Introspective metamodeling and thrifty optimization for simulated physical phenomena.

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Abstract:

Scientists and experts from many domains frequently use computer codes to simulate physical phenomena. It is especially true in the field of nuclear safety, where real experiments might be unsafe. At the French Institute of Nuclear Safety and Radiation risks (IRSN), experts in criticality safety repeat simulations often in an attempt to find the configuration which leads to a worst case scenario as an important information for decision making [3]. For such inverse problem solving, the usual way is to run an optimization algorithm, which automatically triggers many evaluations in different configurations. A key limitation of this process is that simulations are expensive. They need computing resources and time to achieve, and the more precise the expected result is the more it needs to be obtained. To reach to a conclusion with time-consuming simulation codes, experts need thrifty optimization algorithms to conduct their studies.

Algorithms adapted to expensive objective functions have been developed for a long time. The most used one is probably the Efficient Global Optimization (EGO) algorithm [2]. This algorithm is based on a kriging metamodel, that acts as a surrogate for the computer code. A kriging model is built by conditioning a Gaussian process by known simulation results in such a way that it interpolates them. Its predictions are normal distributions and, as a stochastic process, sample trajectories can also be simulated. Kriging allows the EGO algorithm to estimate the point which is expected to lead to the larger improvement from the currently known best configuration. Such criterion makes EGO global in scope in that it looks for the optimum not only close to the previous best iterate but also at regions of the configuration space where information is lacking.

In many cases of practical interest, those algorithms can be further improved by using an additional feature of the simulation: it is common that the simulations are computed by a chain of different codes. The first codes often provide information which is highly correlated to the final simulation at a lower computing cost (see Figure 1 below). This has to be exploited by the optimization algorithm in order to save time or to improve the conclusion confidence.

The first step of the work is to build *introspective* metamodels able to exploit the partial information internal to the simulations chains and thus improve the accuracy of the model at a given computational budget. For this we have devised "co-kriging" models [1], which extend kriging by supposing a linear correlation between the different kinds of information (referring to Figure 1, we need a covariance function not only between $Z(x_1)$ and $Z(x_2)$, but also between $Z(x_1)$ and $Y(x_2)$). Various implementations have been tested and compared. Evaluating the accuracy of a stochastic metamodel such as kriging should go beyond calculating a mean square error, because not only the mean prediction but rather the whole predicted distribution has to be considered.

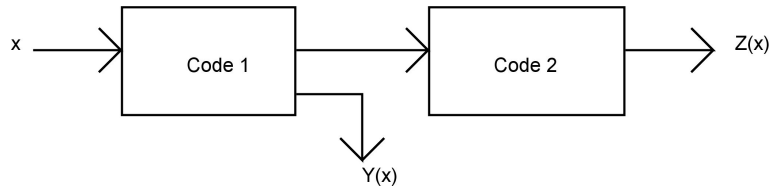

Figure 1: In the industrial application, the simulations are computed by two chained codes. The first one computes, from the given configuration (x), many physical values that are needed by the second code, but also a value $Y(x)$ which is the solution for the simplified physical problem and thus is somehow informative of the higher accuracy value $Z(x)$.

Moreover co-kriging is not the only way to build an introspective metamodel: we have also proposed "hyper-kriging", which works by composing kriging models (we first build kriging models for $Y(x)$ and for $Z(x, y)$, and then build up $Z(x)$ by composition). Tests performed on random functions show that hyper-kriging is more accurate, even when the functions are generated from co-kriging models. Nevertheless hyper-kriging is less practical for numerical purposes due to the loss of the normal distribution property of the predictions, and thus some analytical results (such as those underlying EGO) cannot be directly exploited.

Once a suited introspective metamodel is given, only a few changes are needed to adapt EGO. The new algorithm, called "Step or Stop" (SoS), first uses the classical EGO criterion to choose the most informative configuration to simulate, then runs the first part of the chained code, and with the newly obtained informations, estimates if computing the rest of the chain is worth the additional computing time. The SoS algorithm can easily be generalized to cases where the simulation chain is longer than two codes. In our industrial application, the first part of the simulation is the fastest, about 10 times faster than the second part, so SoS can efficiently save time by not fully computing simulations of low interest. The first tries of SoS on toy functions show noticable time-savings when the hypothesis upon the relation between the first and the second part of the codes are correctly described.

References

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Short biography – Nicolas Garland began this PhD thesis in 2014, after a Master's Degree in Applied Mathematics, specialized in statistics, and an internship at IRSN (Cadarache) about optimization and metamodelling. This PhD thesis is funded by IRSN (Fontenay-aux-Roses).