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Kriging-based optimization algorithms for noisy data

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Abstract. Responses to many real-world problems can only be evaluated perturbed by noise. Intelligent optimization strategies, successfully coping with noisy evaluations, are required in order to enable making efficient optimization of these problems. The surrogate model has been popularly used in the area of design optimization with high computational cost, especially in Kriging-based optimization algorithms. The performance of those algorithms depends on a sequential search of so-called infill points, used to update the Kriging meta-model at each iteration. This article explores the most relevant single and multi-objective infill algorithms used for Kriging-based optimization with noise-handling strategies. Those algorithms explore information about the variance of the predictor and the noise from stochastic simulation.

Keywords: Optimization problem, Kriging metamodeling, noise data, Infill criteria

1 Introduction

Recent computational advances have allowed the mathematical models of engineering problems to become highly complex, including a greater amount of data, details and refinements. Practical examples can be observed when analyzing a beam by considering a higher-order beam model, plasticity, damage theories, and other sources of non-linearity, and approximating the solution using a state-of-the-art finite element model. All of this procedure would still be a rough representation of reality if the intrinsic randomness of materials (rock, soil, concrete) and loads (wind, earthquake motion) were disregarded and a deterministic average was used [1].

A high computational cost optimization problem-solving strategy has been the approach of predictive response surfaces through meta-models. The primary motivation for using meta-models in simulation optimization is to reduce the number of expensive fitness evaluations without degrading the quality of the obtained optimal solution.

There is extensive literature on the different meta-modeling techniques, from which we can highlight the deterministic Kriging meta-model ([2] e [3]), also known as Gaussian Process Regression (GPR) meta-model or Gaussian random field models ([4]), which have traditionally been popular in engineering.

There have been several efforts to extend deterministic Kriging to what is called stochastic Kriging (SK) which employs Gaussian processes for the optimization of functions in the presence of noise or uncertainties, acting as a regressor meta-model that extracts the smooth trend of the data and characterizes both the intrinsic uncertainty inherent in a stochastic simulation and the extrinsic uncertainty about the unknown response surface [5].

The Kriging meta-model performs efficiently because it not only approximates outputs over the entire search space (i.e., the response surface) but quantifies the prediction uncertainty provided through the mean square error (MSE), also known as Kriging variance [6]. Figure 1, adapted from [7], shows an example of Kriging based on noisy observations, where actual function is in bold blue, Kriging mean is in bold black, 90% confidence intervals are represented in mixed line and the circles are the observation values.

The performance of Kriging-based optimization algorithms depends on a sequential search of so-called infill points, used to update the predictor at each iteration. An infill criterion helps to balance local exploitation and global exploration during this search by using the information provided by the Kriging meta-model.

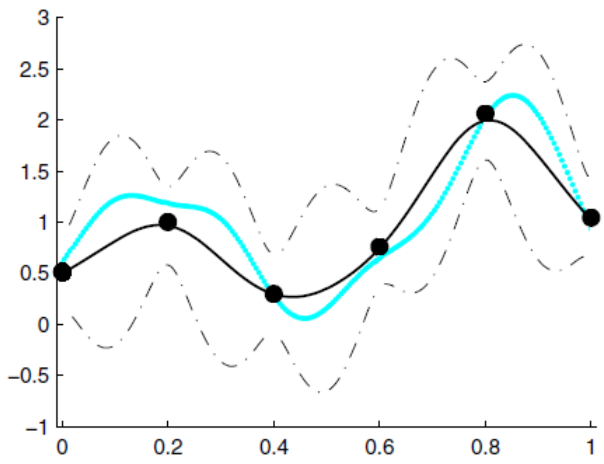

Figure 1. Kriging meta-model on noisy observations

Infill algorithms start by simulating a limited set of input combinations (referred to as the initial design), and iteratively select new input combinations to simulate by evaluating an infill criterion, also referred to as improvement function or acquisition function, that reflects the Kriging information [6].

The goal of this paper is the presentation of the most relevant single and multi-objective infill algorithms and some research carried out in the area that uses Kriging-based optimization with noise-handling strategies popular for expensive black-box functions. This article is organized as follows. Section 2 provides a brief explanation of the Kriging meta-model studied, Section 3 details the infill algorithms used in Kriging-based optimization with noisy handle, and lastly, conclusions are present in Section 5.

2 Kriging metamodeling

2.1 Deterministic Kriging

Kriging [8] is a functional approximation method originally coming from geosciences [2], and having been popularized in computer experiments [4]. To fit a meta-model for the response $f(x)$, the deterministic Kriging assumes that the unknown response surface ($\hat{y}$) can be represented as [5]:

$$\hat{y}(\mathbf{x}) = M(\mathbf{x}) + Z(\mathbf{x}). \tag{1}$$

where $M(\mathbf{x})$ is a vector of known trend functions, while $Z(\mathbf{x})$ represents the extrinsic uncertainty imposed on the problem due to predictor construction. $Z(\mathbf{x})$ is defined as a realization of a Gaussian random field with zero mean and stationary covariance.

What links one observation to another is the covariance function, denoted $\sum_z$, also referred to as *kernel*. Multiple covariance functions exist in the field of Gaussian process, the choice depends on prior hypothesis about the unknown functions. One of the most commonly used *kernel* in Kriging literature is the stationary squared exponential as a Gaussian base [6], Equation 2, which is the focus of this research.

$$\left[\sum\nolimits_z\right]_{ij} = \sigma_z \mathbf{h}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \sigma_z exp\left[-\sum_{k=1}^{n_x} c_k |x_k^{(i)} - x_k^{(j)}|\right]^{p_k}. \tag{2}$$

where σ_z is the variance of uncertainty caused by the construction of the surrogate model, $\mathbf{h}$ is the correlation vector, c_k and p_k are hyperparameters from the meta-model. The hyperparameters of these covariance function are usually estimated using Maximum Likelihood Estimation (MLE). The Kriging prediction and variance for a given point x^+ are, respectively:

$$\hat{y}(x^+) = \hat{\mu} + \mathbf{h}^T \Psi^{-1}(\overline{\mathbf{y}} - 1\widehat{\mu}) \tag{3}$$

$$s^2(x^+) = \hat{\sigma}_z^2 \left[1 - \mathbf{h}^T \Psi^{-1} \mathbf{h} + \frac{(\mathbf{1} - \mathbf{1}^T \Psi^{-1} \mathbf{h})^2}{\mathbf{1}^T \Psi^{-1} \mathbf{1}}\right]. \tag{4}$$

where $\hat{\mu}$ and $\hat{\sigma}_z^2$ is the mean and variance trend of the Kriging meta-model, respectively, Ψ is the covariance matrix of all the support points of Z and $\overline{\mathbf{y}}$ is the vector of the approximate mean value of the objective function at each design point, those parameters are defined in [6].

It is possible to use Kriging to filter or regress the noise inherent in predictor construction. To achieve this objective, the regression parameter must be adjusted to the variance of the meta-model noise. [9] propose to add a regression constant λ to the main diagonal of Ψ, that is, we now have $(\Psi + \lambda\mathbf{I})$ where $\mathbf{I}$ is the identity matrix.

2.2 Stochastic Kriging

To deal with functions on the presence of noise or uncertainties, the extension of deterministic Kriging for stochastic Kriging (SK) was proposed [5]. We thus focus on SK for being capable of accommodating noisy evaluations in the optimization framework.

In the stochastic Kriging (SK) it is added a parcel ϵ for meta-model construction, Equation 5, to account the sampling variability inherent in a stochastic simulation, which represents an intrinsic uncertainty of the problem.

$$\hat{y}(\mathbf{x}) = M(\mathbf{x}) + Z(\mathbf{x}) + \epsilon(\mathbf{x}). \tag{5}$$

where $\epsilon(\mathbf{x})$ has zero mean and is independently and identically distributed across replications.

The SK prediction and variance for a given point x^+ are, respectively:

$$\widehat{y}(x^+) = \hat{\mu} + \hat{\sigma}_Z^2 \mathbf{h}^T \left[\sum{}_Z + \sum{}_\epsilon\right]^{-1} (\overline{\mathbf{y}} - \widehat{\mu}\mathbf{1}). \tag{6}$$

$$s^2(x^+) = \hat{\sigma}_Z^2 - (\hat{\sigma}_Z^2)^2 \mathbf{h}^T \left[\sum{}_Z + \sum{}_\epsilon\right]^{-1} \mathbf{h} + \frac{\delta^T \delta}{\mathbf{1}^T \left[\sum{}_Z + \sum{}_\epsilon\right]^{-1} \mathbf{1}}. \tag{7}$$

where $\delta(\mathbf{x}^+) = \mathbf{1} - \mathbf{1}^T \left[\sum{}_Z + \sum{}_\epsilon\right]^{-1} \hat{\sigma}_z^2 \mathbf{h}(\mathbf{x}^+)$, $\mathbf{h}$ is the correlation vector, $\hat{\mu}$ and $\hat{\sigma}_z^2$ are the mean and variance trend of the SK meta-model, respectively, $\sum{}_Z$ is the covariance matrix of all the support points of Z, $\sum{}_\epsilon$ is the covariance matrix of ϵ and $\overline{y}$ is the vector of the approximate mean value of the objective function at each design point, those parameters are defined in [5].

3 Stochastic Kriging-based optimization

Stochastic optimization in engineering problems has been called robust optimization where the uncertainties are represented probabilistically, using random variables or stochastic processes. Assuming that the system performance is given by the function $f(\mathbf{x}, \theta)$, where θ is the vector of random parameters and $\mathbf{x}$ is the vector of design variables. The expected value (E) and variance (V) in practical problems can hardly be evaluated analytically, so approximations are made using simulation such as Monte Carlo Integration (MCI).

The meta-model approach is just an approximation of the actual function $f(\mathbf{x}, \theta)$ that we want to optimize, so it is prudent to increase the response surface accuracy by using other function calls besides the initial sampling plane, these are called Infill Points (IPs). Those updates points are determined by exploring the meta-model information.

In recent years, several infill criterion have been approched aimed Kriging-based algortihms. For robust optimization problems with significant noise, algortihms that includes information about stochastic function noise has been proving better performance in order to refine the response surface models when performing optimization [10].

The use of Kriging meta-model is attractive because, not only can it give good predictions of complex landscapes, it also provides a credible estimate of the possible error in these predictions. So, in Kriging-based optimization algorithm, the error estimates make it possible to make tradeoffs between sampling where the current prediction is good (local exploitation) and sampling where there is high uncertainty in the function predictor value (global exploration), allowing searching the decision space efficiently [11].

Thus, filling algorithms start by simulating a limited set of input combinations (referred to as initial design) and iteratively select new input combinations to simulate by evaluating a fill criterion, also known as an enhancement function or acquisition function, that reflects information from the Kriging. The response surface is then updated sequentially with information obtained from the newly simulated fill points; the procedure is repeated until the computational budget is exhausted or a desired performance level is reached and the estimated optimum is returned [12].

We distinguish two major categories of infill criteria: single-objective and multi-objective infill criteria. In single-objective infill criteria, the improvement brought by an infill point (IP) is measured in reference to each individual objective, or to a scalarized single objective function. Differently occurs in multi-objective formulating that exploit how to optimize a set of competing objectives, in Kriging predictor could be information about the predictor and its variance [12].

Exists a number of Kriging-based optimization algorithms that explore different point addition metrics - Infill criterion. The traditional Efficient global optimization (EGO) approach of [11] is one of the most popular Kriging-based algorithms for optimizing noiseless simulation. We can still quote expected quantile improvement (EQI) proposed by [13], an adapted version of the sequential Kriging optimization (SKO) approach by [14] and correlated knowledge-gradient (CKG) proposed by [7].

In the following topics, we will introduce some of the most relevant Kriging-based optimization algorithms for single and multi-objective simulation optimization that consider information from the noisy stochastic function on process.

3.1 Single objective infill criteria optimization

In this section the focus is to introduce some single-objective infill criteria with noise-handling strategy applied in Kriging meta-model. In that case, the improvement is measured regarding only one objective, but the selection of infill points is based on the tradeoff between the objectives where the optimum values are and where have high uncertainty prediction.

Those algorithms focused here assume heterogeneous simulation noise, meaning that the variance of the noise depends on support design point, and presents stochastic noise information in its formulation.

Augmented expected improvement (AEI): Addressed by [14], is an extension for stochastic function evaluation of the Expected Improvement (EI) criterion presented by [11] for the deterministic case. Therefore, in the formulation, uncertainties about the noise of the stochastic function and the prediction by Kriging meta-model are taken into account. The maximum AEI as the next infill point is:

$$AEI(x^+) = E[I(x^+)] \left(1 - \frac{\hat{\sigma}_\epsilon^2(x^+)}{\sqrt{\hat{s}^2(x^+) + \hat{\sigma}_\epsilon^2(x^+)}}\right) \tag{8}$$

where $\hat{s}^2$ is the variance of the meta-model expected value and $hat\sigma_\epsilon^2$ is the variance of the function noise.

Some authors approach this technique like [9] that used AEI as infill criterion applying efficient global optimization (EGO) method as optimization algorithm for homogeneous noise. [10] and [15] introduced the variance parcel to reflect the presence of heterogeneous noise. And more recently [16] used AEI as base infill criteria for formulation of a multi-objective engine calibration problem with constraints.

Correlated knowledge-gradient (CKG): Behind this infill criterion is that in noisy environments, the Kriging prediction $\hat{f}(x)$ may be closer to $f(x)$ than the sample mean $\overline{y}$; therefore, points are selected based on their effect on the Kriging prediction [10]. This algorithm allows for revisits and uses a fixed number of simulations replications per iteration. [17] used CKG infill criterion and CKG as optimization algorithm for homogeneous noisy.

A continuous approximation of the knowledge gradient that can be calculated and optimized when the feasible set of decisions is continuous was propose by [18]. The approximation proposal can be calculated at a particular decision, x, along with its gradient at x, allowing to use classical gradient-based search algorithms for maximizing it. The performance is demonstrated in the calibration of an expensive industrial simulator.

Expected quantile improvement (EQI): This criterion was propose by [13]. Starting from the consideration that using only the noisy observations is a highly risky strategy, since the noise may introduce errors in the ranking of the observations. So, it uses the β-quantiles given by the Kriging conditional distribution, for a given level $\beta \in [0.5, 1)$ a point x^* is declared the best over a set of candidates x_n whenever it has the lowest β-quantile:

$$x^* = argmin_{x \in x_n}[q_n(\mathbf{x})] = argmin_{x \in x_n}[\hat{y}(\mathbf{x}) + \Phi^{-1}\beta s^2(x^+)] \tag{9}$$

where q_n is the quantile of the updated Kriging meta-model at x_{n+1}, $\hat{y}$ is Kriging predictor and Φ is the cumulative probability density of the normal distribution. Thus, improvement I is defined to be the a decrease of the lowest β-quantile between the present step n and the forthcoming step $n+1$:

$$I(\mathbf{x}^{n+1}) = \big[\big] min q_n(\mathbf{x}) - q_{n+1}(\mathbf{x}^{n+1})\big]^{+} \tag{10}$$

So the next point is the point with maximum EQI($\mathbf{x}$)=$E[I(x)]$. This calculation requires an estimate of a stochastic function variance.

An EQI as infill criterion and optimization algorithm method for homogeneous simulation noise was use by [13]. [15] used EQI as infill criterion and applying efficient global optimization (EGO) method as optimization algorithm for heterogeneous noise.

3.2 Multi-objective infill criteria optimization

This section introduces some infill criteria approach in optimization of Kriging-based algorithms with noise-handling strategies for multi-objective simulation. In that case, the improvement is measured regarding each separate objective, in general, those methods propose that instead of adapting the Infill criterion for stochastic cases, they use noise-handling strategies.

Static resampling (SR): Replicate the objective values for each design a fixed number of times and take the average over time for short. This method reduces the variance of the objective function estimated increasing the sample size, sampling an individual's objective N times reduces the corresponding standard deviation by a factor of $\sqrt{N}$. In the simple approaches, the number of samples (sample size) for each individual is predefined and fixed. Since each sampling (objective evaluation) could be very expensive, it is desired to reduce the sample size as much as possible without degrading the performance [19]. Assume homogeneous simulation noise.

SR as noise treatment strategies as use by [20] and [21], applying $\mathcal{S}$ Metric Selection based-EGO (SMS-EGO) as optimization algorithm and Lower Confidence Bound (LCB) and Expected Hypervolume Improvement (EHI) as infill criterion.

Kriging with nugget effect (KNE): as defined in [12], the term "nugget" refers to a variation or error in the measurement. This nugget is often used to model the effect of white noise in the observations, under the assumption that the variance of the noise is homogeneous; thus this variance is a constant. The nugget effect is introduced in the kernel structure by adding a hyperparameter that models the variability in the observations; the Kriging metamodel then loses its interpolating nature. Assume homogeneous simulation noise.

[20] also used KNE as noise treatment strategies. Others authors were [22] applying PESMO as optimization algorithm and predictive entropy search (ES) as infill criterion, and [23] applying ϵ-Pal as optimization algorithm and ϵ-Pareto as infill criterion.

***Re-interpolation (RI)* for homogeneous noisy**: Use deterministic experiments to measure the uncertainty in the result due to the noise in the data. So Forrest builds first an initial Regression Kriging metamodel with noise in the data and then fits an interpolating Kriging response surface model with zero error at the sample locations through the values predicted. Observe that Regression Kriging metamodel assumes homogeneous simulation noise. [6] applies in a regressing Kriging (homogeneous noise) model surface that extracts a smooth trend from the data and filters out this noise.

$$\hat{y}(\mathbf{x}_{n+1}) = -\hat{\mu} + \mathbf{h}^T\mathbf{R}^{-1}(\hat{\mathbf{y}}_r - \mathbf{1}\hat{\mu}) \tag{11}$$

where,

$$\hat{\mu} = \frac{1^T\mathbf{R}^{-1}\mathbf{y}}{1^T\mathbf{R}^{-1}\mathbf{1}} \tag{12}$$

where $\mathbf{R}$ and $\mathbf{h}$ are the covariance matrix and the correlation vector, respectively. Those remain unchanged and so it is not necessary to re-optimize the parameters of the meta-model.

RI also was use by [21] as noise treatment strategies. Other authors were [24] applying Efficient Global Optimization (EGO) as optimization algorithm and Expected Improvement (EI) as infill criterion.

***Re-interpolation (RI)* for heterogeneous noisy**: Different of [9], [15] build a model response surface based on heterogeneous noise through the data, meaning that the variance of the noise is not constant, does depend on position of support design point, which is foreseen in covariance matrix $(\sum)$ and the correlation vector $(\mathbf{h})$. He is applying Efficient Global Optimization (EGO) as optimization algorithm and Expected Improvement (EI) as infill criterion.

Rolling Tide Evolutionary Algorithm (RTEA): This algorithm was proposed by [25] which gives a heuristic on how to choose promising settings for re-evaluations and used by [20] in Kriging regression meta-model. The main idea of RTEA is to handle noise by re-evaluating only promising settings, while inferior settings are evaluated only once. In each iteration, after a new point has been proposed using evolutionary operators, k already evaluated points are chosen for re-evaluation. The selection of these k points is based on the dominance relation and the number of prior re-evaluations. An interesting feature is that new points are only proposed in the first part of the optimization, the second part is used to solely refine the archive. [21] used SMS-EGO as optimization algorithm and LCB and EHI as infill criterion. [25] still propose others approaches of learning the variance during optimisation.

4 Conclusions

This paper presented Kriging-based algorithms for optimization via simulation with noise-handling strategy for stochastic black-box simulations. Different infill criteria techniques can be approached which can be distinguished into two major classes, single and multi-objective simulation.

In single objective simulation the improvement is measured regarding only one objective and the stochastic noise is represented directly on formulation. As in the multi-objective infill criteria the improvement is measured regarding each separate objective, in general noise-handling strategies are adopted in the process. The techniques covered in this article require an estimate for the stochastic function noise, this information is critical in the optimization process based on the Kriging metamodel to represent problems with significant noise.

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