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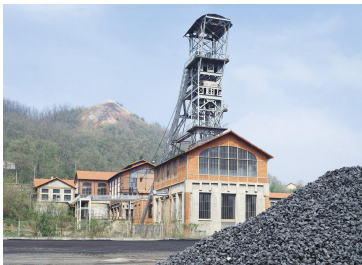


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On Gaussian Processes for Spatial Modeling and Optimization

Didier Rullière and Rodolphe Le Riche
may 16-17, 2023

LIMOS-HUST online workshop on Operations Research, Artificial Intelligence and Networks (ORAIN 2023)



picture: mining headframe (chevalement) at Saint-Etienne

.....

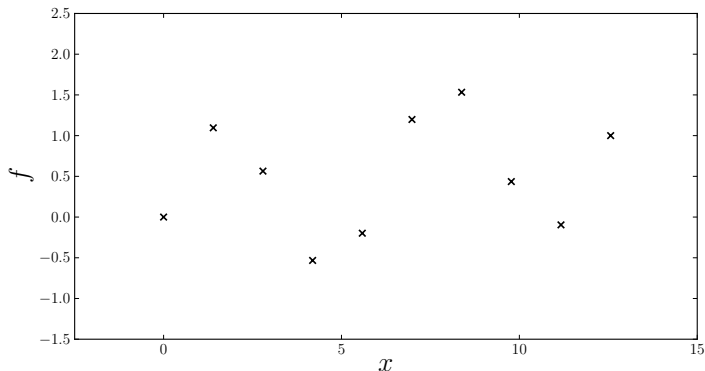
Outline

- 1 Gaussian Process Interpolation
- 2 GPs in decision theory: case studies

Gaussian Process Interpolation

Gaussian process regression (1/4)

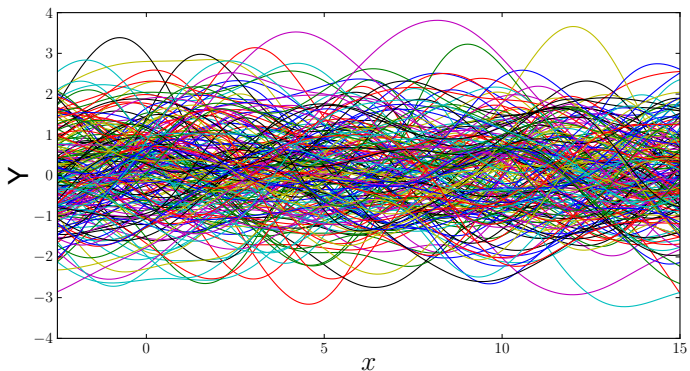
Assume we have observed a function $f(\cdot)$ over a set of points $\mathbb{X} = (x_1, \dots, x_n)$:



Here in 1D. The vector of observations is $\mathbf{y} = f(\mathbb{X})$, i.e. $y_i = f(x_i)$.

Gaussian process regression (2/4)

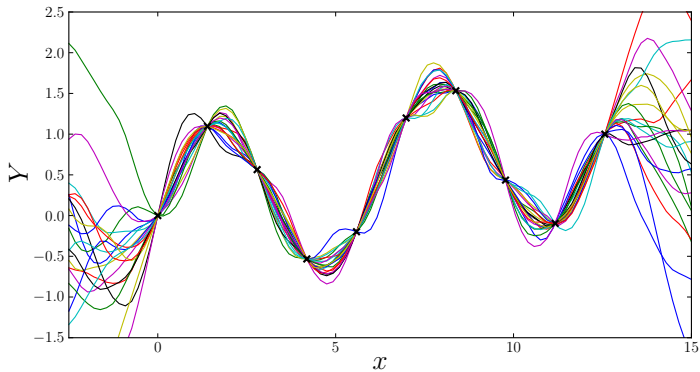
Since $f(\cdot)$ is unknown, we make the general assumption that it is close to the sample path of a Gaussian process $Y \sim \mathcal{N}(\mu(\cdot), k(\cdot, \cdot))$:



(here $\mu(x) = 0$)

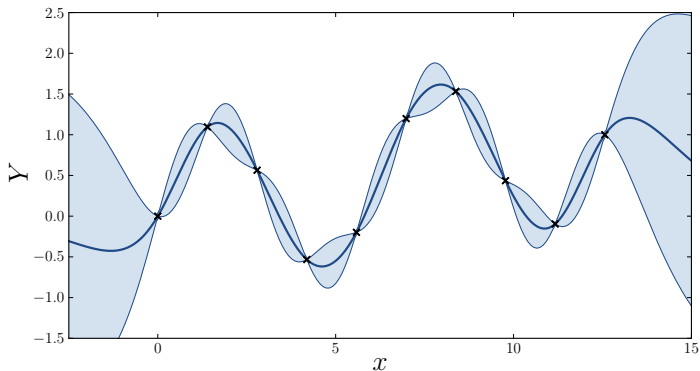
Gaussian process regression (3/4)

If we remove all the samples that do not interpolate the observations we obtain:



Gaussian process regression (4/4)

It can be summarized by a mean function and 95% confidence intervals.



... it is easy to extend to higher dimensions. Formally the mean predictor at one location x is the Best Linear Unbiased Prediction (BLUP) using observations $y_i = f(x_i)$.

You can play here: https://durrande.shinyapps.io/gp_playground/

Kriging equations

The conditional distribution can be obtained analytically:

By definition, (Y_x, \mathbf{Y}) is multivariate normal. Formulas on the conditioning of Gaussian vectors give the distribution of $Y_x | \mathbf{Y} = \mathbf{y}$. It is $\mathcal{N}(m(\cdot), c(\cdot, \cdot))$ with :

$$\begin{aligned}m(x) &= \mu(x) + k(x, \mathbb{X})k(\mathbb{X}, \mathbb{X})^{-1}(\mathbf{y} - \mu(\mathbb{X})) \\c(x, x') &= k(x, x') - k(x, \mathbb{X})k(\mathbb{X}, \mathbb{X})^{-1}k(\mathbb{X}, x')\end{aligned}$$

where $k(\cdot, \cdot)$ is the covariance function of the prior Gaussian Process.

Simple Kriging, Gaussian case

For a centered process, when $\mu(x) = 0$ for all x , the simple Kriging predictor mean and variance are

$$\begin{cases} \mathbb{E}[Y_x | \mathbf{Y} = \mathbf{y}] &= m(x) \\ \text{Var}[Y_x | \mathbf{Y} = \mathbf{y}] &= c(x, x) \end{cases}$$

Problems

Here are few selected problems:

- **Model selection:**
how to choose prior process, prior covariance function family, prior covariance function parameters ?
- **Computation:**
how to compute the predictor when the matrices are huge?
- **Adaptation:**
how to adapt to specific settings (monotony, uncertainty, high dimension...)

Because kriging (GP regression) predicts a full, spatially varying, distribution, it is of great use in decision making.

⇒ a stepping stone to address decision-theoretic problems.

GPs in decision theory: case studies

Input uncertainty

Case of Energy Performance Certificate: measurement are done at an unknown location on a specific area (not averaged on the area)

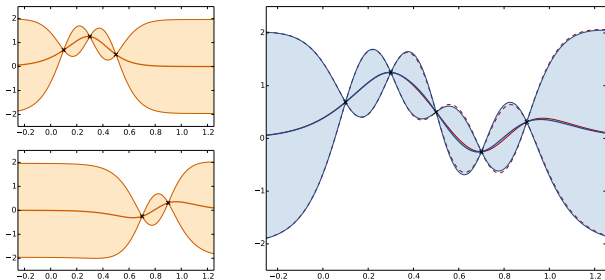


Figure: Left: Prescribed vignette appearing on the French energy performance certificate up to 2021. Label A refers to energy efficient dwellings, G refers to energy intensive dwellings. Right: Map of French inventoried EPCs over a neighborhood of Lyon city.

Adaptation of Kriging to mixtures of Gaussian rv. *Grossouvre et al., 2023*

High Dimension

Large observation number: with (sub)models combinations *Rullière et al., 2018*



Kriging sub-models

aggregation in blue, full model in red.

Figure: Aggregation of two Gaussian process regression models.

Large dimension: with (sub)models combinations *Appriou et al., 2022*

is it better and faster to combine few submodels than to find the best model?

Constrained & robust Bayesian Optimization I

Problem addressed : optimization, with expensive constraints and objectives, in the presence of uncertainties. Cost is twice an issue!

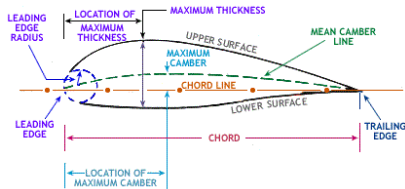
Example : compressor rotor design

Maximize rotor polytropic efficiency

by changing its (parameterized) shape, x

with geometrical, inflow and rotation speed uncertainties, u ,

under flow constraints (angles, no separation, Mach number) indexed by p .



Constrained & robust Bayesian Optimization II

Principle of the method:

- Build GPs of the objective in (x, u) space and of the constraints in the (x, u, p) space.
- Use the GPs to define a figure of merit : the expected feasible improvement (EFI)
- Sequentially (carefully) choose the next variable, uncertainties and constraints to be computed

$$x^{n+1} = \arg \max_x \text{EFI}(x)$$

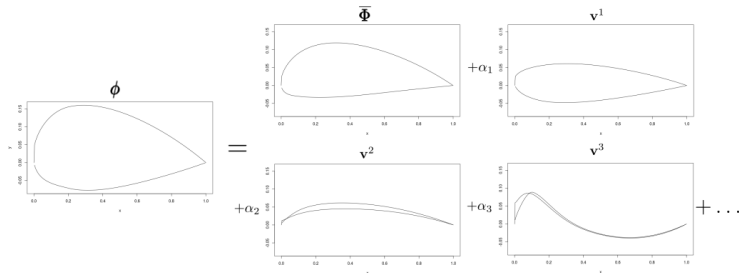
$$u^{n+1}, p^{n+1} = \arg \min_{u,p} \text{Variance of one-step-ahead EFI}(x^{n+1})$$

⇒ faster convergence. More explanations in [Pelamatti et al., 2023](#).

Costly shape optimization I

Example: airfoil minimizing drag. “Infinite” dimensional, and CFD is costly.

Eigendecomposition of the shapes, then work in α -space:



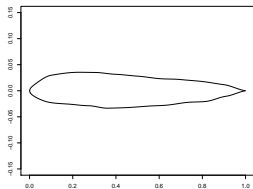
Costly shape optimization II

Principle of the method:

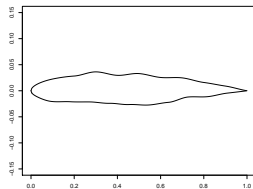
- Learn active components of α from known (inputs, outputs) by maximizing a likelihood plus a term that favors sparsity.
- Build a GP on active components (dimension reduction) + a simple GP on less active components. Perform Bayesian optimization on active space + a random 1D embedding for less active components.
- Project α^{n+1} on manifold of feasible shapes.

⇒ faster convergence, smoother airfoils

(here 100 calls to CFD)



BO on active reduced space



BO on traditional CAD space

More explanations in [Gaudrie et al., 2020](#).

Related recent works by the same team

Quantization of rare events : *Sire et al., 2023*

More Bayesian optimization :

with mixed discrete-continuous variables : *Cuesta Ramirez et al., 2022*

with HSIC-based variable selection : *Spagnol et al., 2019*

with trust regions for higher dimensions : *Diouane et al., 2022*

with constraints (monotonicity, convexity...) : *Maatouk et al., 2023*

testing Bayesian optimization : *Le Riche and Picheny, 2021*

References I

- [1] Appriou, T., Rullièrè, D., and Gaudrie, D. (2022). Combination of High-Dimensional Kriging Sub-models. working paper or preprint.
- [2] Cuesta Ramirez, J., Le Riche, R., Roustant, O., Perrin, G., Durantin, C., and Glièrè, A. (2022). A comparison of mixed-variables bayesian optimization approaches. *Advanced Modeling and Simulation in Engineering Sciences*, 9(1):6.
- [3] Diouane, Y., Picheny, V., Le Riche, R., and Scotto Di Perrotolo, A. (2022). Trego: a trust-region framework for efficient global optimization. *Journal of Global Optimization*, pages 1–23.
- [4] Gaudrie, D., Le Riche, R., Picheny, V., Enaux, B., and Herbert, V. (2020). Modeling and optimization with gaussian processes in reduced eigenbases. *Structural and Multidisciplinary Optimization*, 61:2343–2361.
- [5] Grossouvre, M., Rullièrè, D., and Villot, J. (2023). Spatial interpolation using mixture distributions: A Best Linear Unbiased Predictor. working paper or preprint.
- [6] Le Riche, R. and Picheny, V. (2021). Revisiting bayesian optimization in the light of the coco benchmark. *Structural and Multidisciplinary Optimization*, 64(5):3063–3087.
- [7] Maatouk, H., Rullièrè, D., and Bay, X. (2023). Bayesian analysis of constrained Gaussian processes. working paper or preprint.

References II

- [8] Pelamatti, J., Le Riche, R., Helbert, C., and Blanchet-Scalliet, C. (2023). Coupling and selecting constraints in Bayesian optimization under uncertainties. *Optimization and Engineering*. accepted for publication in April 2023, also available as arXiv 2204.00527.
- [9] Rullière, D., Durrande, N., Bachoc, F., and Chevalier, C. (2018). Nested kriging predictions for datasets with a large number of observations. *Statistics and Computing*, 28(4):849–867.
- [10] Sire, C., Le Riche, R., Rullière, D., Rohmer, J., Pheulpin, L., and Richet, Y. (2023). Quantizing rare random maps: application to flooding visualization. *Journal of Computational and Graphical Statistics*, 0(ja):1–31.
- [11] Spagnol, A., Le Riche, R., and Veiga, S. D. (2019). Global sensitivity analysis for optimization with variable selection. *SIAM/ASA Journal on uncertainty quantification*, 7(2):417–443.