Gaussian Processes: from knowledge-informed Machine Learning to optimization

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Gaussian Processes: from knowledge-informed Machine Learning to optimization

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Why learning with Gaussian Processes ?

Many situations lead to sparse data or uncertain data. Gaussian processes (GPs) offer a mathematically funded framework for learning, optimizing, and other decision-making activities.

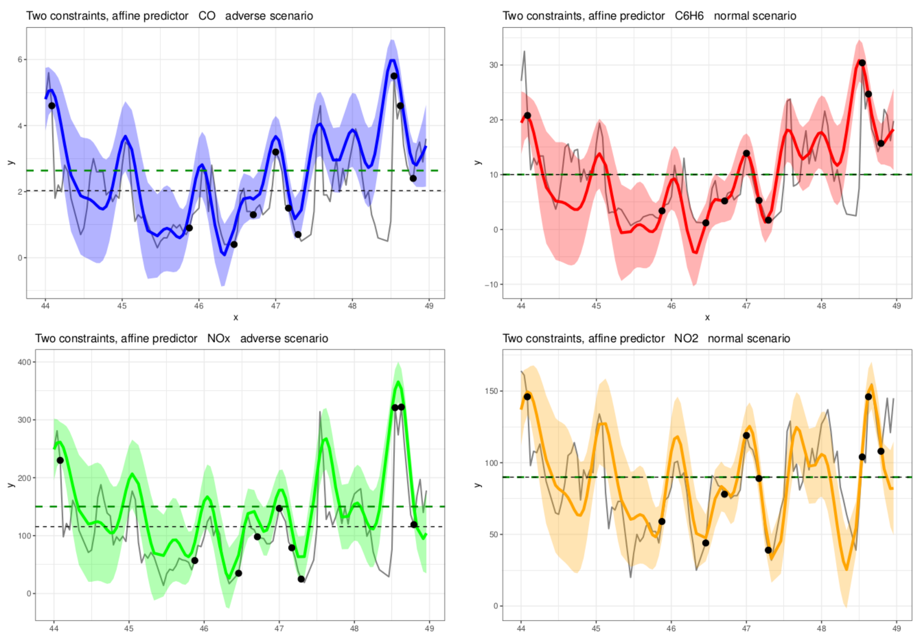
Gaussian process regression framework

- **Problem:** Predict a phenomenon based on few observations
  - Express the GP as a best linear unbiased predictor

$$\hat{Y}(\mathrm{x}) := \sum_{i=1}^{n} \alpha_i(\mathrm{x}) Y(\mathrm{x}_i)$$

$$\text{with } (\alpha_1(\mathrm{x}), \dots, \alpha_n(\mathrm{x})) = \arg\min_{\alpha} \mathbb{E}\left[\left(\hat{Y}(\mathrm{x}) - Y(\mathrm{x})\right)^2\right]$$

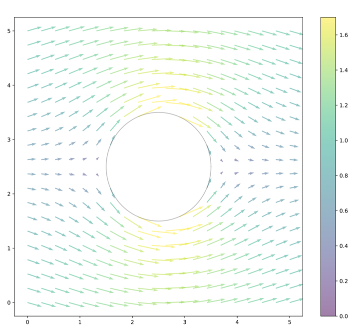
- **Contribution** [1]: Application to multi-output, classification.
  - Add unbiased constraints, linear constraints (e.g. adverse scenarios)
  - Extend to vector interpolation, to classification



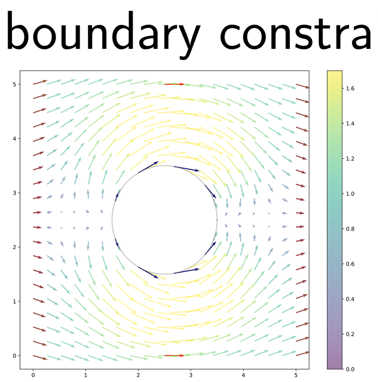
GPs and physics-informed predictions

- **Problem:** Incorporate physical information.
- **Contribution** [2]: Impose linear partial differential equations in a kriging model either as observations or as constraints in the model loss minimization (BLUE). For a potential flow, $\nabla . v(x) = 0$.

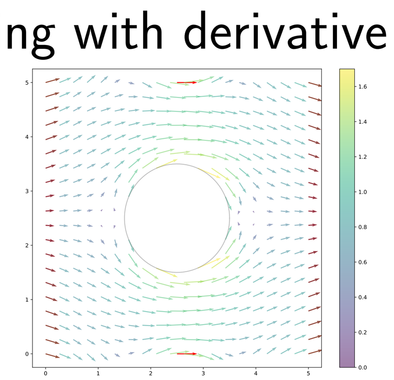
True flow



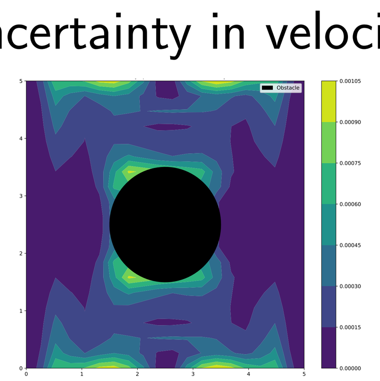
Lagrange boundary constraints pred.



Kriging with derivative obs.

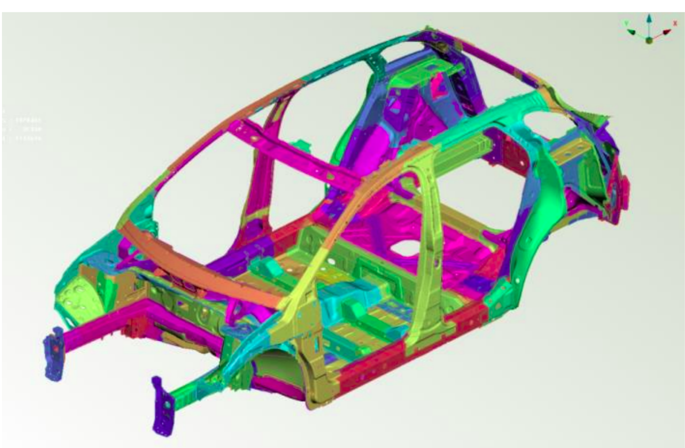


||uncertainty in velocity||



GPs for optimization in high dimension

- **Problem:** Optimize in high dimension.
  GPs are a key asset in the optimization of expensive functions: they can partially replace the true function. But GPs tend to fail in high-dimension, even more so in the context of optimization.



- **Contribution** [3]: Build a GP as a linear combination of GPs with fixed length-scales: more robust, avoid repeated minimizations of the loss. Analytical model. E.g. Optimization of a vehicle structure, 130 variables.
- **Contribution** [4]: Optimize with a GP within an adapted Trust Region. TREGO (Trust Region Efficient Global Optimization)

GPs for optimization with uncertainties

- **Problem:** Optimize with uncertain parameters

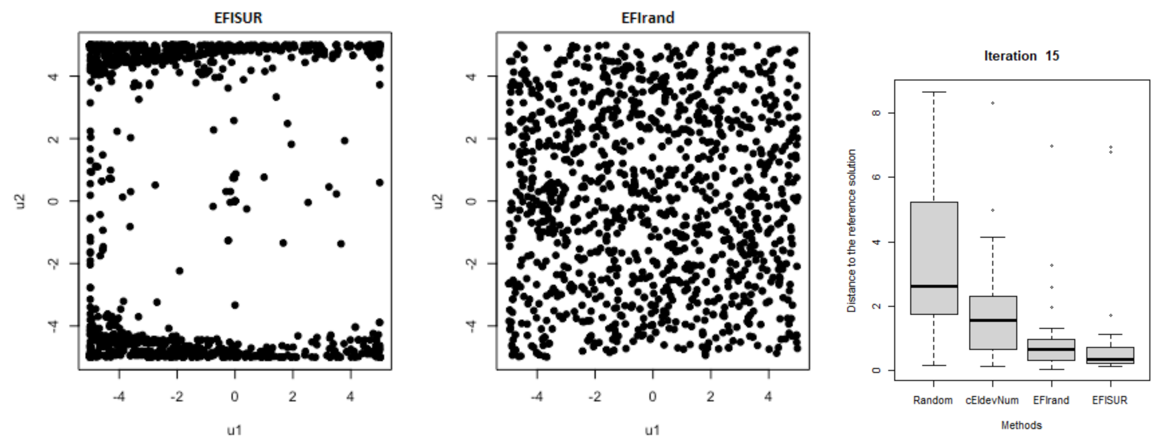
$$x^* = \arg\min_{x \in \mathcal{S}_X} \mathbb{E}[f(x, U)] \text{ s.t. } \mathbb{P}(g(x, U) \le 0) \ge 1 - \alpha \,,$$

where U has a known probability density.

- **Contribution** [5]: EFISUR (Efficient Feasible Improvement with Stepwise Uncertainty Reduction) method alternates between

$$\begin{cases} x^{\text{next}} = \arg\max_{x \in \mathcal{S}_X} \text{ExpectedFeasibleImprovement}(x) \\ u^{\text{next}} = \arg\min_{u \in \mathcal{S}_U} \text{VarianceNextStep}(x^{\text{next}}, u) \end{cases}$$

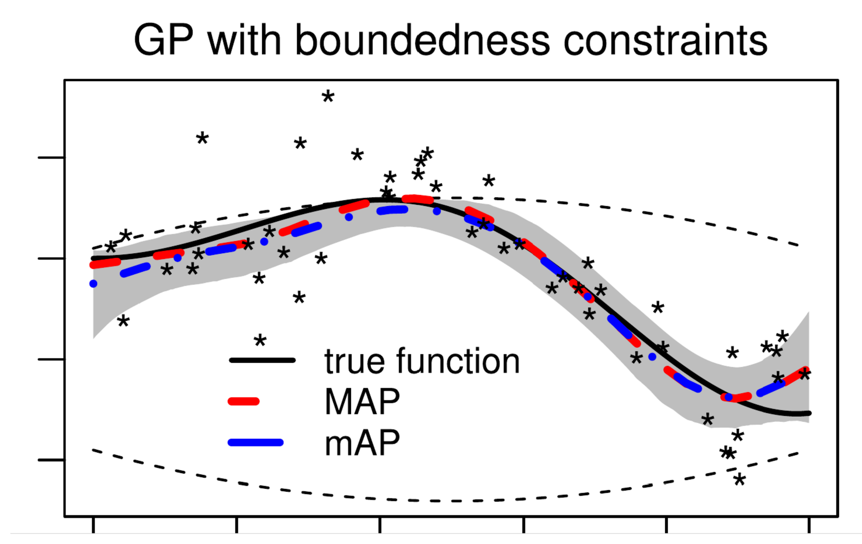
e.g. distribution of uncertain parameters by EFISUR (left) and at random (middle). Effect on the convergence accuracy (right):

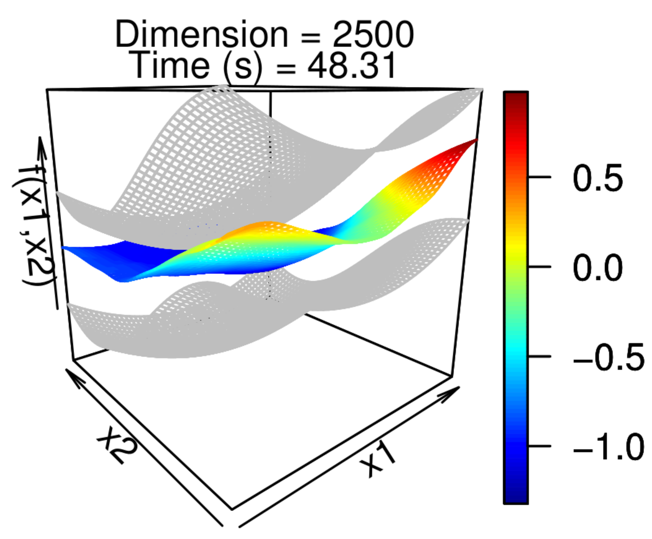


- **Contributions** [6, 7]: More information, continuations.

GPs under shape constraints

- **Problem:** Incorporate constraints: monotonicity, shape constraints.
- **Contributions** [8, 9]:
  - Approximate GP by finite dimensional combination of Gaussian random variables (Karhunen–Loève, hat functions...)
  - Transfer constraints on these Gaussian random variables
  - Sample constrained Gaussian random vectors (MCMC, ESS...)





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