Enhanced Meta-model Based Optimization under Constraints using Parallel Computations

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Meta-models proved to be a very efficient strategy for optimization of expensive black-box models, e.g. Finite Element simulation for electromagnetic devices. It enables to reduce the computational burden for optimization purposes. Kriging is a popular method to build meta-model. Its statistical properties were firstly used in efficient global optimization for unconstrained problems. Afterwards many extensions were introduced in the literature to deal with constrained optimization. This paper presents a comparative study of some infill criteria for constraints handling and a new strategy for parallelization of the expensive computations of models.

***Index Terms*—Constrained optimization, Expensive simulation, Kriging, Parallelization strategy.**

I. Introduction

Meta-models are used in many fields, mainly to replace expensive black-box models. In an optimization problem the objective function and/or constraints are not always cheaply available data, thus these surrogate models aim to give a model able to approximate the expensive black-box models from a limited number of solutions. Optimization using meta-models were first introduced in [1] to tackle unconstrained optimization. Its main advantage is the reduction of the number of calls to the expensive model. However, for problem with high number of parameters the number of evaluations arises exponentially (curse of dimensionality). Thus, the purpose of this paper is to compare methods to handle constraints and propose a new strategy for parallelization, which enables to run several evaluations at each iteration. A brief review of meta-model based optimization and infill criteria for constrained optimization is presented. Then, the parallelization strategy is presented and tested on an analytical model.

II. Meta-model based optimization

Meta-model based optimization can be as in Fig. 1. The first step aims to determine initial set of parameter values (initial design) using a design of experiments, e.g. Latin Hypercube Sampling (LHS). The full (expensive) model is solved for each set of parameters. Afterwards a meta-model is built based on the initial design and the output data. Kriging is well suited for building the meta-model due to its statistical properties. The most important part in the process is to find the infill point which improves the actual best solution and increases the meta-model precision. This point will be evaluated using the full model in the next iteration. In Fig. 1, the arrow that goes out and come back in to the same step means that a sub-optimization problem is dealt with in that step. Finally some stopping criteria are evaluated to terminate the optimization.
Kriging is an interpolation based on a regression term and a stochastic term. The stochastic term aims to eliminate the error due to regression and is constructed based on the location of the sampled points. Kriging is one of the interpolation methods that characterize the variance, or the precision, of the prediction. In [2] an exhaustive presentation and the implementation of kriging predictor are detailed. The developed toolbox is used in the numerical evaluation.

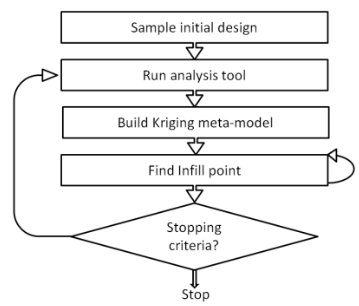

Fig. 1. Flowchart of kriging meta-model based optimization.

III. Infill criteria

The most famous infill criterion to deal with unconstrained optimization is Expected Improvement (*EI*) criterion, presented in [1]. This criterion enables a tradeoff between exploitation and exploration of the design space.

Maximizing *EI* leads to the point with the highest probability of improvement, either by sampling toward the optimum or improving the approximation of the meta-model.

There exist other infill criteria, they often reveal striking similarities, an exhaustive set of infill criteria was presented in [3] for unconstrained and constrained optimization. The probability of feasibility (*PF*) criterion is widely used for constrained optimization.

$$PF(x) = \Phi\left(\frac{-\hat{g}(x)}{\hat{s}_g(x)}\right) \quad (1)$$

where $\hat{g}$ and $\hat{s}_g$ are the expected value and the standard deviation of the kriging predictor for a constraint $g \leq 0$.

To sample point that improves the actual solution and respects constraints both EI and PF should be maximized. Table I summarizes the main formulations.

The first formulation has a statistical derivation. It aims to sample points that maximize the expectation of improvement and constraints satisfaction. However the product of EI and PF reveals high multimodality and algorithms often fail to find the global optimum. Thus, the second formulation was proposed to consider the infill criterion as bi-objective. The points chosen are the ones that maximize both EI and PF and belong to the Pareto front. For both formulations, one concern is that it impacts the search close to the constraints boundary, so if the optimum lies on the constraints boundary these infill criteria may fail to find it. The third formulation was proposed in [3] and considers the problem as a constrained one to reduce the multimodality of the infill criterion and to gain in precision of the solution. $P_{tol}=0.95$ was recommended but it has an effect on the precision. The authors' opinion is that $P_{tol}=0.5$ seems more reasonable because $PF=0.5$ when $\hat{g}=0$.

In the case of many constraints, the first two formulations consider the global PF as the product of the probability of feasibility of each constraint. The third formulation considers each constraint independently and calculates their respective probabilities of feasibility, ending up with the same number of constraints as the original problem. A modified formulation aims to consider the product of the probabilities of feasibility, reducing the number of constraint to only one.

As stopping criterion, the variation of *EI* for successive iterations is less than a specified threshold.

TABLE I

INFILL CRITERIA FOR CONSTRAINED OPTIMIZATION

Formulation	Infill point determination
1	$\max_d EI(d).PF(d)$
2	$\max_d (EI(d), PF(d))$
3	$\max_d \; EI(d)$ $s.t.\; PF(d) \geq P_{tol}$

IV. PARALLELIZATION STRATEGY

In the sequential process, only one point is found by maximizing *EI*. The aim of the parallelization strategy is to find multiple promising points at each iteration to take advantage of and clusters by running distributed evaluations.

In [4] the straightforward extension of EI from sequential to parallel was presented. As the infill criterion has not an analytic expression for more than two points, the authors propose its estimation through Monte Carlo simulation. In [5] a hybrid method was proposed. It adds artificially the point found at each iteration to a subset, evaluate it with the kriging predictor, and reconstruct the meta-model. Afterwards, the next point is found until reaching the number of required points. When the number of evaluated points increases, the construction of the meta-model become a time consuming step which penalize the whole process.

The proposed method is based mainly on the multimodal behavior of *EI* and searches the points that maximize *EI* and exclude its vicinity to find another point. The process is repeated until the number of excluded points equals the number of required parallel evaluations. The exclusion area is defined by the distance from that point.

V. ANALYTICAL TEST

A comparison on an analytical problem from [6] is done. 10 tests for each formulation were done with different initial designs of experiments generated by the LHS. Furthermore SQP algorithm with 10 start points uniformly random chosen from the space, is presented. The averages of the results are shown in Table II. The metrics used for comparison are the convergence rate (*C.R.*) that is the percentage of the 10 tests that converge to the known solution for less than 1% of the range of variable. *dist* is the Euclidean distance to the known solution for the tests that converged, *evals* is the mean number of evaluations of the exact model, and *time* is mean computing time. The table shows that *SQP* and the third formulation with $P_{tol}=0.95$ have the lowest convergence rate. The first and second formulations have good convergence rates but the number of evaluations is higher. Due to the multimodality of the problem, the algorithm often fails to find the global optimum. The modified third formulation shows the best results among the sequential formulations.

For the parallelization strategy, three evaluations of the exact model at each iteration were done. The results show that the number of exact model evaluations has increased by 42%, however the time decreased by 52%.

TABLE II

COMPARISON OF OPTIMIZATION RESULTS

Formulation	C.R	dist	evals	time (s)
SQP	0.3	1.00e-6	31.5	0.13
1	0.8	3.26e-2	47.7	57.24
2	1	4.09e-2	55.3	66.36
3 ($P_{tol}=0.95$)	0.4	3.47e-2	32.5	39.00
3 ($P_{tol}=0.5$)	0.9	1.42e-4	37.4	44.88
3 modified	1	1.27e-5	36.2	43.44
Parallel	1	2.11e-5	52.5	21.00

VI. CONCLUSION

In this communication, we have developed a strategy of optimization based on kriging meta-model and the parallelization of the computations of the full model. The results obtained on an analytical example are promising.

This strategy is currently assessed on the TEAM Workshop problem 22 with 8 variables and will be presented to the conference.

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