Statistical interpretation of an ensemble of surrogate models

.

How to create one stochastic surrogate model out of multiple deterministic surrogate models

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Director : Charles Audet, Co-director : Sébastien Le Digabel

Polytechnique Montréal

10 September 2020

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Surrogate models in black-box optimization

True problem :

$$\begin{aligned} &\min_{x \in \mathbb{R}^n} f(x) \\ &s.t. \quad c_j(x) \leq 0, \quad \forall j \in \{1, 2, \ldots, m\} \end{aligned} \qquad (P)$$

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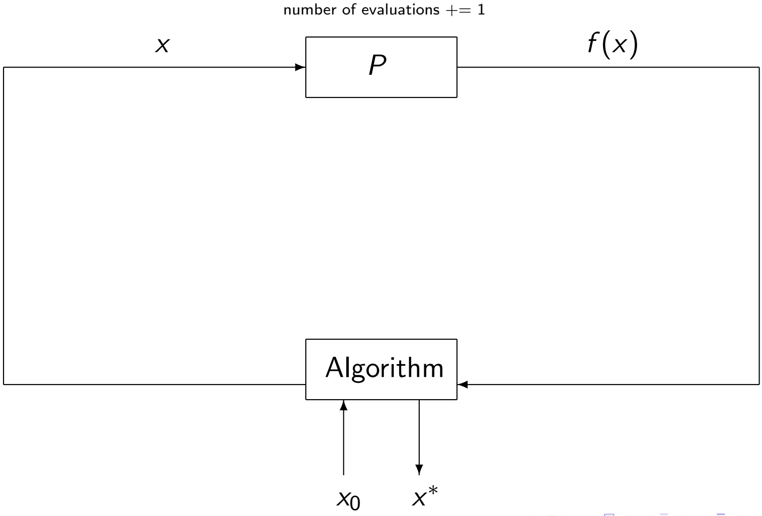
Sample points (cache) :

$$\begin{aligned} \mathbb{X} &= \{x^{(1)}, \dots, x^{(p)}\} \\ \mathbf{y} &= \{f(x^{(1)}), \dots, f(x^{(p)})\} \end{aligned}$$

Surrogate models in black-box optimization



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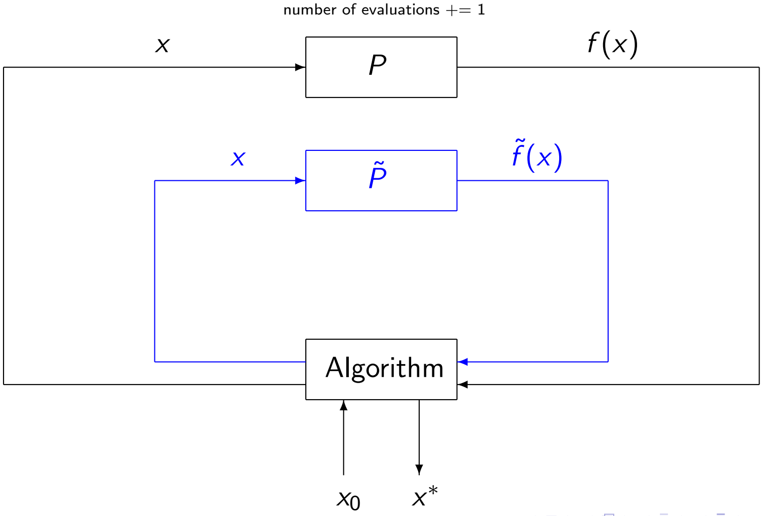
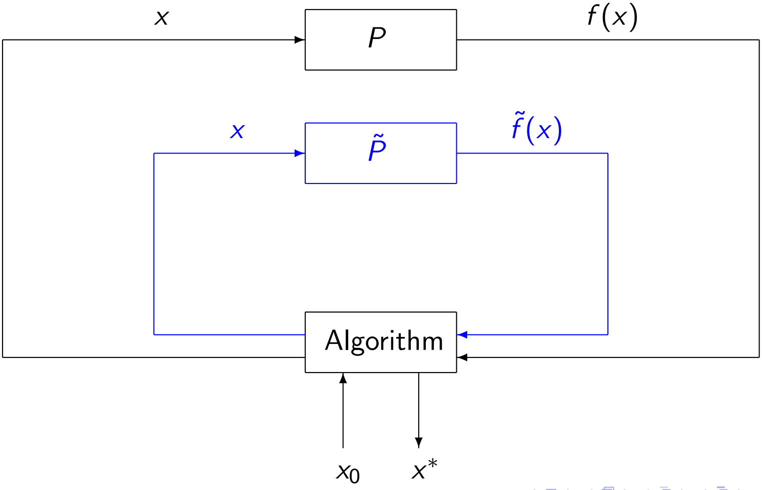


Surrogate models in black-box optimization

$$\mathbb{X} = \mathbb{X} \cup \{x\}$$

$$\mathbf{y} = \mathbf{y} \cup \{f(x)\}$$

number of evaluations += 1



Surrogate models in black-box optimization

Seminal article : Booker et al. (1999) [1]

Types of surrogate models :

- Radial Basis Functions [2, 3]
- Quadratic Models [4, 5]
- Kernel Smoothing [6, 7]
- Gaussian Processes [8, 9, 10]
- . . .

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Stochastic surrogate models

$$x \in \mathbb{R}^n \longrightarrow \tilde{f}(x)$$

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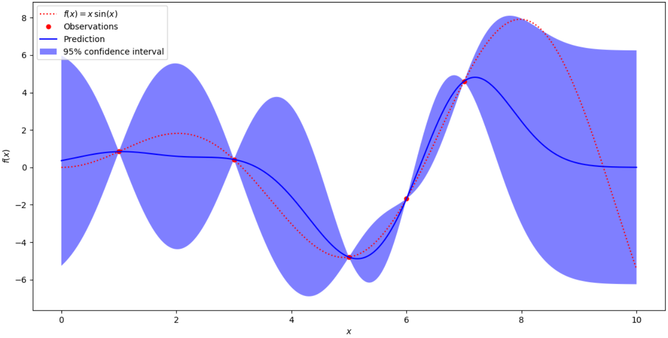

Figure: Gaussian process regression on $f : x \mapsto x \sin x$

Stochastic surrogate models

What is the use of a stochastic surrogate ?

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- Expected Improvement [9] :

$$\begin{aligned} EI(x) &= \mathbb{E}[I(x)] \\ &= \mathbb{E}[\max\{fmin - f(x), 0\}] \end{aligned}$$

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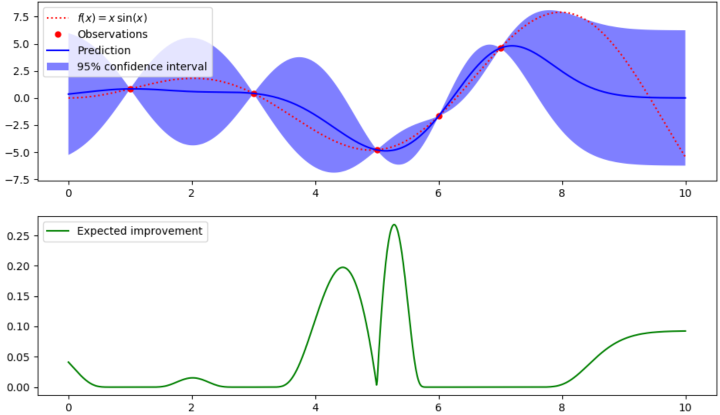
Gaussian process regression and the resulting Expected Improvement



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- Probability of Improvement [11] :

$$PI(x) = \mathbb{P}[I(x) > 0]$$
$$= \mathbb{P}[f_{min} > f(x)]$$

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Stochastic surrogate models

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Statistical Surrogate Formulations for Simulation-Based Design Optimization, 2015 [11]

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8 formulations of the surrogate problem $\tilde{P}$ integrating EI, P, PI, EFI, μ and PFI.

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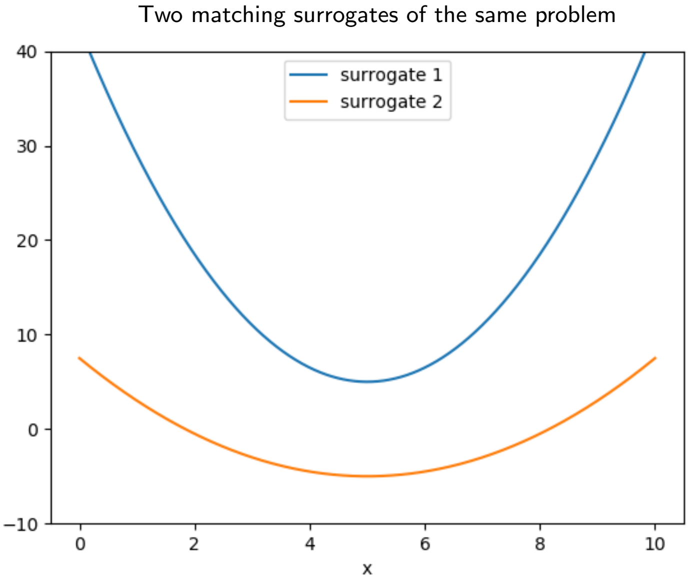

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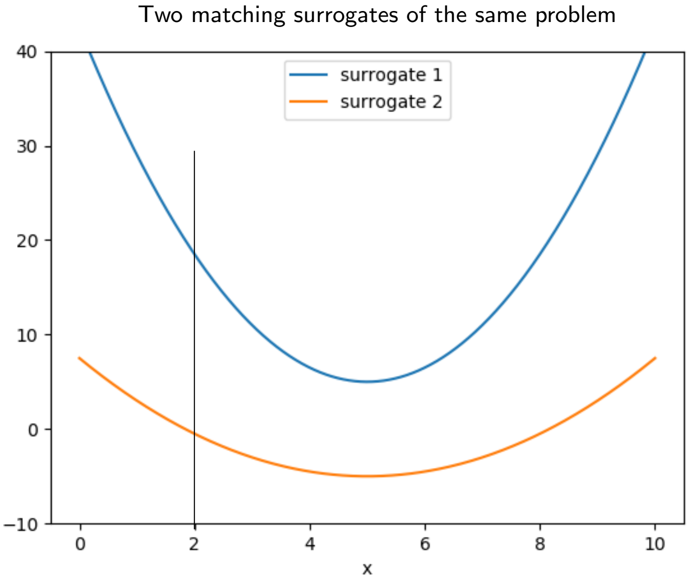

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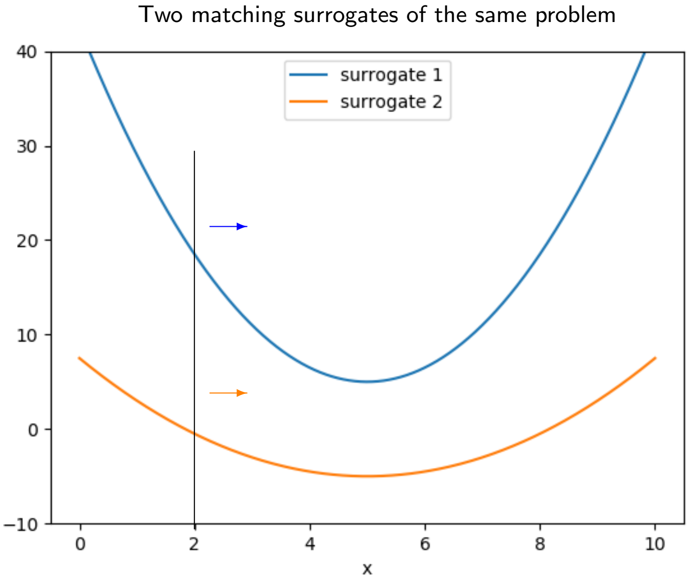

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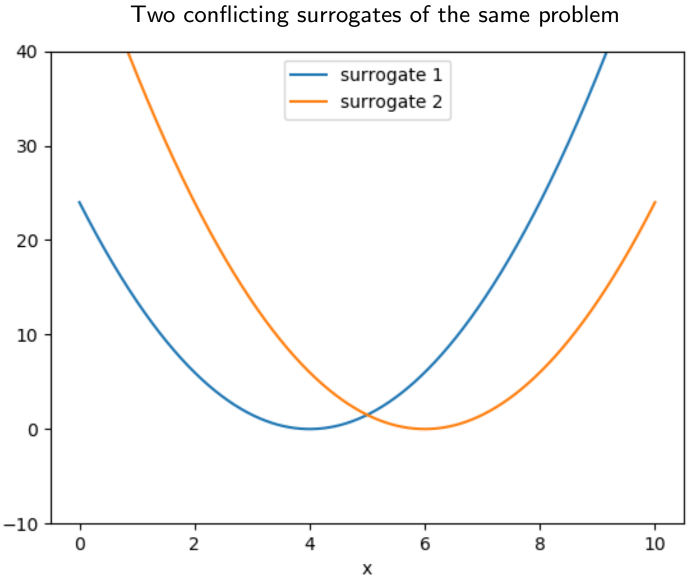

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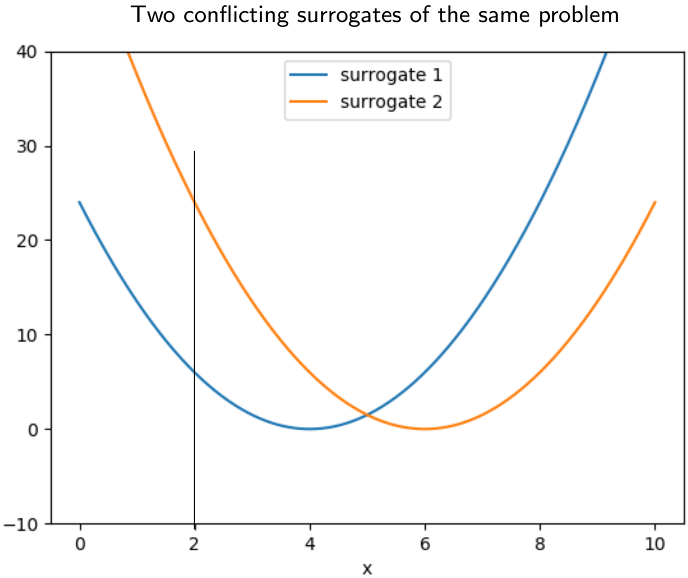

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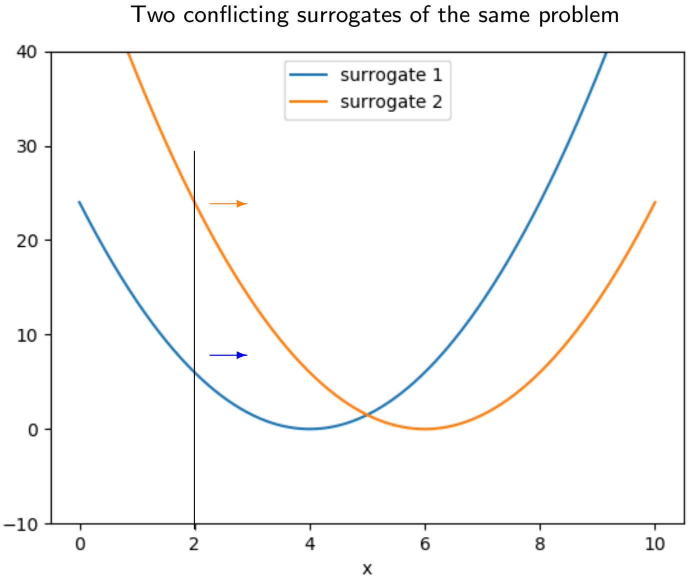

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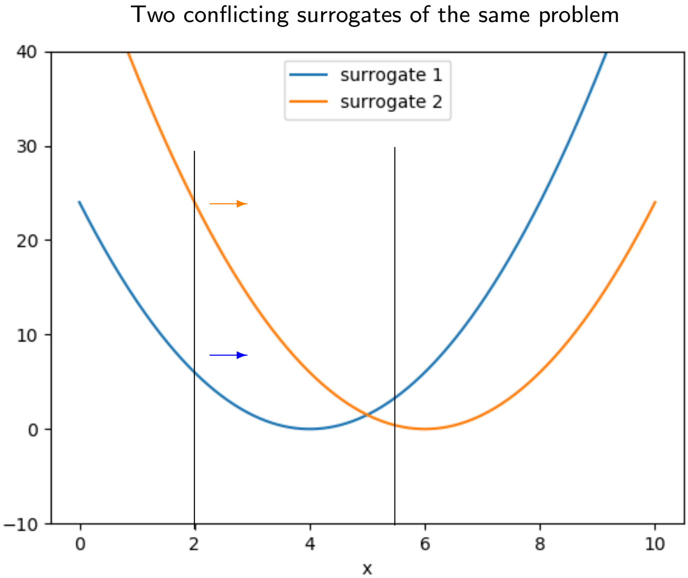

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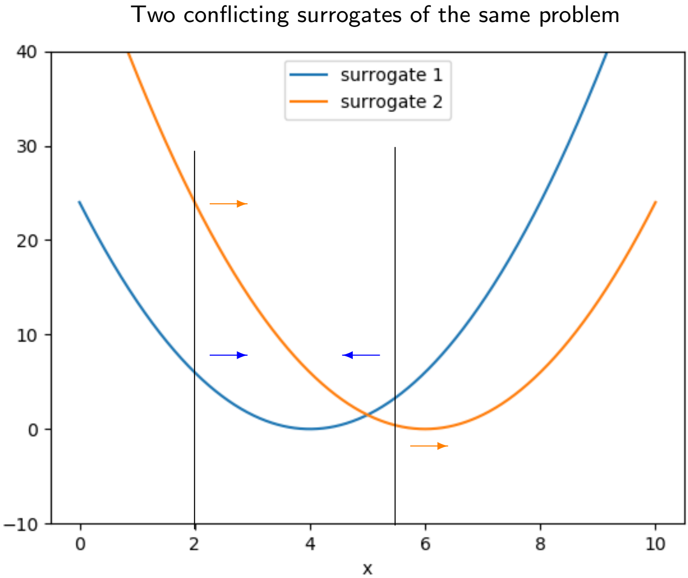

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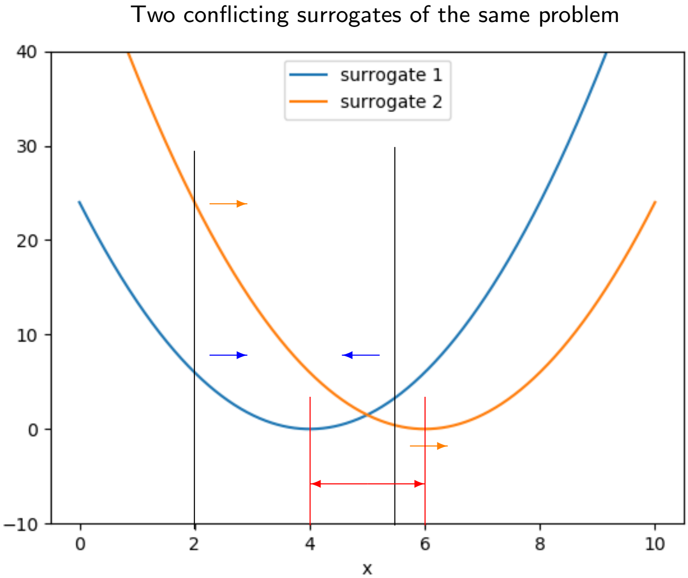

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For a given point $x \in \mathbb{R}^n$, we define :

- The number of surrogates that predict a decrease in the direction $d \in \mathcal{D}$:

$$n_{d<x} = \left|\left\{\tilde{f} \in \mathcal{S} : \; \tilde{f}(x + td) < \tilde{f}(x)\right\}\right|$$

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- The *order-based uncertainty* (inspired by the article [12]) :

$$\mathcal{U}^{f}_{OB}(x) = \frac{1}{|\mathcal{D}|} \sum_{d \in \mathcal{D}} \frac{n_{d<x}(s - n_{d<x})}{(s/2)^2}$$

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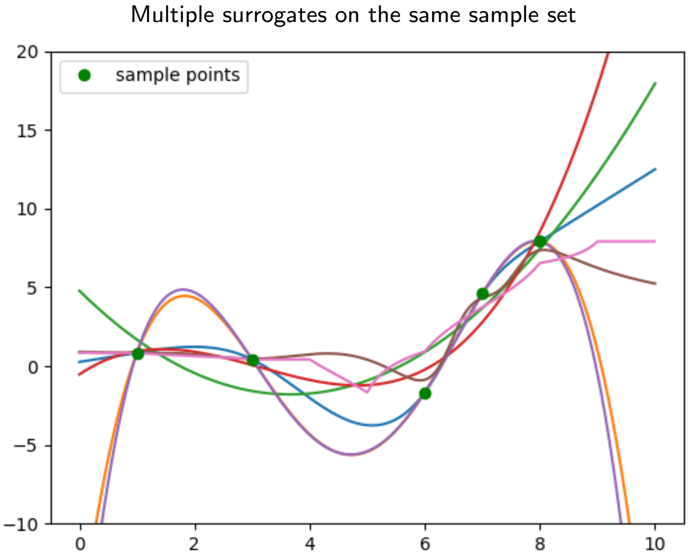

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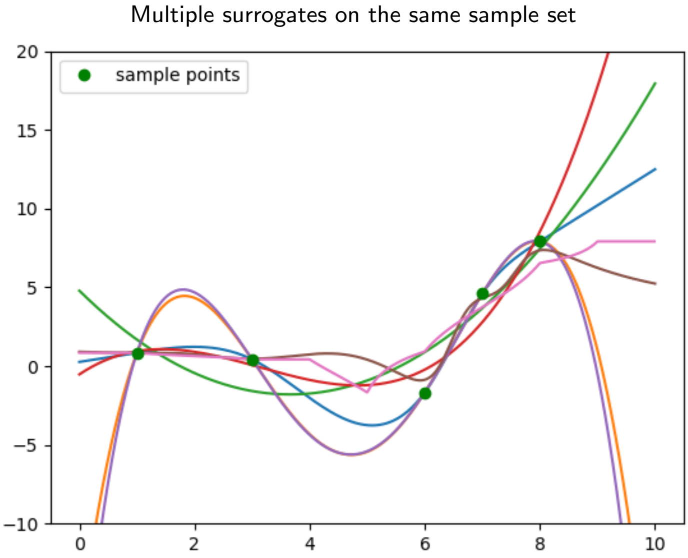

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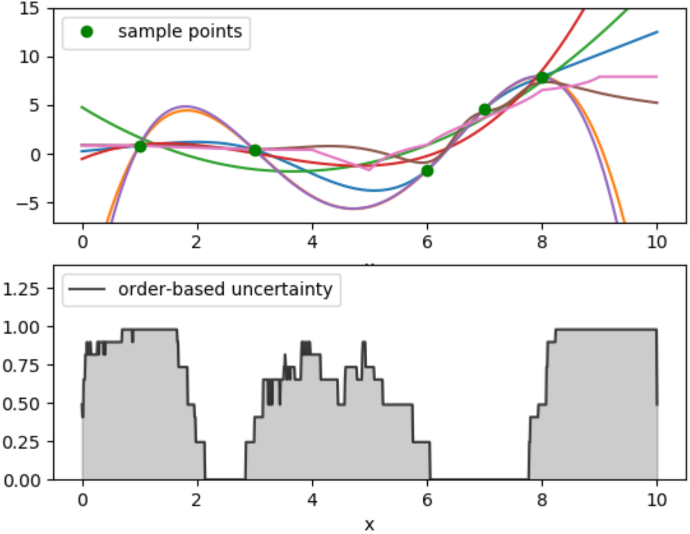
Statistical interpretation of an ensemble of surrogate models

Multiple surrogates on the same sample set
and order-based uncertainty



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Initial objective : recover $\tilde{\sigma}(x)$, $\tilde{\sigma}_j(x)$, $EI(x)$, $P(x)$ and $PI(x)$.

$$\begin{aligned} \tilde{\sigma}(x) &\longrightarrow \mathcal{U}^f_{OB} \\ \tilde{\sigma}_j(x) &\longrightarrow \mathcal{U}^j_{OB} \end{aligned}$$

$$\begin{aligned} EI(x) &\longrightarrow ? \\ P(x) &\longrightarrow ? \\ PI(x) &\longrightarrow ? \end{aligned}$$

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Future work :

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- Adapt EI, P and PI

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