Two Multi-Fidelity Regression Algorithms

Federico Zertuche Celine Helbert Anestis Antoniadis
Laboratoire Jean Kuntzmann, Grenoble

Summary

We present two different regression methods that learn from several training sets produced by a simulator with adjustable precision.

One is an extension of the Gaussian Processes base Cokriging [2, 3] , and the other uses a Coarse to fine multi-fidelity wavelet regression[1].

Motivation

The parameters on a computer fluid dynamics simulation are, in most of the cases, uncertain. Since this simulations tend to be complex and time consuming, we will try to build a reliable meta-model based on a small set of observations to replace the complex code to do a sensitivity analysis.

We study the case where the simulations complexity can be tuned. Precise simulations are very time-consuming whereas fast, imprecise simulations can be too far away from the physical model.

The time-precision relationship is the key point of multi-fidelity: We hope to reduce the time it takes to build a reliable meta-model by using less precise simulations and compensating with faster but imprecise simulations.

Notation

For ease of notation we will consider two training sets:

- $(X_1, Y_1) : \{(x_1^{(1)}, y_1^{(1)}), \ldots, (x_1^{(m1)}, y_1^{(m1)})\}$ - imprecise.
- $(X_2, Y_2) : \{(x_2^{(1)}, y_2^{(1)}), \ldots, (x_2^{(m2)}, y_2^{(m2)})\}$ - precise.

Locally linear Cokriging

We suppose that there are two independent Gaussian Processes Y_1 and D_{12} such that

$$Y_2(x) = \varphi(Y_1(x)) + D_{12}(x)$$

where φ is an unknown function.

Locally linear Cokriging: Learning the parameters

First, we estimate φ by locally linear polynomials by using (Y_1, Y_2). With the estimated relationship $\widehat{\varphi}$, we define the learning set for D_{12} as $(X_2, Y_2 - \widehat{\varphi}(Y_1(X_1))$.

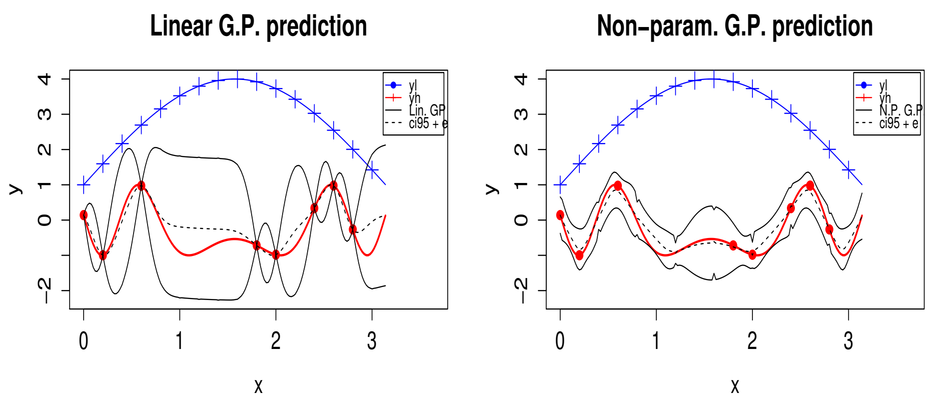
Then, we learn the parameters of

- $Y_1(x) \sim GP(\mu_1, k(x, x; \theta_1))$ by using (X_1, Y_1)
- $D_{12}(x) \sim GP(\mu_{12}, k(x, x; \theta_{12}))$ by using $(X_2, Y_2 - \widehat{\varphi}(Y_1(X_1))$.

We solve 2 separate small optimization problems to fit a fairly complex model.

Example

- Left: Linear relationship hypothesis prediction with confidence intervals.
- Right: Locally linear hypothesis prediction with confidence intervals.



Conclusions: Locally linear Cokriging.

- Simple generalization that keeps all the desirable characteristics of the existing methods.
- Estimating φ is a sensible way to integrating all the training sets.

Perspectives: Locally linear Cokriging.

- Uncertainty propagation of the estimated parameters of the model.
- Consider more general relationships in the form of parametrized curves.

Coarse to fine multi-fi wavelet regression

For each fidelity level we solve

$$\min_{\lambda 1} \sum_{i=1}^{m1} (y_1^i - f_1(x_1^i))^2 \quad \min_{\lambda 2} \sum_{i=1}^{m2} (y_2^i - f_2(x_2^i))^2$$

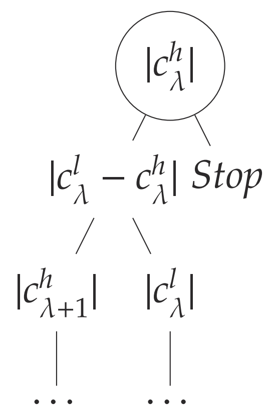
$$f_1(x) = \sum_{\lambda 1 \in \Lambda 1} c_{\lambda 1} \psi_{\lambda 1}(x) \quad f_2(x) = \sum_{\lambda 2 \in \Lambda_2} c_{\lambda 2} \psi_{\lambda 2}(x)$$

Where $\psi_{\lambda 1}$ and $\psi_{\lambda 2}$ are B-spline wavelets of any degree.

Adaptive algorithm

At iteration k, we chose the wavelet basis functions ψ_λ by looking at the size of its coefficients c_λ.

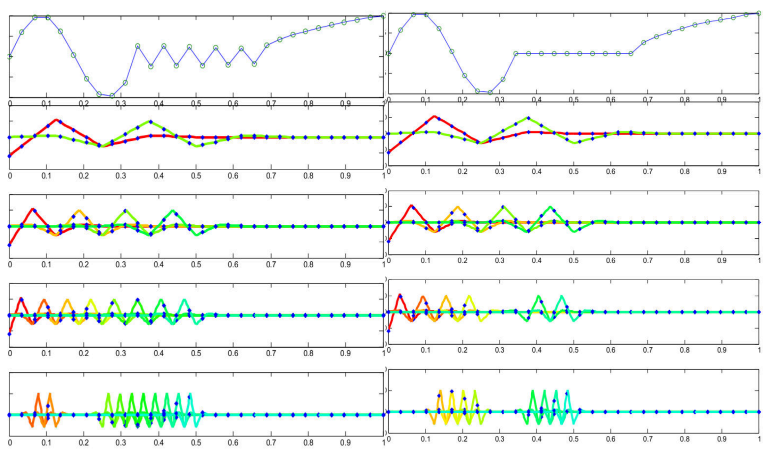
Add observations to solve the least-squares problem when needed.



The idea is to use the similarities between the two levels to add more observations produced by the fast simulator.

Example

- Left: Precise simulation with chosen wavelet basis.
- Right: Rough approximation with chosen wavelet basis.



Conclusions: Coarse to fine multi-fi. wavelet regression.

- Alternative method that does not relies on the Gaussian hypothesis.
- An algorithm that deals with the resource allocation problem.

Perspectives: Coarse to fine multi-fi. wavelet regression.

- Better understanding of the refinement process: Build statistical test.
- Test the algorithm on complex simulations: higher dimension.

Bibliography

Daniel Castaño and Angela Kunoth, *Robust regression of scattered data with adaptive spline-wavelets.*, IEEE transactions on image processing : a publication of the IEEE Signal Processing Society **15** (2006), no. 6, 1621–32.

Loic Le Gratiet, *Bayesian analysis of hierarchical multi-fidelity*, (2012), 1–30.

M Kennedy and A O'Hagan, *Predicting the output from a complex computer code when fast approximations are available*, Biometrika (2000), no. 87, 1–13.

Zertuche.Federico@imag.fr, Celine.Helbert@ec-lyon.fr, Anestis.Antoniadis@imag.fr –