_{|\boldsymbol{\alpha}| \leq P} \hat{J}_{\boldsymbol{\alpha}} \Phi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

Statistical moments using PCE

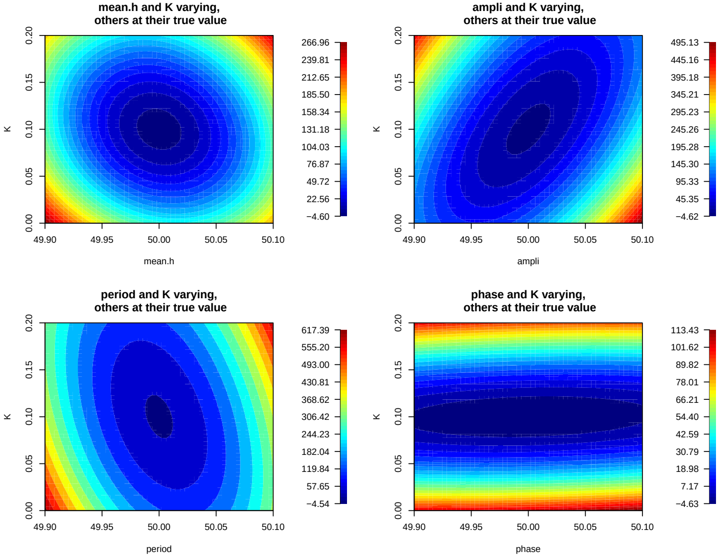
PCE allows us to get easily the statistical moments:

Mean and variance of $\mathcal{J}$ using the coefficients of the expansion

$$\mathbb{E}[\mathcal{J}] = \hat{J}_0 \|\boldsymbol{\Phi}_0\|^2 = \hat{J}_0$$

$$\mathbb{V}\mathrm{ar}[\mathcal{J}] = \mathbb{E}[\mathcal{J}^2] - \mathbb{E}[\mathcal{J}]^2 = \sum_{|\boldsymbol{\alpha}| \leq P} \hat{J}_{\boldsymbol{\alpha}}^2 \|\boldsymbol{\Phi}_{\boldsymbol{\alpha}}\|^2 - \hat{J}_0^2 = \sum_{0 < |\boldsymbol{\alpha}| \leq P} \hat{J}_{\boldsymbol{\alpha}}^2 \|\boldsymbol{\Phi}_{\boldsymbol{\alpha}}\|^2$$

PCE on the response



Principle of Kriging

$\mathcal{X} = \{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n_s)}\}$ and $\mathcal{Y} = j(\mathcal{X})$
We assume that the deterministic model $j(\boldsymbol{x})$ is the realization of a GP [Krige, 1951, Matheron, 1969]:

Kriging formalism

$$\underbrace{J(\boldsymbol{x})}_{\text{r.v.}} = \underbrace{\boldsymbol{f}(\boldsymbol{x})^T\boldsymbol{\beta}}_{\text{deter}} + \underbrace{\varepsilon(\boldsymbol{x})}_{\text{r.v.}}$$

$$\mathbb{E}[\varepsilon(\boldsymbol{x})] = 0 \quad \text{and} \quad \mathrm{Cov}(\varepsilon(\boldsymbol{x}), \varepsilon(\boldsymbol{x'})) = \sigma_J^2 \underbrace{R(\boldsymbol{x}, \boldsymbol{x'})}_{\text{Chosen}}$$

$$\bar{J}(\boldsymbol{x}) \sim J(\boldsymbol{x})|\mathcal{Y}$$

Kriging predicator

$$\boldsymbol{F} = \{f_j(\boldsymbol{x}^{(i)})\}_{\substack{1\le i\le n_s\\ 1\le j\le n_\beta}}$$

$$\boldsymbol{R} = \{R(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)})\}_{1\le i,j\le n_s}$$

$$\boldsymbol{r}(\boldsymbol{x}) = \left[R(\boldsymbol{x}^{(1)}, \boldsymbol{x}), \dots, R(\boldsymbol{x}^{(n_s)}, \boldsymbol{x})\right]^T$$

Joint distribution of $\mathcal{Y}$ and J

$$\begin{bmatrix} \mathcal{Y} \\ J(\boldsymbol{x}) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{F}\hat{\boldsymbol{\beta}} \\ \boldsymbol{f}(\boldsymbol{x})^T\hat{\boldsymbol{\beta}} \end{bmatrix}, \sigma_J^2 \begin{bmatrix} \boldsymbol{R} & \boldsymbol{r}(\boldsymbol{x}) \\ \boldsymbol{r}(\boldsymbol{x})^T & 1 \end{bmatrix} \right)$$

Kriging predicator $\bar{J}$

$$\begin{aligned} \bar{J}(\boldsymbol{x}) &\sim J(\boldsymbol{x})|\mathcal{Y} \\ &\sim \mathcal{N}(\hat{m}_J(\boldsymbol{x}), \hat{s}_J^2(\boldsymbol{x})) \end{aligned}$$

Kriging predicator

$$
\begin{aligned}
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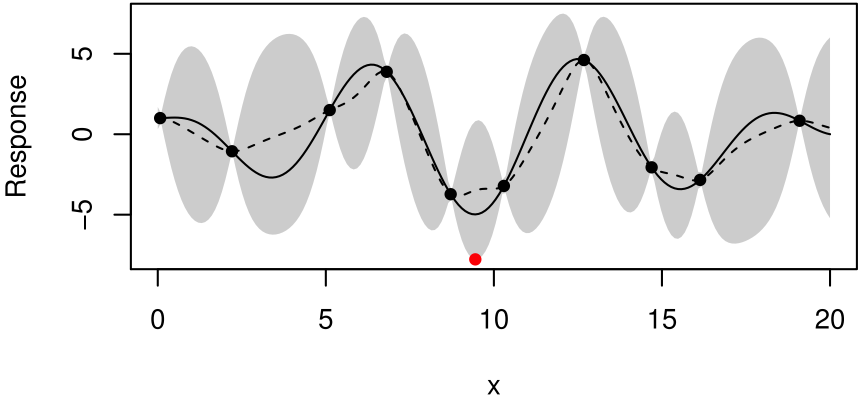
Example of kriging



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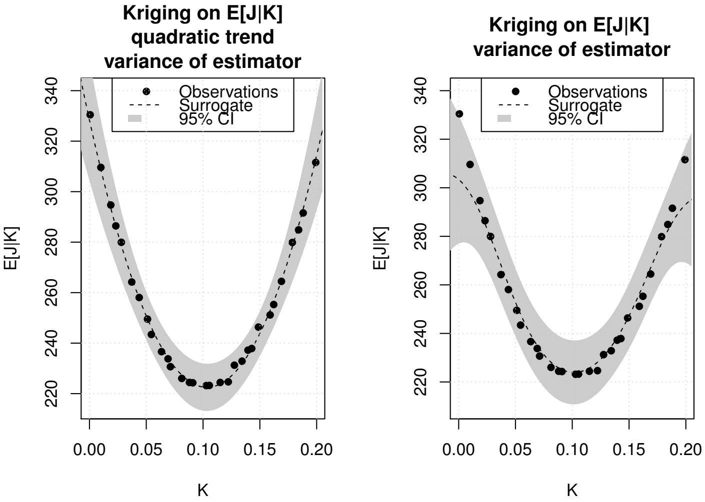

Figure : Kriging with and without trend of the estimate mean. Variance of observations based on the variance of the estimate

Multi-objective problem: general vocabulary

Vector of objective functions $\boldsymbol{f} = (f_1, \ldots, f_r)$:

Pareto domination relation

$$\boldsymbol{f}(\boldsymbol{x}) \prec \boldsymbol{f}(\boldsymbol{x}') \text{ if } \begin{cases} f_j(\boldsymbol{x}) \leq f_j(\boldsymbol{x}') & \forall j \leq r \\ f_j(\boldsymbol{x}) < f_j(\boldsymbol{x}') & \text{for one } j \leq r \end{cases}$$

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Pareto set, front

Pareto set:

$$\mathfrak{P} = \{\boldsymbol{x} \text{ s.t. } \nexists \boldsymbol{x}', \boldsymbol{f}(\boldsymbol{x}') \prec \boldsymbol{f}(\boldsymbol{x})\}$$

Pareto front:

$$\{\boldsymbol{z} \text{ s.t. } \exists \boldsymbol{x} \in \mathfrak{P}, \boldsymbol{z} = \boldsymbol{f}(\boldsymbol{x})\}$$

Kriging to estimate the Pareto front [Dellino et al., 2012]

Minimization of the vector $(\mu(K), \sigma^2(K))$
Idea: Replace expensive computations of $(\mu(K), \sigma^2(K))$ by cheap computations of the metamodel

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- Initial design on $\mathcal{K}$, compute for each one $\hat{\mu}$ and $\hat{\sigma}^2$, and generate a surrogate

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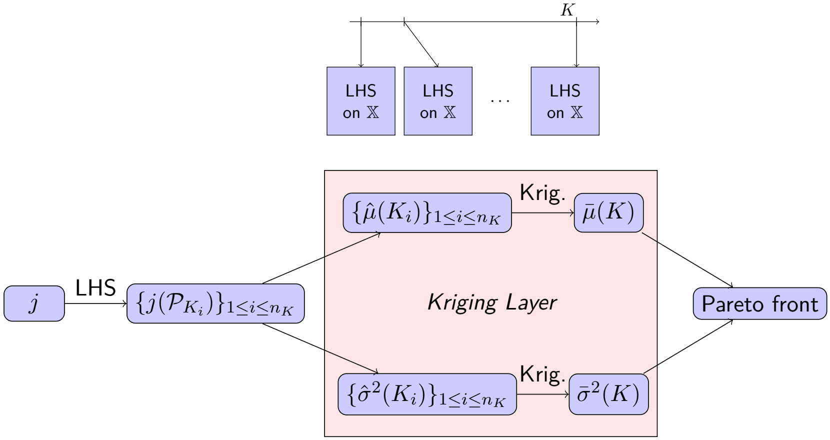
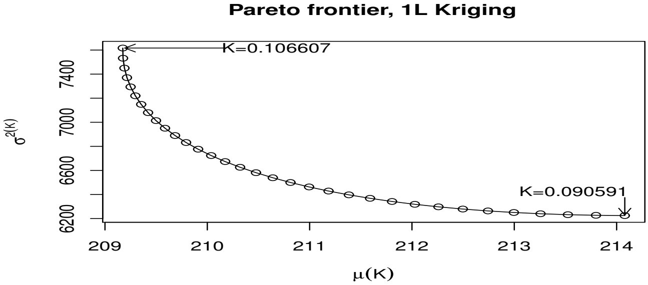
- Initial design on $\mathbb{X} \times \mathcal{K}$, and use a surrogate to estimate mean and variance

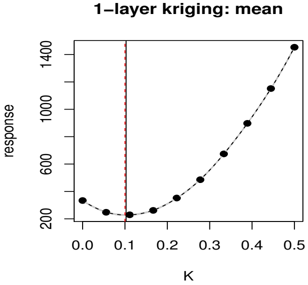
1L-Kriging

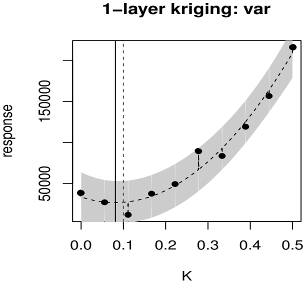


K
LHS on $\mathbb{X}$
LHS on $\mathbb{X}$
...
LHS on $\mathbb{X}$
j
LHS
$\{j(\mathcal{P}_{K_i})\}_{1\leq i\leq n_K}$
$\{\hat{\mu}(K_i)\}_{1\leq i\leq n_K}$
Krig.
$\bar{\mu}(K)$
Kriging Layer
$\{\hat{\sigma}^2(K_i)\}_{1\leq i\leq n_K}$
Krig.
$\bar{\sigma}^2(K)$
Pareto front

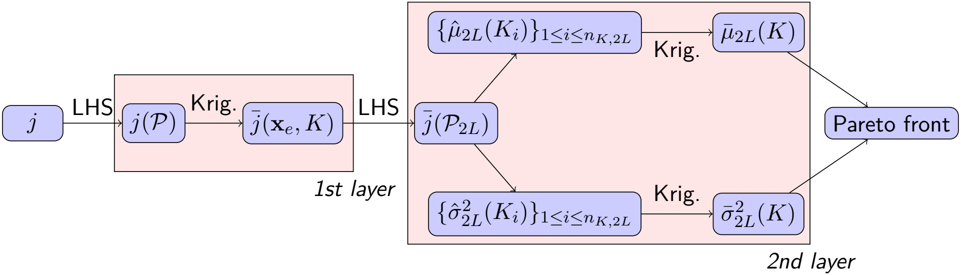
1L-Kriging


Pareto frontier, 1L Kriging
K=0.106607
K=0.090591
σ^2(K)
7400
7000
6600
6200
209
210
211
212
213
214
μ(K)

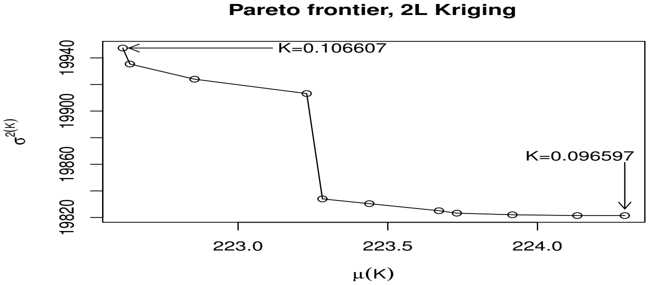

1−layer kriging: mean
response
1400
1000
600
200
0.0
0.1
0.2
0.3
0.4
0.5
K

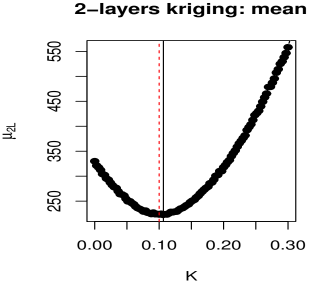

1−layer kriging: var
response
150000
50000
0.0
0.1
0.2
0.3
0.4
0.5
K

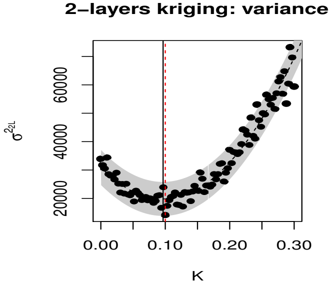
2L-Kriging


j
LHS
$j(\mathcal{P})$
Krig.
$\bar{j}(\mathbf{x}_e, K)$
1st layer
LHS
$\bar{j}(\mathcal{P}_{2L})$
$\{\hat{\mu}_{2L}(K_i)\}_{1\leq i\leq n_{K,2L}}$
Krig.
$\bar{\mu}_{2L}(K)$
$\{\hat{\sigma}^2_{2L}(K_i)\}_{1\leq i\leq n_{K,2L}}$
Krig.
$\bar{\sigma}^2_{2L}(K)$
Pareto front
2nd layer

2L-Kriging


Pareto frontier, 2L Kriging
K=0.106607
K=0.096597
19940
19900
19860
19820
223.0
223.5
224.0
$\mu(K)$
$\sigma^{2}(K)$


2−layers kriging: mean
550
450
350
250
0.00
0.10
0.20
0.30
K
μ_{2L}


2−layers kriging: variance
60000
40000
20000
0.00
0.10
0.20
0.30
K
σ^{2}_{2L}

Steepest descent using PCE [Miranda et al., 2016]

For a given K, expansion of $J(\boldsymbol{X}_e, K)$ and $\frac{\partial J}{\partial K}(\boldsymbol{X}_e, K)$

$$J(\boldsymbol{X}_e, K) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} \hat{J}_{\boldsymbol{\alpha}}(K) \Phi_{\boldsymbol{\alpha}}(\boldsymbol{X}_e) \quad \text{and} \quad \frac{\partial J}{\partial K}(\boldsymbol{X}_e, K) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} \hat{G}_{\boldsymbol{\alpha}}(K) \Phi_{\boldsymbol{\alpha}}(\boldsymbol{X}_e)$$

Relation between $\hat{J}_{\boldsymbol{\alpha}}(K)$ and $\hat{G}_{\boldsymbol{\alpha}}(K)$

$$\Rightarrow \frac{\mathrm{d}\hat{J}_{\boldsymbol{\alpha}}}{\mathrm{d}K}(K) = \hat{G}_{\boldsymbol{\alpha}}(K), \quad \forall \boldsymbol{\alpha} \in \mathcal{A}$$

Steepest descent using PCE [Miranda et al., 2016]

Recalling that

$$\hat{\sigma}_J^2(K) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} \hat{J}_{\boldsymbol{\alpha}}(K)^2 \|\Phi_{\boldsymbol{\alpha}}\|^2$$

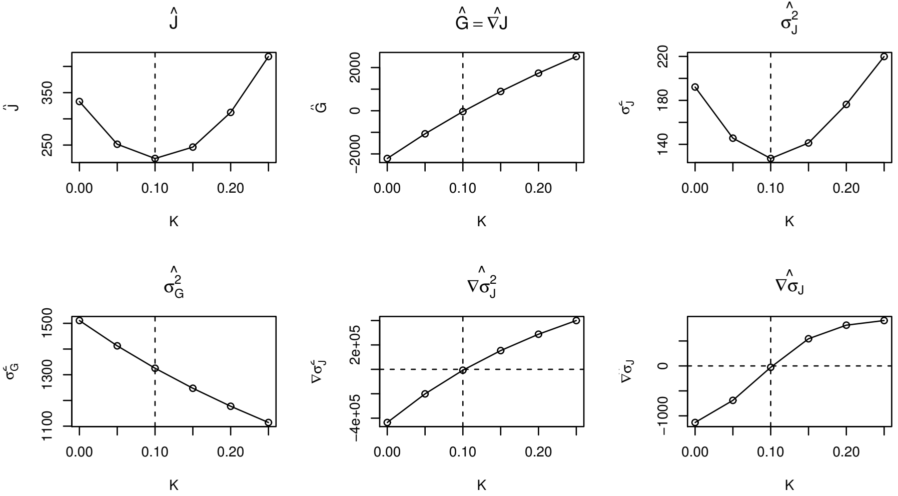
By differentiating with respect to K:

Gradient of the variance

$$\frac{\mathrm{d}\hat{\sigma}_J^2}{\mathrm{d}K}(K) = 2\sum_{\boldsymbol{\alpha}\in\mathcal{A}} \hat{J}_{\boldsymbol{\alpha}}(K)\frac{\mathrm{d}\hat{J}_{\boldsymbol{\alpha}}}{\mathrm{d}K}(K)\|\Phi_{\boldsymbol{\alpha}}\|^2 = 2\sum_{\boldsymbol{\alpha}\in\mathcal{A}} \hat{J}_{\boldsymbol{\alpha}}(K)\hat{G}_{\boldsymbol{\alpha}}(K)\|\Phi_{\boldsymbol{\alpha}}\|^2$$

We have the gradient of the mean $\hat{G}_0$ and the gradient of the variance
$\Rightarrow$ Gradient descent algorithm.

Expansion for different K



Gradient descent algorithm on ρ

$$\rho(K,\lambda) = \lambda\mu(K) + (1-\lambda)\sigma(K)$$