Multi-Point Infill Sampling Strategies Exploiting Multiple Surrogate Models

P. Beaucaire
Cenaero
B-6041 Gosselies, Belgium
paul.beaucaire@cenaero.fr

Ch. Beauthier
Cenaero
B-6041 Gosselies, Belgium
charlotte.beauthier@cenaero.be

C. Sainvitu
Cenaero
B-6041 Gosselies, Belgium
caroline.sainvitu@cenaero.be

ABSTRACT

This work presents interesting multi-point search algorithms exploiting several surrogate models, implemented in MINAMO, the multi-disciplinary optimization platform of Cenaero. Many types of surrogate models are used in the literature with their own strengths and weaknesses. More generally, each one models differently a given problem and provides its own representation of the reality. The idea of this paper is to exploit simultaneously different types of surrogate models in order to catch automatically their strengths and to outshine some of their weaknesses. This strategy is based on a multi-point enrichment at each iteration, each candidate point being provided by one kind of surrogate model and/or criterion. This strategy can be tuned by selecting different infill criteria, based on different surrogate models, in order to improve more specifically different aspects such as feasibility, exploration and/or exploitation. The performance of this surrogate-based optimization framework is illustrated on well-known constrained benchmark problems available in the literature (such as GX-functions and MOPTA08 test cases). Good performance both in terms of identification of feasible regions and objective gains is demonstrated.

CCS CONCEPTS

• **Theory of computation** → **Online learning algorithms**; **Active learning**; • **Computing methodologies** → *Machine learning approaches*; *Modeling methodologies*; • **Mathematics of computing** → *Evolutionary algorithms*.

KEYWORDS

surrogate-based optimization, infill sampling criteria, multi-point, constrained design problems.

GECCO '19 Companion, July 13–17, 2019, Prague, Czech Republic

ACM ISBN 978-1-4503-6748-6/19/07...$15.00
https://doi.org/10.1145/3319619.3328527

ACM Reference Format:
P. Beaucaire, Ch. Beauthier, and C. Sainvitu. 2019. Multi-Point Infill Sampling Strategies Exploiting Multiple Surrogate Models. In *Genetic and Evolutionary Computation Conference Companion (GECCO '19 Companion), July 13–17, 2019, Prague, Czech Republic.* ACM, New York, NY, USA, 9 pages. https://doi.org/10.1145/3319619.3328527

1 INTRODUCTION

A globally effective approach to optimization problems based on computationally expensive high-fidelity computations lies in the exploitation of surrogate models. They act as cheap-to-evaluate alternatives to the original model reducing the computational cost, while still providing improved designs. A wide variety of techniques are available to build these models, such as Radial Basis Function Networks (RBFN) or Kriging, which all have their advantages and drawbacks, see [11]. The underlying principle of Surrogate-Based Optimization (SBO) consists in accelerating the optimization process by essentially exploiting surrogates for the objective and constraint evaluations, with a minimal number of function calls to the high-fidelity model for keeping the computational time within affordable limits [10]. The SBO design cycle considered in this contribution consists of several major elements as shown in Figure 1.

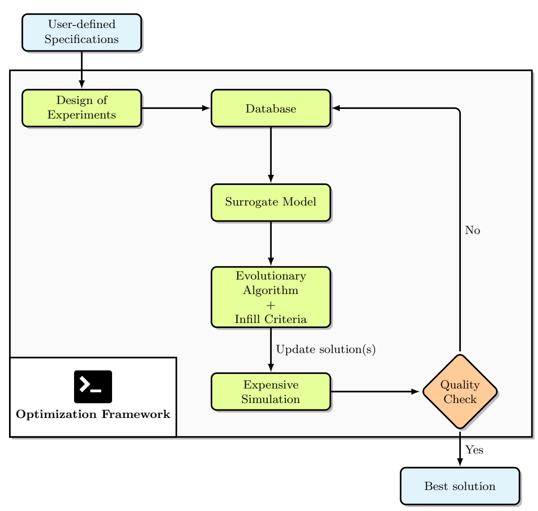


Figure 1: Online surrogate-based optimization framework.

Key to efficient SBO is above all the exploitation of a useful accuracy level as a compromise for fast but sufficiently reliable surrogate models. Surrogate-based approaches can be categorized as *online* or *offline* approaches, according to how the model interacts with the simulation and the optimizer. The advantage of the considered optimization strategy is its online modeling framework in which a model is created and is adaptively improved during the course of the optimization, while in an offline approach, the optimization is performed based on an *a priori* trained model. It is therefore beneficial to consider an online SBO context where the surrogate models are refined at each iteration, because a dynamic training of the surrogates during the optimization is much more efficient than having to rely on static surrogates. This online SBO, carried out by Minamo (see [27]), consists on several steps. First of all, a Design of Experiments (DoE) is defined using an *a priori* space filling technique LCVT (Latinized Centroidal Voronoi Tessellations). The objective is to extract as much information as possible from a minimum number of experiments for a pertinent knowledge base over the design space. After the evaluation of the DoE by the high-fidelity models, the next step is then the online SBO process. The surrogate models are trained based on the available information in the database, and an evolutionary optimization step is launched to generate new best candidates for the given optimization problem. These candidates are then evaluated by the high-fidelity models and their accurate performance is checked afterwards. Finally, the new candidates are added to the database and the online SBO is repeated until a satisfactory performance is achieved.

Two important questions are induced from this surrogate-based optimization scheme :

(1) how can we use the approximation models to suggest new, improved designs in order to balance exploration, exploitation and feasibility ?
(2) how to know which kind of meta-model is the more appropriate to resolve our problem ?

1.1 Infill sampling criteria

Recently, Yondo et al. [37] provide a comprehensive and present-day overview of surrogate-based optimization steps, like design of experiments, choice of the type of the surrogate models and infill criteria. Wang and Shan [36] give an overview of the meta-modeling techniques.

The first objective of infill sampling criteria (ISC) aims to extract knowledge from the surrogate models to find potential interesting areas for model refinement in order to strike a balance between model exploitation and exploration (and possibly feasibility). The goal with an infill search criterion is therefore to extract a maximum information from a minimum number of samples by balancing between :

- exploiting regions of the design space where the surrogate model indicates there might be a minimizer;
- exploring regions that are under-sampled and of high estimated surrogates' error;
- searching for feasible regions, i.e. regions where all constraints are satisfied.

One of the more popular approaches to select update points is the maximization of the Expected Improvement (EI). This criterion has been used by a number of authors for solving a variety of problems ; notably, in the Efficient Global Optimization (EGO) algorithm developed by Jones et al. [15], the generalized EI [29, 30], the weighted EI [32] and multi-objective EI [16]. Further studies have adapted EI to find multiple update points [12, 30], which is the topic of this study.

Parr et al. [22] provide a review of single update infill criteria for constrained problems showing that a probabilistic approach to constraint handling outperforms the penalty approach on a number of problems. This probabilistic approach, suggested by Schonlau [30], uses a product of the EI of the objective function and the probability of feasibility calculated from the constraint functions (see e.g. [24]). Parr et al. [21] treat the EI and the probability of feasibility separately and explicitly consider trade-offs between them by using multi-objective optimization. Similarly, Féliot [31] uses a sequential Monte Carlo techniques to compute and optimize the constrained EI extended for multi-objective optimization.

1.2 Multi-point strategy

In today's industrial setting it is commonplace for parallel computing architectures to be available to the designer and this option is very valuable in surrogate-based optimization. The updating strategy can be parallelized in the sense that several points can be evaluated by the simulation and added to the database at each design iteration. Furthermore, mono-point infill search criteria generally suffers from the complexity of combining and adjusting exploitation/exploration/feasibility in a unique point. It is therefore interesting to work on strategies that can add more than one point per design iteration in an online optimization scheme.

Using multiple updates is far from a new idea, having been notably explored by Schonlau [30]. With the availability of parallel computing becoming commonplace, formulation of multiple update infill criteria has received further attention in past years [35]. Ginsbourger et al. [12] have provided an extension to Schonlau's early work by providing a sound analytical expression for finding multiple updates based on the EI.

Some works highlight the benefits of using a probabilistic approach to handle inequality constraints when selecting single updates [22]. Motivated by these finding, some existing methods used to select multiple updates are modified to handle constraints using a probabilistic approach. By exploiting a smart blend of interpolation/regression (RBFN) and classification (Probabilistic Support Vector Machines (PSVM)), interesting mono- and multi-point infill sampling criteria have been proposed, to improve the evolutionary algorithm's ability to quickly reach feasible zones in order to tackle the challenges of highly constrained problems, see [2, 4].

1.3 Exploiting surrogate models

Surrogate modeling is at the core of the proposed strategy. The surrogates being problem dependent may produce unreliable results, if a wrong surrogate is selected. Many works have been done on the use of multiple surrogates with success to enhance the robustness of the optimization process, see e.g. [1, 28, 33]. Most of these approaches are based on either the building of several types of surrogate models and the selection of the best ones (based on quality metrics) or the aggregation of different types of surrogates by weighting them with a "quality" factor. These approaches help to overcome the *a priori* choice of type of surrogate models, see e.g [8, 13, 20, 34]. Viana and Haftka [35] notably propose an algorithm for adding several points per optimization cycle based on the use of multiple surrogates. They proposed an approach that enables running the EGO algorithm with multiple surrogates simultaneously. Recently, Dong et al. [9] use dynamically three types of surrogate models (Kriging, RBF and Quadratic Response Surfaces). A multi-point infilling criterion is presented to capture the new sample points on the three models per iteration by using a score-based strategy.

The purpose of this paper is to use multi-point strategy with multiple surrogate models based on multiple instance of evolutionary algorithms. In the next section, some reminders on basic concepts (surrogate models and infill criteria) are exposed. Our proposed multi-point strategies exploiting different surrogate models and infill criteria are described in Section 2.3. Then Section 3 shows the performance of the proposed strategies on well-known benchmark problems. Finally Section 4 gives some conclusions and perspectives for this work.

2 MULTIPLE SURROGATES-BASED OPTIMIZATION STRATEGY

The idea of this work is to define infill criteria that can use the information from several kinds of surrogate models, or to consider several times the same criterion but based on different surrogate models. These strategies are promising because each surrogate model can induce its own representation of the real expensive function and by combining them, it can profit from complementary information of the surrogate models. As explained in the introduction, the advantages of combining several surrogate models have already been studied via selection or aggregation of surrogate models strategies but are generally limited to one instance of the optimization algorithm. The idea of our strategy is to exploit the information yield by multiple surrogate models in a multi-point strategy within multiple instance of evolutionary algorithms (EAs). In order to define our strategy, we will first remind some basics concepts on surrogate models and infill criteria.

2.1 Surrogate models

In this study, we will consider two different surrogate models : auto-Tuned Radial Basis Function (TRBF) network and Kriging. RBF are linear models expressed as follows [5] :

$$y(x) = \sum_{i=1}^{n} w_i \; h\left(||x - c_i||_2, \sigma_i\right), \tag{1}$$

where n is the number of points in the database, the model y is defined as a linear combination of n radial basis functions, w_i's are the weights, h is called the hidden unit function or the basis function, c_i's and σ_i's denote, respectively, the centers and the widths of the basis functions. The parameter σ is a parameter controlling the smoothness of the interpolation. The goal of the approximator is to find the weights w_i minimizing the error between the real outputs and those predicted by the model. The considered auto-tuned RBF model implements a tuning so as the surrogate models are generated without having to prescribe the type of basis function (multiquadric or Gaussian) and hyper-parameter values (fixed and variable widths heuristics), see [27].

The mathematical form of a Kriging model is

$$y(x) = \mu(x) + Z(x) \tag{2}$$

where x is an m-dimensional vector (m design parameters), see [11]. The "global trend" $\mu(x)$ approximates globally the design space. *Ordinary Kriging* assumes a constant but unknown mean : $\mu(x) = \mu$. The second term of Equation (2), $Z(x)$, represents the local deviation from the global trend and is expressed using a stochastic process with zero mean and covariance

$$cov(Z(x_i), Z(x_j)) = \sigma^2 R(x_i, x_j),$$

where σ^2 is the process variance and $R(x_i, x_j)$ is the *correlation function* between points x_i and x_j defined by

$$R(x_i, x_j) = \exp\left(-\sum_{k=1}^{m} \theta_k |x_{i,k} - x_{j,k}|^{p_k}\right),$$

where $0 < \theta_k \leq \infty$ is the kth element of the correlation parameter denoted by θ and $p_k = 2$ in our study. The parameter θ_k is essentially a width parameter that affects how far a sample point's influence extends.

The best choice for the values of vectors θ_k can be obtained by maximizing the following likelihood function

$$-\frac{1}{2}\left(n \ln \sigma^2 + \ln(\det(R))\right), \tag{3}$$

over the domain $\theta_k > 0$. Maximizing the likelihood function (Equation (3)) is a multi-dimensional and multi-modal optimization problem. In this work, in order to reduce its computational training cost, the Kriging hyper-parameters are estimated by a BFGS local optimizer instead of a global optimizer like an evolutionary algorithm (EA).

2.2 Constraints management within an SBO framework

At each design iteration of an SBO process, new candidate points are generally selected based on an Infill Sampling Criterion (ISC) in order to extract a maximum of information from a minimal number of samples, aiming to promote a balance between exploration, exploitation and feasibility.

In highly constrained problems, one of the key ingredients towards the eventual location of the global optimum first lies in the identification of the potential feasible region(s). For this purpose, most classical constraint handling techniques [6] are based on penalty functions penalizing unfeasible samples, but suffer from necessary penalty parameters tuning. To efficiently search the feasible domain, Deb [7] has proposed a constrained tournament selection that unconditionally favors feasible (and successful) samples without any required tuning. This constraint handling technique works as follows :

- when two individuals are compared, the feasible one is always preferred to the unfeasible one ;
- if both individuals are feasible, the one with the best objective function value is chosen ;
- if both individuals are unfeasible, the one with the least violation of the constraints is preferred.

The most classical ISC used with Kriging surrogate model is the Expected Improvement (EI) which benefit from the variance provided by the surrogate itself. Let $f_{\min}$ be the best sampled function value after n evaluations of the function $y = f(x)$. For simplicity, we will leave out the dependence on x in this section, notating the predicted value $\hat{y}(x)$ as $\hat{y}$ and the Kriging variance $\hat{\sigma}^2(x)$ as $\hat{\sigma}^2$. Then the EI is defined as

$$EI = \begin{cases} (f_{\min} - \hat{y})\,\Phi(z) + \hat{\sigma}\phi(z), & \text{if } \hat{\sigma} > 0 \\ 0, & \text{if } \hat{\sigma} = 0 \end{cases} \tag{4}$$

where $\phi(\cdot)$ and $\Phi(\cdot)$ denote the probability density function and the cumulative distribution function of the standard normal distribution, respectively, and z is defined by :

$$z = \frac{f_{\min} - \hat{y}}{\hat{\sigma}}.$$

The Probability of Feasibility (PF) has been proposed by Schonlau [30] in order to deal with constraints. The criterion is similar to the probability of improvement for the objective. We denote by $\hat{g}(x)$ the Kriging prediction on the constraint. Suppose that the uncertainty in the predicted value at a position x can be described in terms of a normally distributed random variable $G(x)$ with mean $\hat{g}(x)$ and variance $\hat{\sigma}^2(x)$. The PF gives the area of the distribution $G(x)$ that is below the constraint limit $g_{\min}$, i.e. :

$$P[H(x) < g_{\min}] = \Phi\left(\frac{g_{\min} - \hat{g}(x)}{\hat{\sigma}(x)}\right)$$

where $H(x) = g_{\min} - G(x)$ is a measure of feasibility, $\hat{g}(x)$ is the Kriging prediction of the constraint function and $\hat{\sigma}^2(x)$ is its associated Kriging variance, see e.g. [10]. Therefore, the PF gives an indication of possible feasible regions in the domain.

The Constrained Expected Improvement (CEI) can therefore be defined as the product of EI of the objective and the probability of feasibility of the constraint, see [21, 23] :

$$CEI = EI(x) * P[H(x) < g_{\min}].$$

A suitable infill criterion for constrained problems is then obtained by maximizing the CEI. The criterion can easily be extended to several constraints by using the total probability of feasibility, which is given by the product of the individual probability of feasibility of each constraint.

2.3 Proposed multi-point strategies

Two infill criteria have been considered in this work :

- Deb's constraint tournament selection criterion [7] ;
- Constrained expected improvement (CEI) [23].

The main idea of our multi-point surrogate-based optimization framework is to perform two EAs in parallel either based on different types of surrogate models or based on different infill criteria. The principle of our multi-point strategies is illustrated in Figure 2. In these strategies, two points will be evaluated at each iteration. In future work, it should be interesting to compare with a strategy selecting only one point of the two points using a quality criterion based on the surrogate models in order to evaluate only this point with the real function, as proposed in [3]. In our study, the EA which is considered to optimize the surrogate models is a real-coded genetic algorith with traditional line and box recombination crossover operators and mutation operators that randomly disturb parameters values with a probability of 0.01.

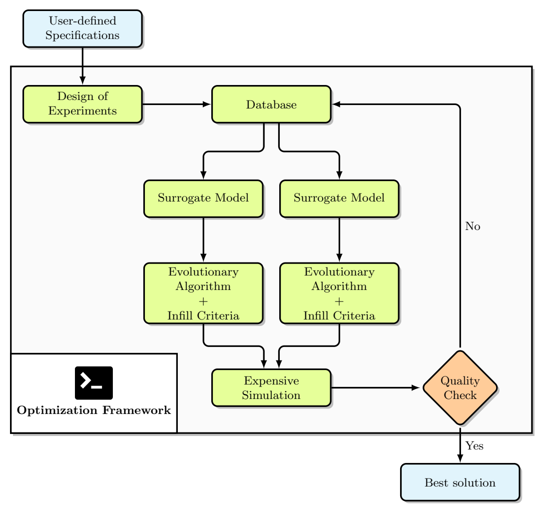


Figure 2: Parallel multi-point strategy in online surrogate-based optimization framework.

The following mono- and multi-point strategies will be compared in Section 3.

- `MonoTRBF` : Mono-point strategy using an auto-tuned RBF (TRBF) meta-model and Deb's constraint tournament selection to deal with contraints (framework of Figure 1) ;
- `MonoCEI` : Mono-point strategy using a Kriging model and CEI as infill strategy (framework of Figure 1) ;
- `MultiCEI` : Multi-point strategy with two evolutionary algorithms, the first one exploiting Deb's constraint tournament selection with a TRBF model, the second one based on CEI infill criterion with a Kriging metamodel. This strategy combines `MonoTRBF` and `MonoCEI` strategies (framework of Figure 2) ;
- `MultiMeta` : Multi-point strategy with two evolutionary algorithms, both searches are based on Deb's constraint

tournament selection but with either a TRBF model or a Kriging model (framework of Figure 2).

These strategies have also been compared to basic selection and aggregation of surrogate models strategies. They are not presented in this paper for lack of space and also because it has been shown that the multi-point strategies with multiple surrogate models outperform these selection and aggregation strategies.

3 NUMERICAL RESULTS

In this section, the different mono- and multi-point strategies described above are compared on well-known constrained benchmark problems available in the literature (such as GX-functions defined in e.g. [18, 26]). In order to achieve a fair comparison, the different strategies are executed in the same conditions : 100 independent runs, started from an initial database (LCVT) of size $n+1$, n being the number of design variables. The results are presented on different graphs for each test case :

- a graph showing the evolution of the objective function (mean of 100 runs with 95% confidence interval). At each iteration, the best point from the optimizer which satisfies all the constraints and which has the minimal objective value is extracted and used to compute the mean. Therefore, this graph depicts the curve only for feasible points (respecting all the constraints) ;
- a graph showing the evolution of the number of violated constraints (mean of 100 runs) when it is relevant.

Furthermore, performance profiles (introduced in [19]) give information about the global trend of the different strategies on the whole set of benchmark problems. They act as principle that an algorithm solves the problem (each of test cases) when the objective function (mean here) passed a fixed threshold. Two kinds of thresholds are considered. The large threshold (`LargeThres`) allows to identify the strategies which gives the best performance in an approaching phase of the optimum zone while the fine threshold (`FineThres`) is more interesting for the final convergence of the algorithm, for the fine-grained search of the best optimum. Since the feasibility concept is not present in the original version of these profiles, each run has been considered independently so that one run will solve the problem if the objective of a feasible point is lower than the given threshold.

Note that all graphs are drawn based on the number of iterations. This is an conscious choice because as a reminder, we put ourselves in the context where the simultaneous costly evaluation of several points is possible ; otherwise multi-point strategies are less relevant.

Figures 3-6 show the objective function and the constraint violation evolution (when it is relevant) on the analytical constrained optimization problems GX. For lack of space in this paper, evolution graphs are only shown on some interesting cases but the following GX functions are considered in the performance profiles for the global comparison : G1, G2 (10D with plog transformation), G3MOD (20D with plog transformation), G5MOD, G6, G7, G8, G9, G10, G13MOD, G16, G18, G19 and G24.

On these benchmark problems, the `MultiCEI` strategy reaches faster feasible zones and obtains a better objective function convergence than the mono-point strategies `MonoTRBF`. On the other hand, the `MultiMeta` strategy allows to quickly identify the feasible zone with a good convergence of the objective function. It also obtains better results than the mono-point strategies on all benchmark problems. The association of TRBF and Kriging models seems to be very effective and very complementary, taking advantages of the strengths of both types of models.

Furthermore, Figures 7-8 allow to compare globally the different strategies on the whole set of benchmark problems via the performance profiles. The performance profiles represent the part of solved problems for a given budget, fixed by the α parameter, representing a multiplier of the needed number of iterations such that the best version solves the problem. For example, Figure 7 indicates that `MultiMeta` strategy solved first 60% of problems (in a fine way) ($\alpha = 1$) and that it has solved 80% of problems in a budget equal to twice the minimum budget (limited here to 100 iterations). To simplify, look at the profile for $\alpha = 1$ gives the strategies which are faster and the more efficient and look at $\alpha = \infty$ shows the strategies which are the more robust (no matter the budget). Then we can observe that both multi-point strategies are very interesting compared to mono-point strategies, in terms of efficiency as well as robustness. Concerning the `MonoCEI` strategy, even if it can bring good performance punctually (as seen on G7 problem notably), it seems to be less efficient than the `MonoTRBF`, which can explain that the `MultiCEI` strategy is slightly behind the `MultiMeta` strategy.

Finally, Figures 6(a) and 6(b) compare the proposed multi-point strategies with respect to mono-point strategies in terms of number of functions evaluations, if a parallel computing system is not available. These results show that our multi-point strategy `MultiMeta` allows to quickly converge also in terms of number of functions evaluations while being also very interesting in terms of confidence interval.

The proposed strategies have also been compared on the MOPTA08 automotive problem, a benchmark test defined by Jones [14] which enables to assess the efficiency of optimization algorithms in a highly constrained, high-dimensional design space. The MOPTA08 case is representative for a complex multi-disciplinary mass minimization problem that takes into account vehicle crash performance, noise vibration, harshness, and durability. It defines a design space with 124 parameters, for an optimization problem with a single objective and 68 inequality constraints. Note that it is many times larger than test problems typically used by researchers in surrogate-based optimization. Note that the MOPTA08 problem is build based on Kriging surrogate models so by its nature, solving this problem by a Kriging-based optimization strategy (such as `MultiCEI`) is a little bit biased.

In the literature, the expectations for the benchmark are to find a feasible solution, respecting all constraints, that

Table 1: Comparison with state-of-the-art results for MOPTA08 problem starting from an initial database with 125 unfeasible points.

Algorithms	Best objective value without including initial feasible point	Mean number of iterations/evaluations to reach a feasible point
MonoTRBF	261.24 with 275 evaluations	70.05 / 195.05
MultiCEI	225.46 with 425 evaluations	8.480 / 141.96
MultiMeta	230.47 with 425 evaluations	19.44 / 163.88
COBRA (4 runs)[25, 26]	228 with 751 evaluations	243 / 367.5

achieves at least 80% of potential mass reduction in less than 1800 evaluations. For the original benchmark problem, Jones [14] provides one feasible initial point (with an objective value of 251.0706). Since for real-world industrial applications, feasible points are typically not always available, the real challenge is to investigate the performance of our strategies if only unfeasible initial points are considered. For this purpose, a DoE of 125 points has been generated without including the feasible initial point, and the optimization has been launched in these unfavorable conditions.

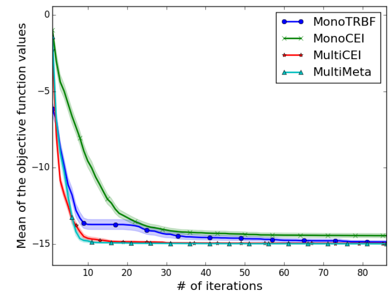
Figure 9 shows the convergence in terms of objective function and constraint violations (mean of 50 independent runs with 95% confidence interval) for the MOPTA08 problem. The mean number of iterations to reach a feasible point with our strategies is very competitive compared to state-of-the-art results presented in [17, 25, 26], see Table 1. As observed previously on analytical benchmark problems, the `MultiCEI` and `MultiMeta` multi-point strategies can help to reach faster the feasible region and here with a good evolution of the objective function convergence compared to the classical mono-point strategy.

4 CONCLUSIONS

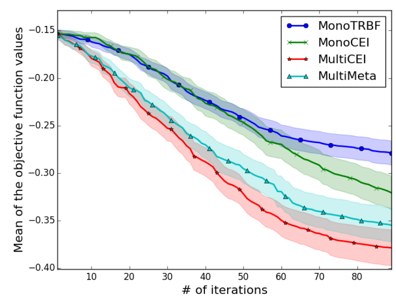
An interesting SBO framework, exploiting simultaneously different types of surrogates and different infill criteria has been presented. More specifically, the information retrieved from these distinct types of surrogates has been conjointly used in order to provide efficient infill sampling criteria that extract a maximum of knowledge from a minimal number of evaluations. This helps to promote an enhanced balance between exploitation, exploration and feasibility, which may be considered as the Graal quest for SBO.

The performance of the proposed parallel multi-point SBO framework has been illustrated on recognized constrained benchmark problems available in the literature. Good performance both in terms of identification of feasible regions and objective gains has been demonstrated compared to mono-point strategies.

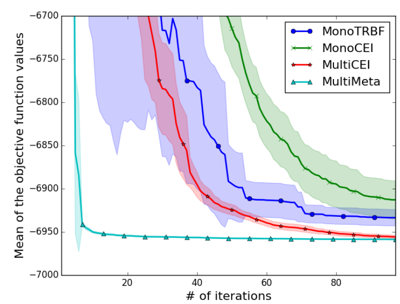
In future, it would be interesting to use more diverse surrogate models in our multi-point strategies, like e.g., Random Forest or Support Vector Regression. Further research will focus on the development of multi-point strategies with multiple dynamic search zones within the SBO process.



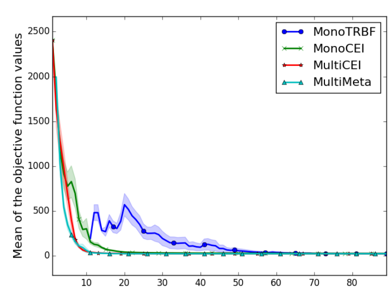
(a) G1 - Evolution of the objective function



(b) G2 - Evolution of the objective function

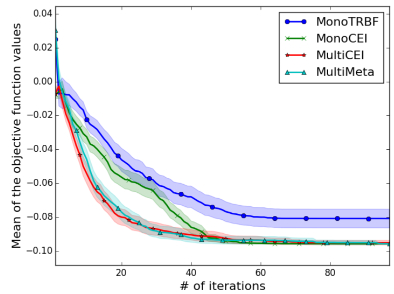


(c) G6 - Evolution of the objective function

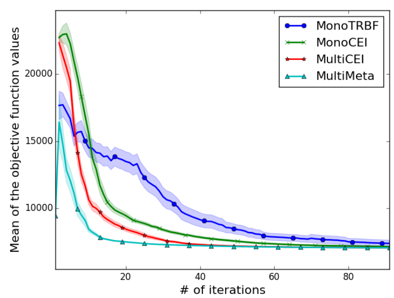


(d) G7 - Evolution of the objective function

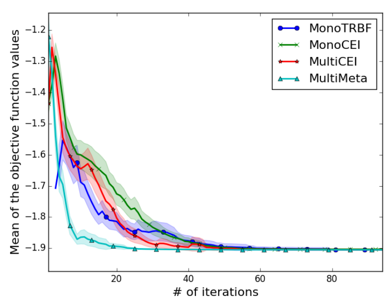
Figure 3: Evolution of the optimization in terms of design iterations for the G1, G2, G6 and G7 test cases.



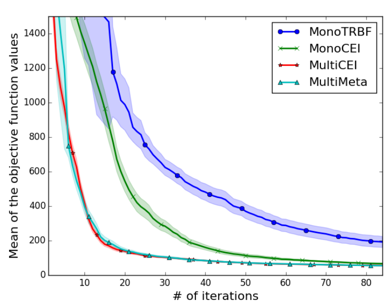
(a) G8 - Evolution of the objective function



(b) G10 - Evolution of the objective function

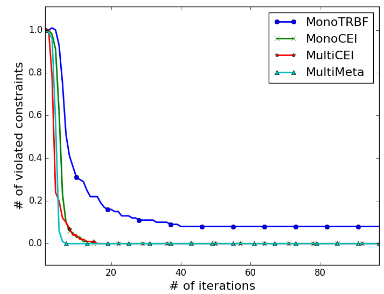


(c) G16 - Evolution of the objective function

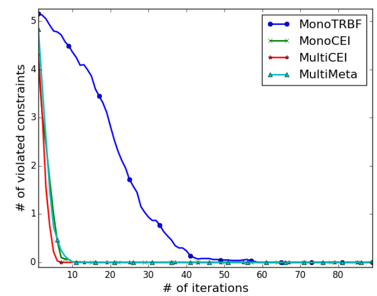


(d) G19 - Evolution of the objective function

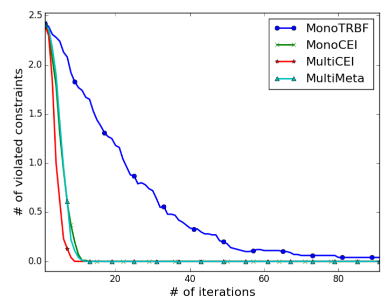
Figure 4: Evolution of the optimization (objective function) in terms of design iterations for the G8, G10, G16 and G19 test cases.



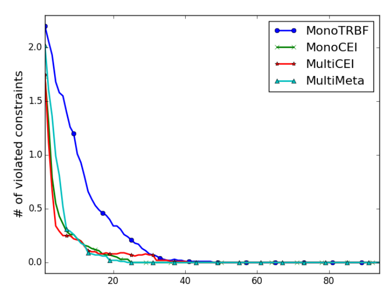
(a) G6 - Evolution of the number of violated constraints



(b) G7 - Evolution of the number of violated constraints

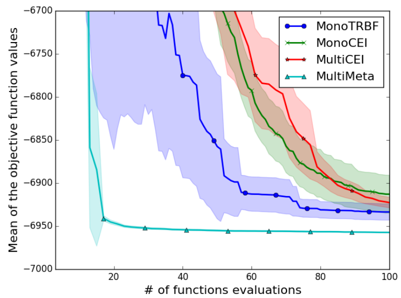


(c) G10 - Evolution of the number of violated constraints

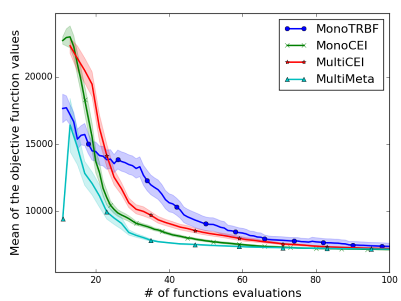


(d) G16 - Evolution of the number of violated constraints

Figure 5: Evolution of the optimization (number of violated constraints) in terms of design iterations for the G6, G7, G10 and G16 test cases.



(a) G6 - Evolution of the objective function



(b) G10 - Evolution of the objective function

Figure 6: Evolution of the optimization in terms of functions evaluations for the G6 and G10 test cases.

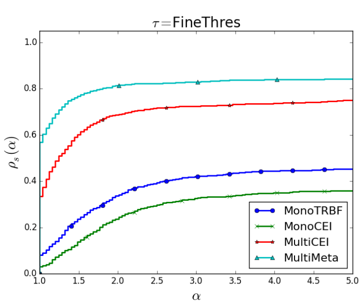


Figure 7: Performance profiles (fine threshold) of the different strategies on the GX test cases. Percentage of solved problems with respect to α.

ACKNOWLEDGMENTS

Safran Aircraft Engines' permission to publish this work is gratefully acknowledged.

The present research benefited from computational resources made available on the Tier-1 supercomputer of the Federation Wallonie-Bruxelles, infrastructure funded by the Walloon Region under the grant agreement n^o 1117545.

The authors would also like to thank the anonymous referees for their valuable comments and helpful suggestions.

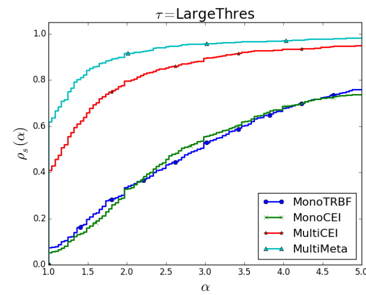
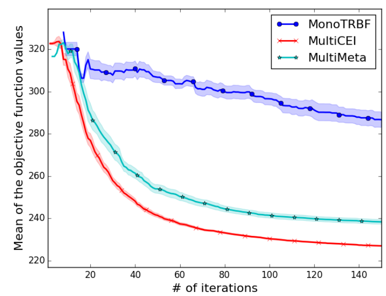
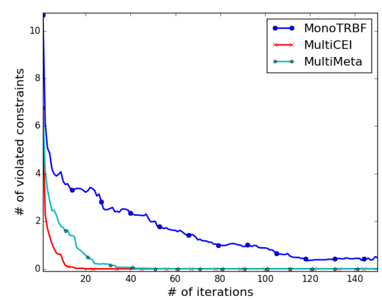


Figure 8: Performance profiles (large threshold) of the different strategies on the GX test cases. Percentage of solved problems with respect to α.



(a) Evolution of the objective function



(b) Evolution of the number of violated constraints

Figure 9: Evolution of the optimization in terms of design iterations for MOPTA08 test case (based on 50 independent runs starting from an initial database with 125 unfeasible points).

REFERENCES

[1] R. Badhurshah and A. Samad. 2015. Multiple surrogate based optimization of a bidirectional impulse turbine for wave energy conversion. *Renewable Energy* 74 (2015), 749–760.

[2] L. Baert, P. Beaucaire, M. Leborgne, C. Sainvitu, and I. Lepot. 2017. Tackling highly constrained design problems : Efficient optimisation of a highly loaded transonic compressor. In *ASME Turbo Expo 2017 : Turbine Technical Conference and Exposition, GT2017, Charlotte, USA*.

[3] S. Bagheri, W. Konen, and T. Bäck. 2016. Online Selection of Surrogate Models for Constrained Black-Box Optimization. In *2016 IEEE Symposium Series on Computational Intelligence (SSCI), Athens, Greece*.

[4] C. Beauthier, P. Beaucaire, and C. Sainvitu. 2017. Surrogate-based evolutionary algorithm for highly constrained design problems. In *International conference on evolutionary and determinitic methods for design optimization and control with applications to industrial and societal problems, Madrid, Spain*.

[5] C.M. Bishop. 1995. *Neural Networks for Pattern Recognition*. Oxford University Press.

[6] C. Coello. 2002. Theoretical and numerical constraint-handling techniques used with evolutionary algorithms: a survey of the state of the art. *Computer Methods in Applied Mechanics and Engineering* 191 (2002), 1245–1287.

[7] K. Deb. 2000. An efficient constraint handling method for genetic algorithms. *Computer Methods in Applied Mechanics and Engineering* 186 (2000), 311–338.

[8] A. Diaz-Manriquez, G. Toscano-Pulido, and W. Gomez-Flores. 2011. On the selection of surrogate models in evolutionary optimization algorithms. *IEEE Congress of Evolutionary Computation (CEC)* (2011), 2155–2162.

[9] H. Dong, S. Sun, B. Song, and P. Wang. 2018. Multi-surrogate-based global optimization using a score-based infill criterion. *Structural and Multidisciplinary Optimization* (2018).

[10] A. I. J. Forrester and A. J. Keane. 2009. Recent advances in surrogate-based optimization. *Progress in Aerospace Sciences* 45, 1-3 (2009), 50–79.

[11] A. I. J. Forrester, A. Sóbester, and A. J. Keane. 2008. *Engineering Design via Surrogate Modelling: A Practical Guide*. John Wiley & Sons.

[12] D. Ginsbourger, R. L. Riche, and L. Carraro. 2010. Kriging is well-suited to parallelize optimization. *Computational intelligence in expensive optimization problems* (2010), 131–162.

[13] D. Gorissen, I. Couckuyt, E. Laermans, and T. Dhaene. 2010. Multiobjective global surrogate modeling, dealing with the 5-percent problem. *Engineering with computers* 26, 1 (2010), 81–98.

[14] D. Jones. 2008. Large-scale multi-disciplinary mass optimization in the auto industry. *Presented at the Modeling and Optimization: Theory and Applications (MOPTA) 2008 Conference* (2008).

[15] D. R. Jones, M. Schonlau, and W. J. Welch. 1998. Efficient global optimization of expensive black-box functions. *Journal of Global Optimization* 13 (1998), 455–492.

[16] A. J. Keane. 2006. Statistical improvement criteria for use in multiobjective design optimization. *American Institute of Astronautics and Aeronautics Journal* 44, 4 (2006), 879–891.

[17] P. Koch, S. Bagheri, W. Konen, C. Foussette, P. Krause, and T. Bäck. 2015. A New Repair Method For Constrained Optimization. In *Proceedings of the 17th Genetic and Evolutionary Computation Conference (GECCO'15)*.

[18] Z. Michalewicz and M. Schoenauer. 1996. Evolutionary algorithms for constrained parameter optimization problems. *Evolutionary Computation* 4, 1 (1996), 1–32.

[19] J. More and S. Wild. 2009. Benchmarking derivative-free optimization algorithms. *SIAM J. OPTIM.* 20, 1 (2009), 172–191.

[20] J. Müller and R. Piché. 2010. Mixture surrogate models based on Dempster-Shafer theory for global optimization problems. *Journal of Global Optimization* (2010).

[21] J. M. Parr, A. I. J. Forrester, A. J. Keane, and C. M. E. Holden. 2012. Enhancing infill sampling criteria for surrogate-based constrained optimization. *Journal of Computational Methods in Sciences and Engineering - Special issue on Advances in Simulation-Driven Optimization and Modeling* 12 (2012), 25–45.

[22] J. M. Parr, C. M. E. Holden, A. I. J. Forrester, and A. J. Keane. 2010. Review of efficient surrogate infill sampling criteria with constraint handling. In *2nd International Conference on Engineering Optimization*.

[23] J. M. Parr, A. J. Keane, A. I. J. Forrester, and C. M. E. Holden. 2012. Infill sampling criteria for surrogate-based optimization with constraint handling. *Engineering Optimization* 44, 10 (2012), 1147–1166.

[24] R. G. Regis. 2011. Stochastic radial basis function algorithms for large-scale optimization involving expensive black-box objective and constraint functions. *Computers and Operations Research* 38 (2011), 837–853.

[25] R. G. Regis. 2014. Constrained optimization by Radial Basis Function interpolation for high-dimensional expensive black-box problems with infeasible initial point. *Engineering Optimization* 46, 2 (2014), 218–243.

[26] R. G. Regis. 2014. Evolutionnary programming for high-dimensional constrained expensive black-box optimization using radial basis functions. *IEEE Transactions on Evolutionary Computation* 18, 3 (2014), 326–347.

[27] C. Sainvitu, V. Iliopoulou, and I. Lepot. 2010. *Global optimization with expensive functions - Sample turbomachinery design application*. Springer Berlin Heidelberg, 499–509.

[28] A. Samad, T. Goel, R. T. Haftka, and W. Shyy. 2008. Multiple Surrogate Modeling for Axial Compressor Blade Shape Optimization. *Journal of Propulsion and Power* 24, 2 (2008), 302–310.

[29] M. J. Sasena, P. Papalambros, and P. Goovaerts. 2002. Exploration of metamodeling sample criteria for constrained global optimization. *Engineering Optimization* 34 (2002), 263–278.

[30] M. Schonlau. 1997. *Computer experiments and global optimization*. Ph.D. Dissertation. University of Waterloo.

[31] M. Schonlau. 2017. *Une approche Bayésienne pour l'optimisation multi-objectif sous contraintes*. Ph.D. Dissertation. Université Paris-Saclay.

[32] A. Sóbester, S. J. Leary, and A. J. Keane. 2005. On the design of optimization strategies based on global response surface approximation models. *Journal of Global Optimization* 33 (2005), 31–59.

[33] F. A. C. Viana and R. T. Haftka. 2008. Using multiple surrogates for metamodeling. In *7th ASMO-UK/ISSMO International Conference on Engineering Design Optimization, UK*.

[34] F. A. C. Viana, R. T. Haftka, and V. Steffen Jr. 2009. Multiple surrogates : how cross-validation errors can help us to obtain the best predictor. *Structural and Multidisciplinary Optimization* 39 (2009), 439–457.

[35] F. A. C. Viana, R. T. Haftka, and L. Watson. 2010. Why not run the efficient global optimization algorithm with multiple surrogates?. In *51st AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*. American Institute of Aeronautics and Astronautics.

[36] G. Wang and S. Shan. 2007. Review of metamodeling techniques in support of engineering design optimization. *Journal of Mechanical Design* 129, 4 (2007).

[37] R. Yondo, K. Bobrowski, E. Andrés, and E. Valero. 2019. *A review of surrogate modeling techniques for aerodynamic analysis and optimization: current limitations and future challenges in industry*. Springer International Publishing, Cham, 19–33.