Sensitivity maps of complex systems with a functional output

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Part I

Introduction

Aim

Let us consider a *time-consuming* simulator.
Assume that the output is a *function* of z = time, space, etc.

Goals

- To **compute *fastly* a sensitivity map (SM)**, which contains the influence of input variables on the output *for all values of* z
- To **account for *estimation* error**
- To **account for *(meta)modeling* error**
  $\rightarrow$ *approximation error of the model, assumed to be well-specified*

A motivating example

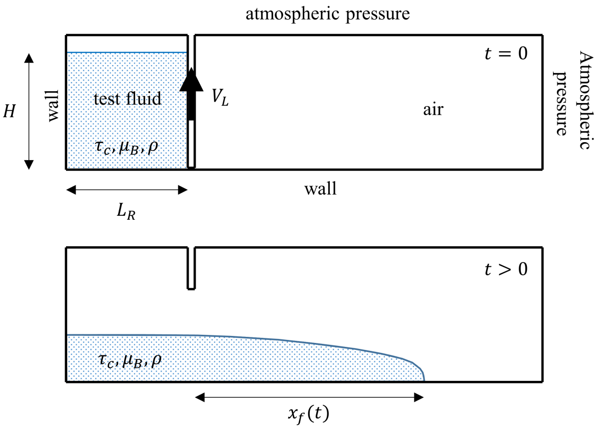

Figure: Schematic of the idealized gradual dam-break case with boundary conditions and input variables.

Sensitivity maps, with estimation error

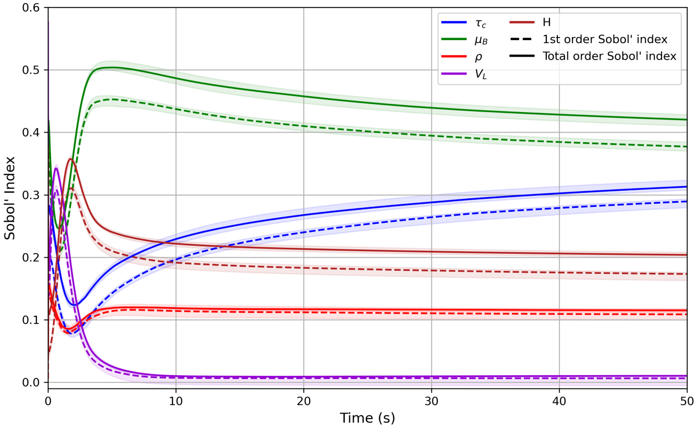

Figure: Total and first-order SMs of all input variables.

Sensitivity maps, with estimation error

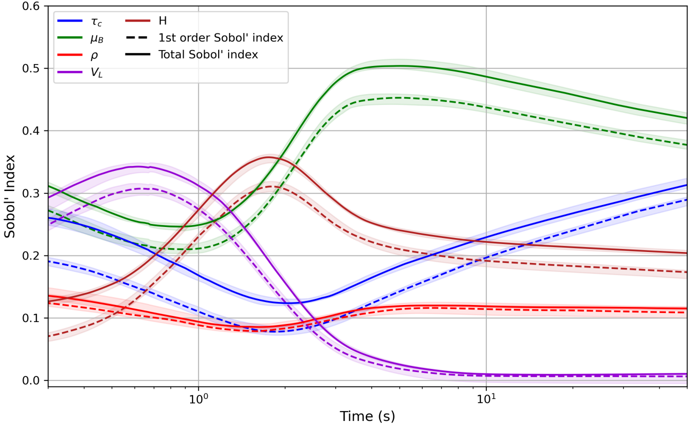

Figure: Total and first-order SMs of all input variables.

Sensitivity maps, with estimation + metamodel error

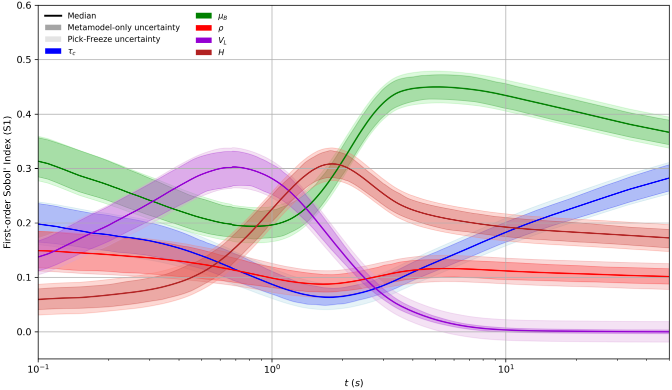

Figure: First-order SMs of all input variables.

Sensitivity maps, with estimation + metamodel error

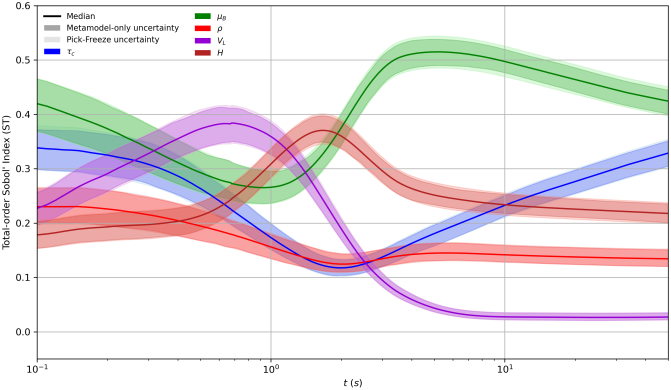

Figure: Total SMs of all input variables.

Part II

Computation of sensitivity maps with basis expansions

Framework and notations

The simulator is modeled by a high-dimensional vector-valued function

$$\begin{array}{ccc} \mathbb{X} \subseteq \mathbb{R}^d & \longrightarrow & \mathbb{R}^L \\ x & \longmapsto & y(x) = (y_\ell(x))_{\ell=1,\dots,L} \end{array} \quad (1)$$

We assume that it is well approximated with a linear basis expansion (e.g. B-splines, wavelet, principal component analysis, etc.)

$$y_\ell(x) \approx \sum_{q=1}^{n_b} c_q(x) v_{q,\ell}, \qquad \ell = 1, \dots, L \quad (2)$$

The idea is to compute the sensitivity maps of $y(x)$ from the low-dimensional vector $c(x) = (c_1(x), \dots, c_{n_b}(x))$.

Variance-based sensitivity analysis (scalar-valued case)

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a function. Let $X = (X_1, \dots, X_d)$ be a random vector with independent components, and $Y = f(X)$, assumed to be square integrable.

The Sobol-Hoeffding decomposition is written

$$f(X) = \sum_{I \subseteq \{1,\dots,d\}} f_I(X_I)$$

with orthogonal terms, leading to the variance decomposition

$$\mathbb{V}\mathrm{ar}(f(X)) = \sum_{I \subseteq \{1,\dots,d\}} \mathbb{V}\mathrm{ar}(f_I(X_I))$$

Variance-based sensitivity analysis (scalar-valued case)

Denote $D = \mathbb{V}\mathrm{ar}(f(X))$ the overall variance.
We will consider the closed Sobol' indices

$$\underline{D}_I(f) = \mathbb{V}\mathrm{ar}(\mathbb{E}[f(X)|X_I]) \qquad \underline{S}_I(f) = \frac{\underline{D}_I}{D} \tag{3}$$

and the total Sobol' indices

$$\overline{D}_i(f) = \sum_{J \supseteq \{i\}} \mathbb{V}\mathrm{ar}(f_J(X)) \qquad \overline{S}_i(f) = \frac{\overline{D}_i}{D} \tag{4}$$

Example : $I = \{i\}$.

- $\underline{S}_i$ coincides with the first-order Sobol' index, measuring the ratio of variance of $f(X)$ explained only by X_i.
- $\overline{S}_i$ measures the ratio of variance explained by X_i and its interactions. We have $\overline{S}_i = 1 - \underline{S}_{-i}$ where $-i = \{1, \dots, d\} \setminus \{i\}$.

Variance-based sensitivity analysis (vector-valued case)

Let consider a vector-valued function $y : \mathbb{R}^d \to \mathbb{R}^L$. Then all 'variances' are covariance matrices, and the interpretation is more complex.

Thus, the overall covariance and *unnormalized* closed Sobol' index are

$$\mathbf{D}(y) = \mathbb{C}\mathrm{ov}(y(X)) \qquad \underline{\mathbf{D}}_I(y) = \mathbb{C}\mathrm{ov}(\mathbb{E}[y(X)|X_I])$$

A meaningful scalar sensitivity index is the *generalized sensitivity index* (GSI). The closed GSI is defined by

$$\underline{\mathrm{GSI}}_I(y) = \frac{\mathrm{Tr}\left[\mathbb{C}\mathrm{ov}(\mathbb{E}[y(X)|X_I])\right]}{\mathrm{Tr}\left[\mathbb{C}\mathrm{ov}(y(X))\right]} = \frac{\sum_{\ell=1,\dots,L} \underline{D}_I(y_\ell)}{\sum_{\ell=1,\dots,L} D(y_\ell)} \tag{5}$$

Fast computation of sensitivity maps

Assume that the basis expansion is exact:

$$y_\ell(x) = \sum_{q=1}^{n_b} c_q(x) v_{q,\ell}, \qquad \ell = 1, \dots, L$$

Then,

Fast computation of sensitivity maps

Assume that the basis expansion is exact:

$$y_\ell(x) = \sum_{q=1}^{n_b} c_q(x) v_{q,\ell}, \qquad \ell = 1, \dots, L$$

Then,

$$\mathbb{E}[y_\ell(X)|X_I] = \sum_{q=1}^{n_b} \mathbb{E}[c_q(X)|X_I] v_{q,\ell}$$

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$$\begin{aligned}
\mathbb{E}[y_\ell(X)|X_I] &= \sum_{q=1}^{n_b} \mathbb{E}[c_q(X)|X_I] v_{q,\ell} \\
\mathbb{V}\mathrm{ar}(\mathbb{E}[y_\ell(X)|X_I]) &= \sum_{q,q'=1}^{n_b} \underbrace{\mathbb{C}\mathrm{ov}(\mathbb{E}[c_q(X)|X_I], \mathbb{E}[c_{q'}(X)|X_I])}_{\left(\underline{\mathbf{D}}_I(c)\right)_{q,q'}} v_{q,\ell} v_{q',\ell}
\end{aligned}$$

Fast computation of sensitivity maps

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\end{aligned}$$

i.e., matricially,

$$\underline{D}_I(y_\ell) = v_{.,\ell}^\top \, \underline{\mathbf{D}}_I(c) \, v_{.,\ell}$$

Fast computation of sensitivity maps

Proposition ([Li et al., 2020, Sáo et al., 2026])

The sensitivity map of $\mathbf{y}(X)$ *can be computed with the basis coefficients as*

$$\underline{S}_I(y_\ell) = \frac{v_{\cdot,\ell}^\top \, \underline{\mathbf{D}}_I(c) \, v_{\cdot,\ell}}{v_{\cdot,\ell}^\top \, \mathbf{D}(c) \, v_{\cdot,\ell}}, \qquad \ell = 1, \dots, L \tag{6}$$

Computing $\underline{\mathbf{D}}_I(c)$ is much cheaper than directly computing $\underline{S}_I(y_\ell)$ for all ℓ.

Fast computation of GSI

Proposition ([Sáo et al., 2026])

Generalized sensitivity indices can be computed from the basis coefficients as

$$\underline{\mathrm{GSI}}_I(y) = \frac{\mathrm{Tr}\,[\underline{\mathbf{D}}_I(c)\,\mathbf{G}]}{\mathrm{Tr}\,[\mathbf{D}(c)\,\mathbf{G}]} \qquad (7)$$

where $\mathbf{G}$ *is the Gram matrix of the basis vectors:* $\mathbf{G}_{q,q'} = \langle \mathbf{v}_{q,.}, \mathbf{v}_{q',.} \rangle_{\mathbb{R}^L}$

A similar expression can be found in [Perrin et al., 2021] for functional PCA.

Part III

Estimation of sensitivity maps with basis expansions

General remark

In general the **estimate** of sensitivity maps may be **computed pixel by pixel** (or time by time) **from the basis expansion** (see e.g. [Marrel et al., 2011])

$$y_\ell(x) = \sum_{q=1}^{n_b} c_q(x) v_{q,\ell}, \qquad \ell = 1, \dots, L$$

We can do **much better** when using **pick-freeze estimators**.

Pick-freeze estimators (closed Sobol' index)

The pick-freeze (PF) estimators are built on two independent copies X, X' drawn from μ_X, and the evaluations

$$Y = f(X) = f(X_I, X_{-I}), \qquad Y^I = f(X_I, X'_{-I}).$$

Then, we have:

$$\underline{D}_I(Y) = \mathbb{C}\mathrm{ov}(Y, Y^I)$$

Pick-freeze estimators (closed Sobol' index)

Now, consider two indep. N samples, $X^1, \ldots, X^N$ and $X^{*1}, \ldots, X^{*N}$ of μ. Denote

$$Y^k = f\left(X^k\right), \qquad Y^{I,k} = f\left(X_I^k, X_{-I}^{*k}\right) \qquad (k = 1, \ldots, N).$$

Using the empirical version of mean, covariance leads to the PF estimator

$$\widehat{\underline{S}_I}^{\mathrm{pf}} = \frac{\widehat{\underline{D}_I}^{\mathrm{pf}}}{\widehat{D}^{\mathrm{pf}}}$$

with

$$\widehat{\underline{D}_I}^{\mathrm{pf}} = \frac{1}{N}\sum_{k=1}^{N} Y^k Y^{I,k} - \left(\widehat{f_0}^{\mathrm{pf}}\right)^2, \quad \widehat{f_0}^{\mathrm{pf}} = \frac{1}{N}\sum_{k=1}^{N}\left[\frac{Y^k + Y^{I,k}}{2}\right]$$

$$\widehat{D}^{\mathrm{pf}} = \frac{1}{N}\sum_{k=1}^{N}\left[\frac{(Y^k)^2 + (Y^{I,k})^2}{2}\right] - \left(\widehat{f_0}^{\mathrm{pf}}\right)^2$$

This estimator is unbiased, asympt. normal and efficient [Janon et al., 2014, Gamboa et al., 2014]

Pick-freeze estimators (vector-valued case)

The definition of the PF estimator is immediately extended to the vector-valued case, replacing all products of the form $YY^\star$ by $Y(Y^\star)^\top$, e.g.

$$\widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}} = \frac{1}{N}\sum_{k=1}^{N} Y^k (Y^{I,k})^\top - \widehat{f_0}^{\mathrm{pf}} \left(\widehat{f_0}^{\mathrm{pf}}\right)^\top$$

Notice that $\widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}}$ is a **quadratic form** of the PF sample

$$Y^1, \dots, Y^N, Y^{I,1}, \dots, Y^{I,N}$$

In particular, with $y_\ell(x) = v_{.,\ell}^\top c(x)$, we obtain

$$Y^k = v_{.,\ell}^\top C^k, \qquad Y^{I,k} = v_{.,\ell}^\top C^{*k}$$

and thus

$$\widehat{\underline{D}_I}^{\mathrm{pf}}(y_\ell) = v_{.,\ell}^\top \widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}}(c) v_{.,\ell}$$

Fast computation of sensitivity maps

Assume that the basis expansion is exact:

$$y_\ell(x) = \sum_{q=1}^{n_b} c_q(x) v_{q,\ell}, \qquad \ell = 1, \dots, L$$

Proposition ([Sáo et al., 2026])

The PF estimator of the closed sensitivity map can be computed in function of the (matrix-valued) PF estimators of the vector of basis coefficients:

$$\widehat{\underline{S}_I}^{\mathrm{pf}}(y_\ell) = \frac{v_{\cdot,\ell}^\top \, \widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}}(c) \, v_{\cdot,\ell}}{v_{\cdot,\ell}^\top \, \widehat{\mathbf{D}}^{\mathrm{pf}}(c) \, v_{\cdot,\ell}}$$

Using $\widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}}(c)$ is enough to estimate $\underline{S}_I(y_\ell)$ for all ℓ.

Theoretical numerical gain

Method	Computational cost
Dimension-wise approach	$\approx 4n_b \times N \times L$
Basis-derived approach	$\approx 3n_b^2 \times (2N + L)$

The basis-derived approach is faster by a factor of (at least)

$$\frac{H(2N, L)}{3n_b}$$

where $H(.,.)$ is the harmonic mean, $H(a, b) = \left(\frac{a^{-1}+b^{-1}}{2}\right)^{-1}$.

The smaller n_b is compared to N, L, the higher the gain.

Assessment of the estimation error

- Obtain by **bootstrap** a B-sample of the law of $\widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}}(c)$ and $\widehat{\mathbf{D}}^{\mathrm{pf}}(c)$ by repeating B times:
  - Draw $k_1, \dots, k_N$ independently from $\mathcal{U}\{1, \dots, n\}$
  - Compute $\widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}}(c)$ and $\widehat{\mathbf{D}}^{\mathrm{pf}}(c)$ replacing the PF sample $Y^1, Y^{I,1}, \dots, Y^N, Y^{I,N}$ by the resampled one $Y^{k_1}, Y^{I,k_1}, \dots, Y^{k_N}, Y^{I,k_N}$

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- Deduce a B-sample of the **joint** law of the vector $(\widehat{\underline{S}_I}^{\mathrm{pf}}(y_\ell))_{\ell=1,\dots,L}$ with

$$\widehat{\underline{S}_I}^{\mathrm{pf}}(y_\ell) = \frac{v_{.,\ell}^\top \widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}}(c)\, v_{.,\ell}}{v_{.,\ell}^\top \widehat{\mathbf{D}}^{\mathrm{pf}}(c)\, v_{.,\ell}}$$

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- Main usage: Draw a boxplot of the marginal distributions $\widehat{\underline{S}_I}^{\mathrm{pf}}(y_\ell)$

As a by-product, we obtain (at a low computational cost) a B-sample of the law of *statistics involving the joint distribution*, such as $\max_\ell \widehat{\underline{S}_I}^{\mathrm{pf}}(y_\ell)$

Comments

The link between the PF estimators of y_ℓ and c can be extended to *any PF estimator that is a* ***quadratic form*** *of the PF sample*

$$Y^1, Y^{I,1}, \dots, Y^N, Y^{I,N}$$

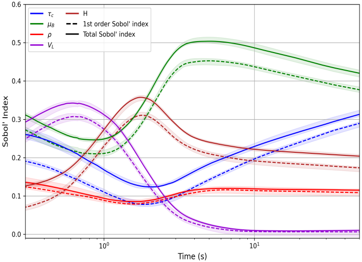
This includes the PF estimator of the total effect from Jansen's formula

$$\widehat{\overline{S}_I}^{\mathrm{pf}} = \frac{\widehat{\overline{D}_I}^{\mathrm{pf}}}{\widehat{D}^{\mathrm{pf}}}, \qquad \widehat{\overline{D}_I}^{\mathrm{pf}} = \frac{1}{2N}\sum_{k=1}^{N}\left(Y^k - Y^{-I,k}\right)^2$$

and the PF estimators of GSI

$$\widehat{\underline{\mathrm{GSI}}_I}^{\mathrm{pf}} := \frac{\mathrm{Tr}\left[\widehat{\underline{\mathbf{D}}_I}^{\mathrm{pf}}\right]}{\mathrm{Tr}\left[\widehat{\mathbf{D}}^{\mathrm{pf}}\right]}, \qquad \widehat{\overline{\mathrm{GSI}}_I}^{\mathrm{pf}} := \frac{\mathrm{Tr}\left[\widehat{\overline{\mathbf{D}}_I}^{\mathrm{pf}}\right]}{\mathrm{Tr}\left[\widehat{\mathbf{D}}^{\mathrm{pf}}\right]}$$

Application to the motivating example



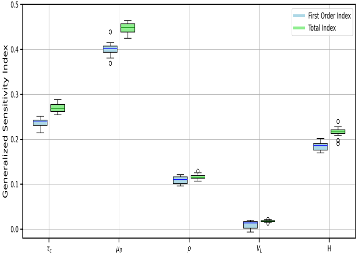


Figure: Sensitivity maps and GSI (time period: [0, 50 s]).

Application to the motivating example

Modeling and computational details

- Modeling
  - We used a space-filling design of experiment of size $\mathbf{n = 200}$
  - The basis expansion used is PCA, with $\mathbf{n_b = 10}$ (**% of variance > 99.9**).
  - Each basis coefficient is modeled by a Gaussian process, independently.
  - The accuracy of the whole model is evaluated on a test set, $Q^2 > 0.9$.
- Sensitivity analysis
  - Input variables are assumed independent and uniformly distributed.
  - Size of pick-freeze samples: $N = 5\,000$.
  - Number of output dimensions: $\mathbf{L = 5\,000}$.
  - Number of bootstrap replicates: 50.
  - Theoretical computational gain : **252**. Observed gain: **35**.
    $\rightarrow$ *Improve coding should even increase the observed gain.*

An example with a spatial output

We consider the Campbell2D function (see e.g. [Marrel et al., 2011]), with:

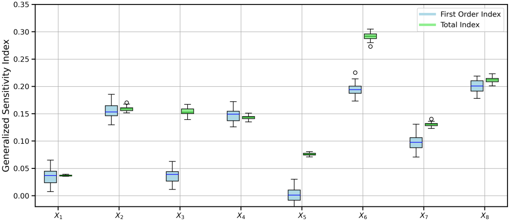
$$f : [-1, 5]^8 \to \mathbb{L}^2([-90, 90]^2)$$

Here we discretize the output on a fine grid of size 64×64, thus $\mathbf{L} = \mathbf{4\,096}$.

The computational setting is similar to the previous application, with the following modifications:

- Modeling
  - For PCA, we chose $\mathbf{n_b} = \mathbf{7}$ (% of variance > 99.2).
  - Here, $Q^2 > 0.95$.
- Sensitivity analysis
  - Theoretical computational gain : **330**. Observed gain: **30**.

An example with a spatial output



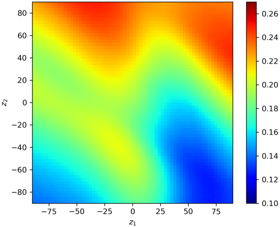


Figure: Left: Estimated GSI - Right: Estimated map of total index for X_8.

Part IV

Estimation of sensitivity maps with model error

Context

In the basis expansion

$$y_\ell(x) = \sum_{q=1}^{n_b} c_q(x) v_{q,\ell}, \qquad \ell = 1, \dots, L$$

the basis coefficients $c_1(x), \dots, c_{n_b}(x)$ **are only known when x belongs to the design of experiments $\mathcal{X}$**, and must be **predicted elsewhere**.

The model error aims at quantifying the approximation error of $c_1(x), \dots, c_{n_b}(x)$ when $x \notin \mathcal{X}$

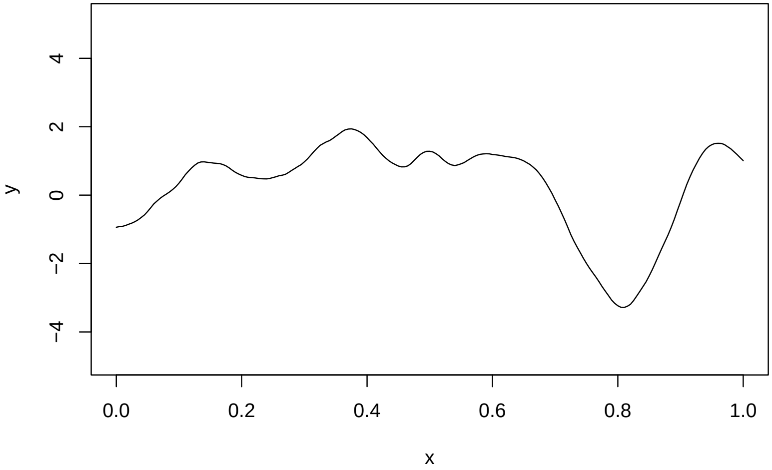
The Gaussian process framework

Let us first consider the scalar output c_q.

We assume that $x \mapsto c_q(x)$ is a sample path of a Gaussian process (GP) Z.

- (Gaussian prior) $\forall x_1, \dots, x_m$ the law of $(Z(x_1), \dots, Z(x_m))$ is Gaussian. A GP is characterized by
  - a mean function $x \mapsto \mathbb{E}_{\mathbb{P}_{\mathbf{Z}}}(Z(x))$
  - a covariance function (kernel) $k : (x, x') \mapsto \mathbb{C}\text{ov}_{\mathbb{P}_{\mathbf{Z}}}(Z(x), Z(x'))$.
- (Gaussian posterior) $\forall x_1, \dots, x_m$ the law of $(Z(x_1), \dots, Z(x_m))$ conditionally on the data $Z(x^i) = z_i$ $(i = 1, \dots, n)$ is still Gaussian
  - Explicit formulas for the conditional mean and conditional kernel

GP simulations



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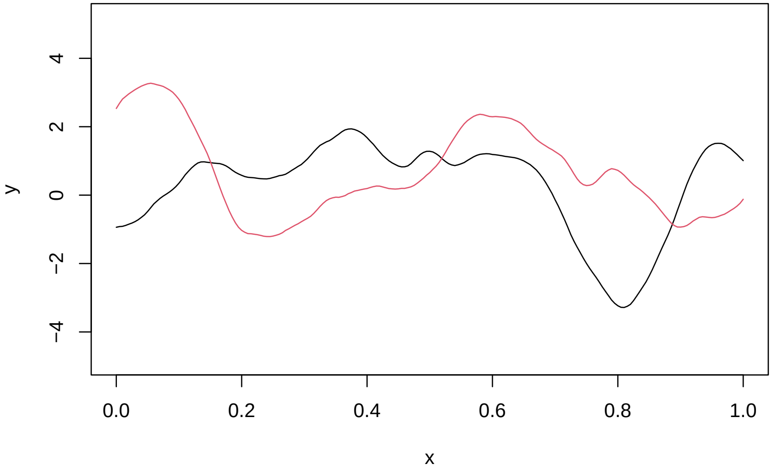

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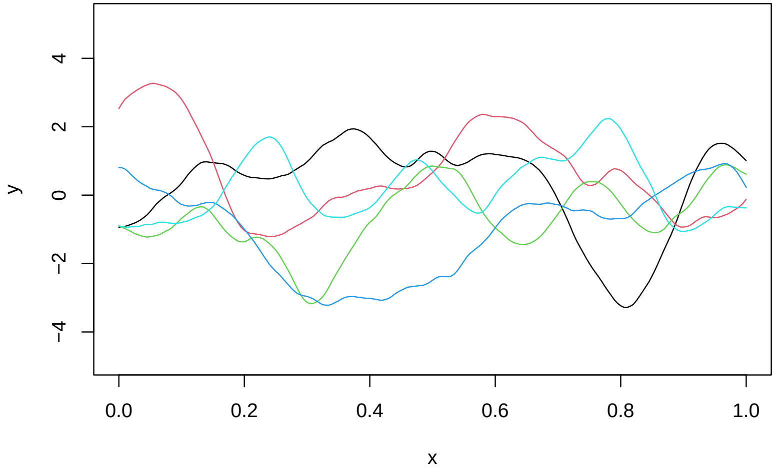
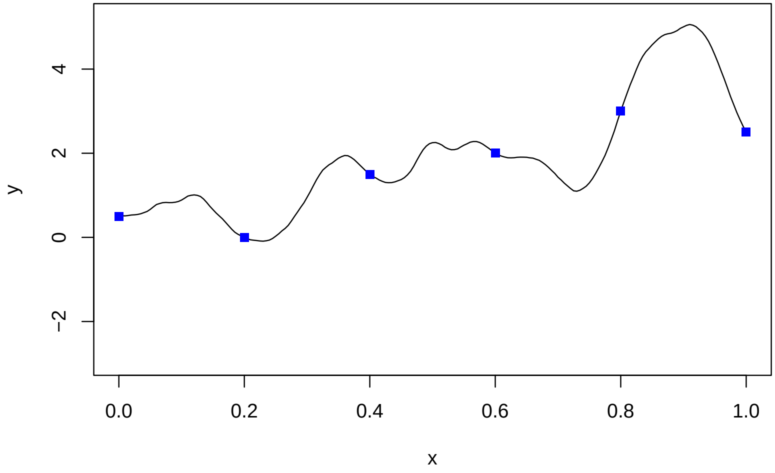


GP conditional simulations



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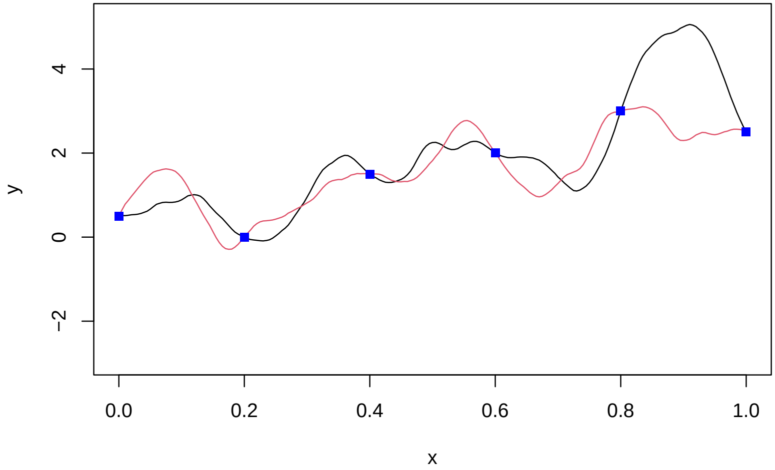

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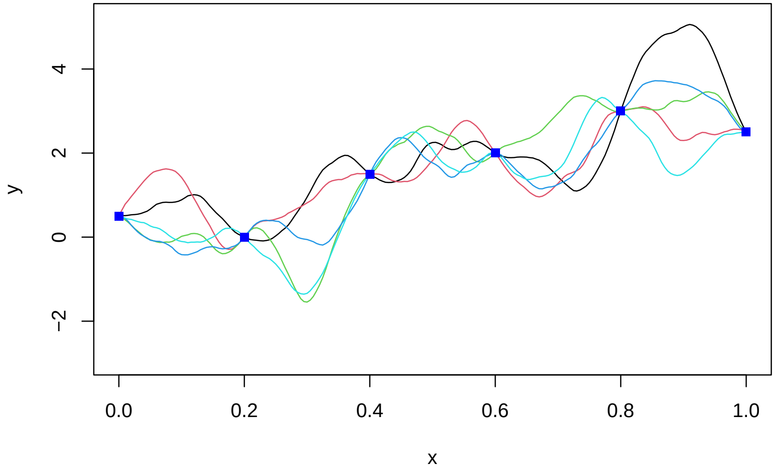

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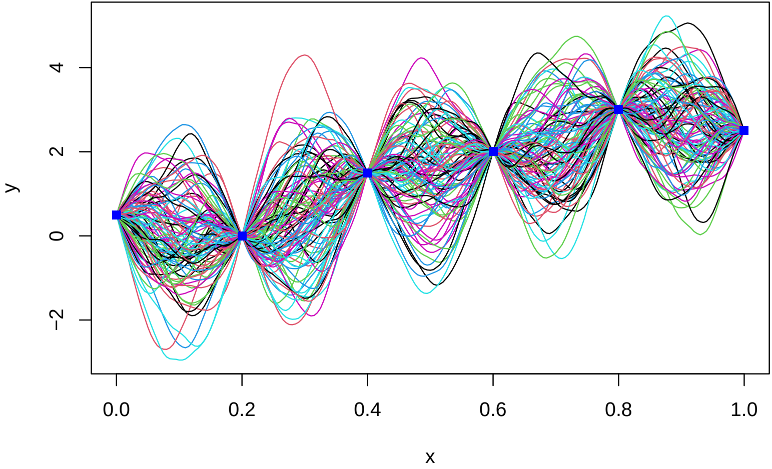


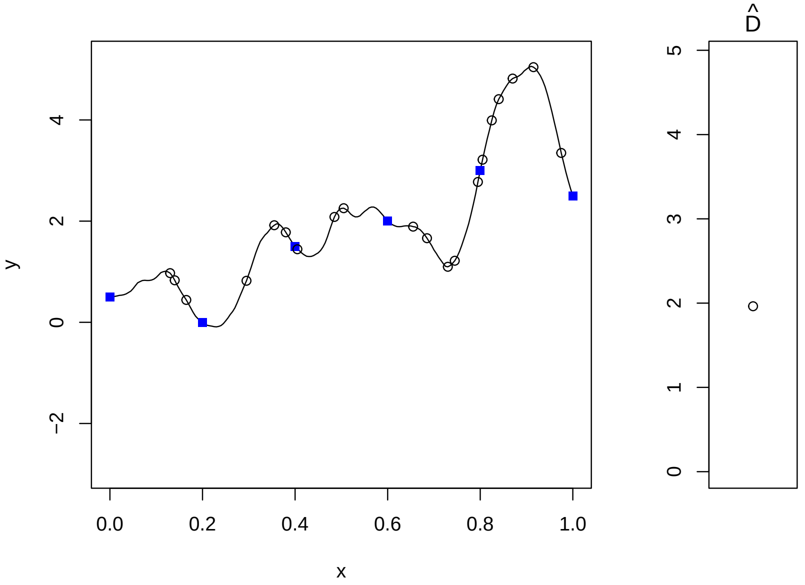
Principle for a scalar output

We now present the methodology proposed by [Le Gratiet et al., 2014], for a scalar output.

- To assess the **model error**, draw GP sample paths (w.r.t $\mathbb{P}_Z$)
- To assess the **estimation error**, draw PF input samples (w.r.t. $\mathbb{P}_X$) on one GP path
  - $\rightarrow$ Use resampling (bootstrap) to reduce GP sampling cost
- To assess both **model + estimation errors**, draw PF input samples (w.r.t. $\mathbb{P}_X$) on sampled GP paths (w.r.t. $\mathbb{P}_Z$)

y_ℓ.

Assessment of model error



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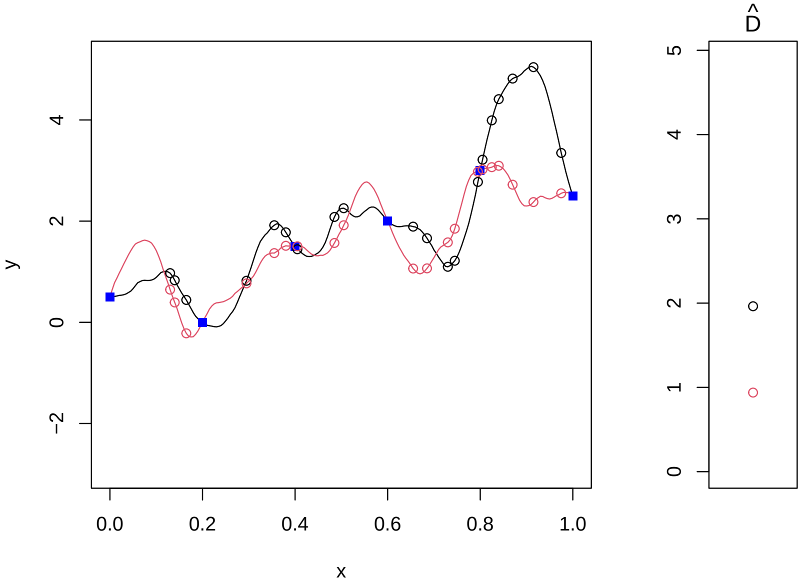

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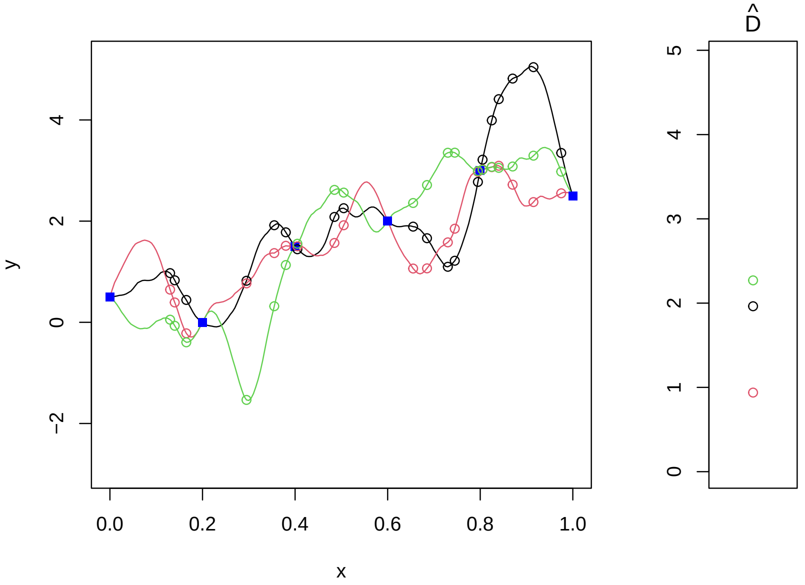

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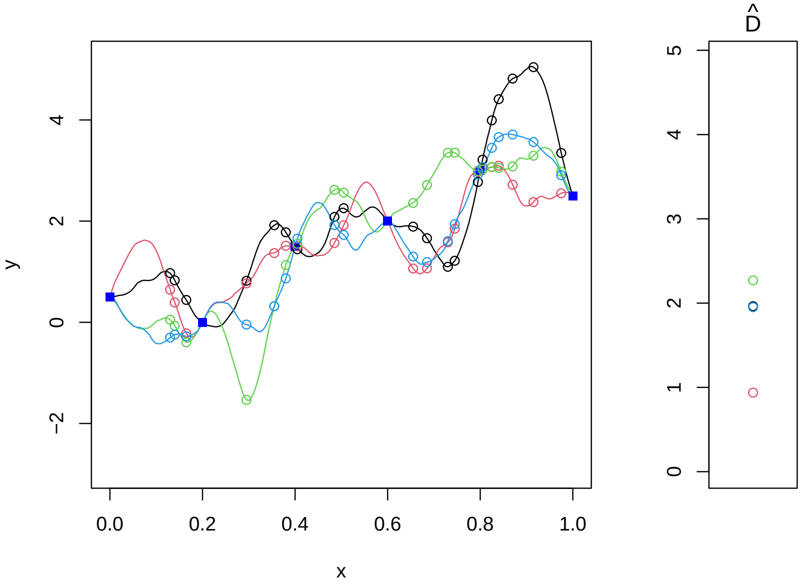

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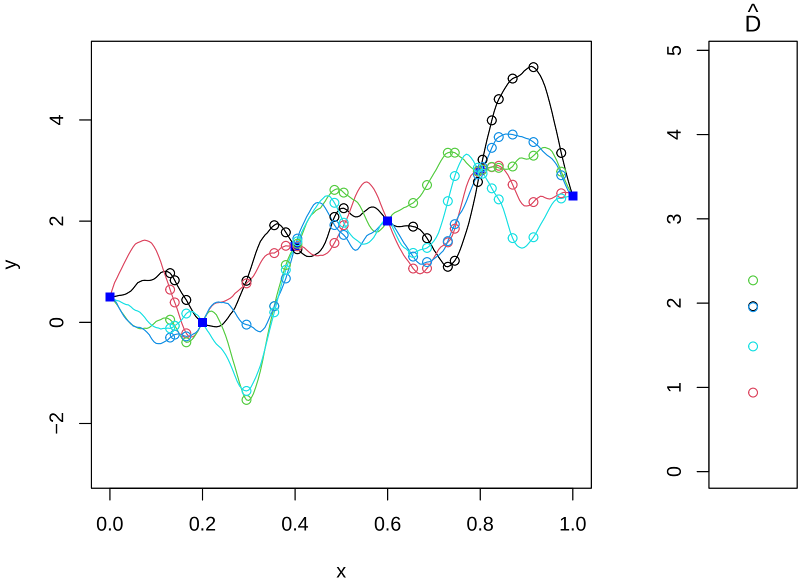
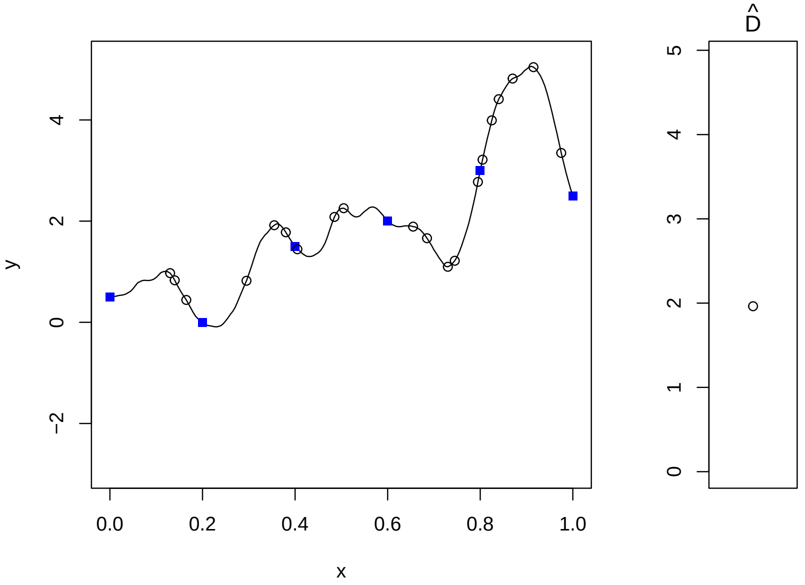


Assessment of estimation error by bootstrap



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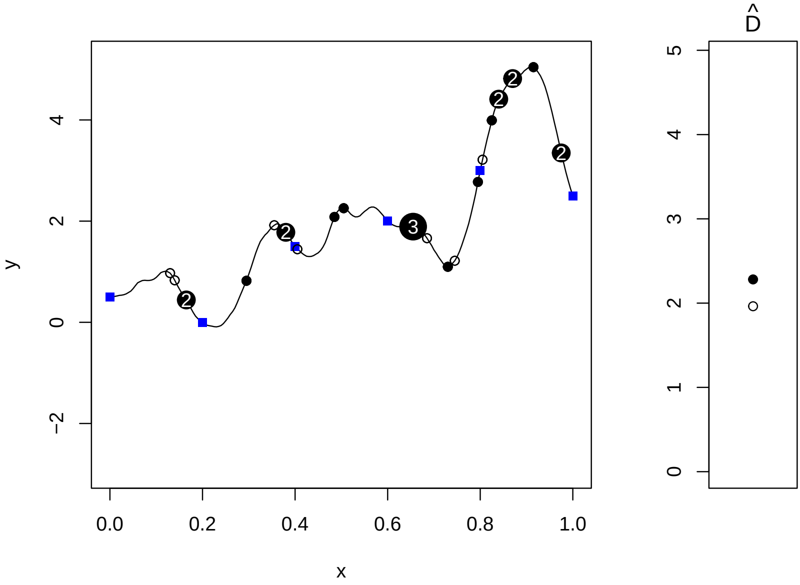

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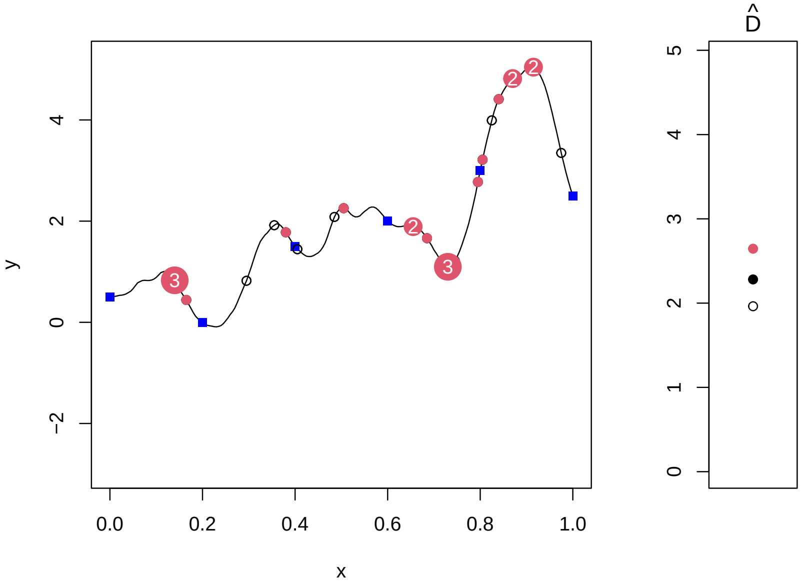

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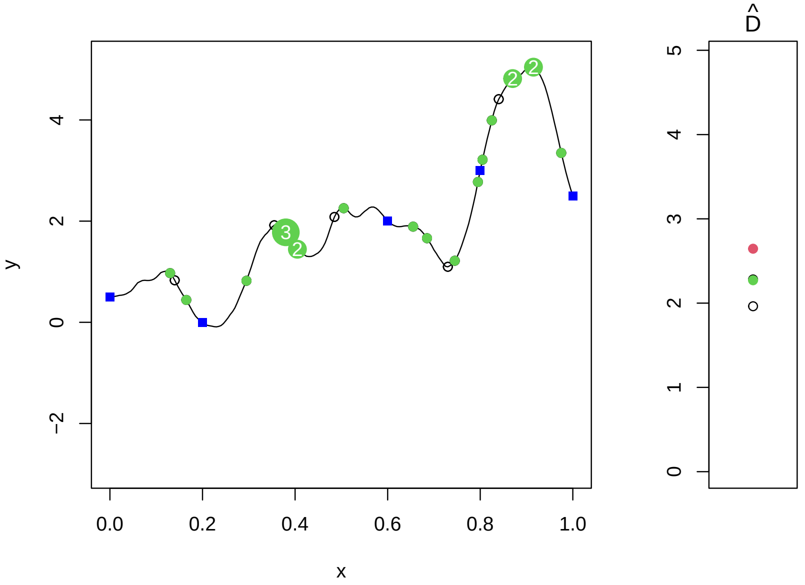

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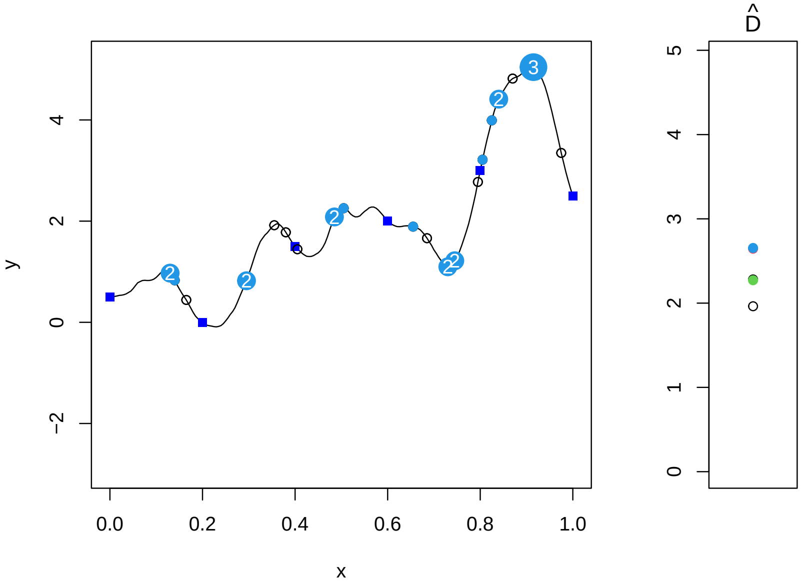

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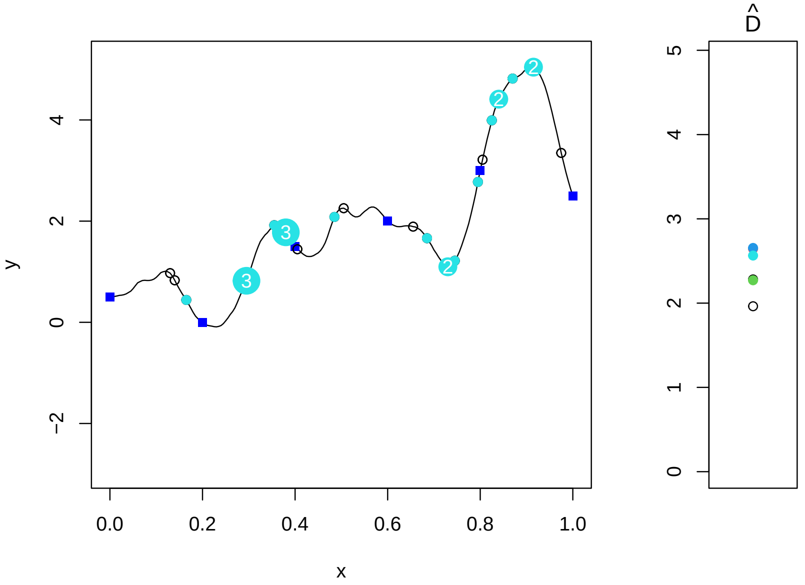


Extension to functional output

We consider the basis expansion:

$$y_\ell(x) = \sum_{q=1}^{n_b} c_q(x) v_{q,\ell}, \qquad \ell = 1, \dots, L$$

We assume that $x \mapsto c_q(x)$ are sample paths of independent Gaussian processes (for $q = 1, \dots, n_b$).

We can adapt the methodology of [Le Gratiet et al., 2014] with our **fast formulas based on coefficients** to assess model + estimation error on

- sensitivity maps
- GSI

by propagating the errors on the coefficients to all the outputs y_ℓ.

Sensitivity maps, with estimation + metamodel error

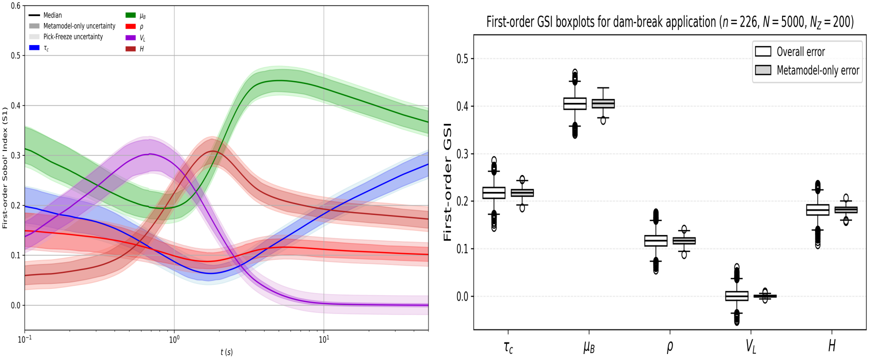
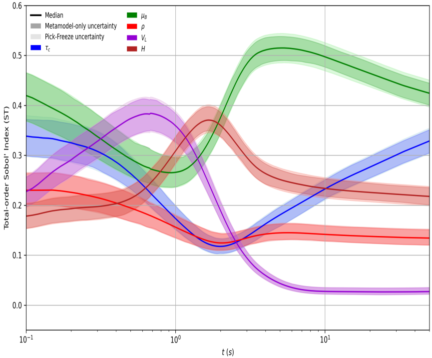
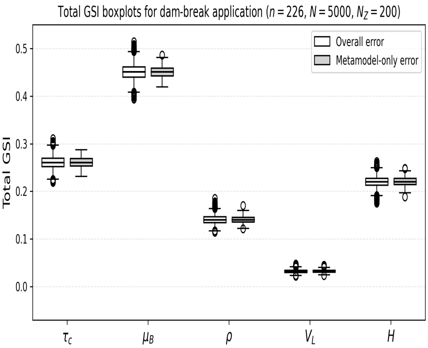


Figure: Estimation of first-order and total SMs, including model error.

Sensitivity maps, with estimation + metamodel error





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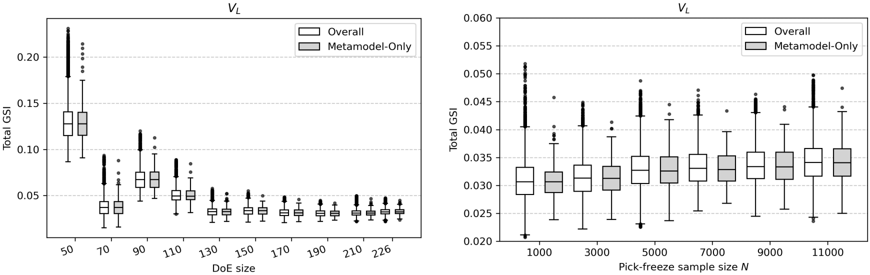

Figure: Total GSI of V_L vs DoE size (N = 5000)/ PF sample size ($n = 226$).

Computational time

The code has been run in an Apple M3 with 8 cores.

- Config 'low': $N = 1\,000$, $N_Z = 10$, $N_X = 10$
- Config 'high': $N = 11\,000$ ($5\,000$ for Campbell), $N_Z = 200$, $N_X = 50$
- S (Standard): Assess the model error for all scalar output dimensions.
- B (Basis-derived): The proposed algorithm, i.e., assess the model error on the vector of basis components and propagate it to the outputs.

\ Method Config \	S	B
low	35s	2 s
high	7h ?	25 mn

Table: Campbell function

\ Method Config \	S	B
low	30s	2 s
high	8h ?	32 mn

Table: Dam-break

Part V

Conclusion and perspectives

Main messages

- Using **any *linear* basis expansion** we obtain **fast formulas of pick-freeze estimates** of (gen.) Sobol' indices for functional outputs
  - → Fast because the PF estimator of the sensitivity map is **deduced from** the PF estimator of **basis coefficients**.
  - → Works for all estimator which is a ***quadratic form* of the PF input samples**
  - → Works for 1st order, 2nd and higher order interactions + total indices.
  - → Gives the **joint distribution of errors**

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  - $\rightarrow$ Gives the **joint distribution of errors**
- Using a GP model for basis coefficients, we can also assess **model error**
- With other estimators, the estimate of the sensitivity maps may be computed pixel by pixel (or time by time) from the basis expansion

$$y_\ell(x) = \sum_{q=1}^{n_b} c_q(x) v_{q,\ell}, \qquad \ell = 1, \dots, L$$

This is always possible but slower.

A short list of references...

Gamboa, F., Janon, A., Klein, T., and Lagnoux, A. (2014).
Sensitivity analysis for multidimensional and functional outputs.
Electronic Journal of Statistics, 8(1):575 – 603.

Janon, A., Klein, T., Lagnoux, A., Nodet, M., and Prieur, C. (2014).
Asymptotic normality and efficiency of two Sobol' index estimators.
ESAIM: Probability and Statistics, 18:342–364.

Le Gratiet, L., Cannamela, C., and Iooss, B. (2014).
A bayesian approach for global sensitivity analysis of (multifidelity) computer codes.
SIAM/ASA Journal on Uncertainty Quantification, 2(1):336–363.

Li, M., Wang, R.-Q., and Jia, G. (2020).
Efficient dimension reduction and surrogate-based sensitivity analysis for expensive models with high-dimensional outputs.
Reliability Engineering & System Safety, 195:106725.

Marrel, A., Iooss, B., Jullien, M., Laurent, B., and Volkova, E. (2011).
Global sensitivity analysis for models with spatially dependent outputs.
Environmetrics, 22(3):383–397.

Perrin, T., Roustant, O., Rohmer, J., Alata, O., Naulin, J., Idier, D., Pedreros, R., Moncoulon, D., and Tinard, P. (2021).
Functional principal component analysis for global sensitivity analysis of model with spatial output.
Reliability Engineering & System Safety, 211:107522.

Sáo, Y. T., Roustant, O., and Maciel, G. d. F. (2026).
Fast pick-freeze estimation of Sobol' sensitivity maps using basis expansions.
Reliability Engineering & System Safety, 265(Part A):111504.

... to be completed by all the references cited in them and many others :)