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ADAPTIVE UPDATE OF SURROGATE MODELS FOR RELIABILITY-BASED DESIGN OPTIMIZATION: A REVIEW

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Abstract: *Meta-models (or surrogate models, formerly response surfaces) are getting popular in engineering designs. They are used to simulate the behaviour of structures with less computational demands than the original model (e.g. finite element models). It is still necessary to evaluate this expensive original model few times in some specified points called Design of Experiments (DoE). The first DoE is usually just space-filling to cover up the whole design space and the meta-model built with an initial DoE is therefore not very accurate everywhere. Other points are added to the meta-model to improve accuracy at important regions. In this paper, various updates of meta-models are reviewed from different points of view. Unfortunately, there is a distinction between updates even in reliability assessment and reliability-based design optimization research areas.*

Keywords: Surrogate models, Adaptive update, Reliability-based design optimization, Design of Experiments.

1. Introduction

Realistic simulations of a structural behaviour require usage of complex and very detailed models. If those models are used for an engineering design, it is inevitable to enumerate them several times. These so-called *true functions* or *performance functions* (based on e.g. a finite element method) can be quite expensive to evaluate several times consecutively. If even one evaluation of the true function is very time consuming, the optimization used for the engineering design can last for ages. To speed up the design process, the true model can be replaced by some model of the original model that has a very similar behaviour; however, it is less time consuming. Those models of models are called *meta-models* or *surrogate models* and require just few evaluations of the costly true function. Those evaluations are then used to create the meta-model. Proper locations where to evaluate the true function (called *support points*) have to be chosen properly usually by a *Design of experiments* with support points usually uniformly distributed in the whole design space. It is better to start with just a couple of support points and then find the correct positions where to add other support points to improve the meta-model mimicking the true model (called *updating*). Initial meta-models do not have the same accuracy as the true models particularly in locations that are most interesting for an engineering design such as the vicinity of the border between the safe and the failure domain called a *limit state*. Adaptive updating of meta-models can make the meta-model more accurate in those interesting locations.

2. Meta-Models and Updates

Meta-models can be divided into two fundamental parts: *non-interpolating* models minimizing sum of squares errors from some predetermined functional form (e.g. *polynomial surfaces*) and *interpolating* models intersecting all support points based on the idea of linear combination of some basis functions. Interpolating models can contain fixed basis functions (e.g. *thin-plate splines* or *multiquadrics*) or basis functions to be tuned, e.g. *Radial Basis Functions Networks* or *Kriging* (Jones, 2001). If the interpolating meta-model is trained only with few support points, it is too stiff to approximate the original behaviour of the true function and conversely, fitting the true function with plenty of points makes the model too

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flexible and causes over-fitting (Forrester et al., 2008). In addition, Kriging allows computing the mean squared error (MSE) of any predicted outcome, which is frequently used for the meta-model updates. If any other meta-model type is more suitable for a specific problem, the generic updates have to be utilized.

2.1. Update for reliability assessment

The type of a meta-model update depends on a field of the model application. Despite appearing similar, a reliability assessment and a reliability optimization require a different updating approach. Consider the evaluation of the failure probability p_f in an n-dimensional space of random variables $X_1, \ldots, X_n$ as a multiple integral of a joint probability density function $f_X(x)$ over the failure domain $g(\mathbf{X}) \leq 0$. In the standard normal space, the Hasofer-Lind reliability index β is then defined as an inverse cumulative distribution function of the standard normal distribution $\beta = \Phi^{-1}(1-p_f)$. It can be geometrically understood as the shortest connecting line between the origin and the *most probable failure point* (MPFP). To improve the behaviour of the meta-model for the reliability assessment, the update is most essential around this MPFP, because this region contributes most to the total failure probability. Bucher & Bourgund (1990) came with the idea to update the response surface utilizing second-order polynomials.

2.2. Updates for reliability-based design optimization

One possible approach to define the reliability-based design optimization is

$$\min_{d \in D} c(\mathbf{v}, \mathbf{d}) \qquad \text{s.t.} \qquad \begin{cases} h_i(\mathbf{d}) \leq 0, & i = 1, \ldots, n_e, \\ p_{f,j}(\mathbf{v}, \mathbf{d}) \leq p_{f,j}^{tol}, & j = 1, \ldots, n_p. \end{cases} \tag{1}$$

The cost function $c(\mathbf{v}, \mathbf{d})$ is to be minimized with optimal values of design variables arranged in **d** vector. Design variables are chosen from a design space **D**. Uncertain parameters are arranged in vector **v**. n_e is the total number of deterministic constraints defined by $h_i(\mathbf{d})$, $p_{f,j}(\mathbf{v}, \mathbf{d})$ stands for a probability of occurrence of j^{th} event and $p_{f,j}^{tol}$ is a prescribed tolerable threshold. n_p us the total number of probabilistic constraints. Design variables usually represent mean values of random variables and their optimal combination coincide with the minimum of the cost function under the fulfilled constraints.

Meta-models can replace both the cost function and the deterministic and probabilistic constraints. Nevertheless, there is a difference in their consecutive update. If the meta-model is used to compute the values of the objective function, an improvement of the meta-model is necessary in the vicinity of the best-so-far optimum found so as to allow for a convergence to the global optimum. Several strategies are used, namely *minimizing a response surface* (Jones, 2001), *maximizing the probability of improvement* (Kushner, 1964; Jones, 2001), *maximizing the expected improvement* (Jones et al., 1998) or *goal seeking* (Jones, 2001). On the other hand, if a meta-model is utilized for the constraint replacement, some contour (e.g. a limit state) has to be approximated. Algorithms as the *Efficient Global Reliability Analysis* (EGRA) (Bichon et al., 2008), modified *Active Kriging + Monte Carlo Simulation* (Echard et al., 2011) or *Meta-model-based importance sampling* (Dubourg, 2011) can be effectively employed. The latter algorithms utilize some special meta-models' features that are not available for all types of meta-models. The generic update can be carried out through placing new support points in a vicinity of the limit state still ensuring the uniform space-filling criterion e.g. by the MiniMax metric which leads to the multi-objective optimization (Myšáková et al., 2013). Although the replacement of probabilistic constraint seems to be the similar problem as in the reliability assessment, the layout is different due to its repeated evaluation for different designs. The limit state function can be understood as a collection of the MPFPs for different design variables combinations and thus the meta-model updating only in the one MPFP vicinity is not sufficient, but the vicinity of the whole contour needs to be updated.

2.2.1. Updates for meta-models replacing an objective function in RBDO

Minimizing a response surface approach (Jones, 2001) is independent of a used meta-model type. New support points are added sequentially into the best-so-far optimum found on the meta-model. In case of multi-modal problems, this method can converge prematurely in a local optimum or fail in the worst possible case. Additional points in DoE for the non-interpolating meta-models with fixed number of degrees of freedom need not help at all and this method can be misleading in finding any optima. The interpolating meta-models converge to the local optimum in most cases. To ensure that the local optimum is found the local search is carried out in its vicinity.

Maximizing the probability of improvement (Kushner, 1964; Jones et al., 1998) utilizes the ability of Kriging to compute MSE of a prediction. An uncertainty in the prediction is lesser (low MSE) in areas with higher concentration of support points and reversely. The output y^* at the point x^* not identical with any support point is not known, therefore y^* can be modelled as a random normal variable Y with a mean equal to the Kriging prediction $\hat{y}(x)$ and standard deviation s equal to the Kriging standard error. For more details about Kriging, see e.g. Jones et al. (1998). To find the global optimum, the minimum value $y_{\min}$ of the true function evaluated on initial DoE is determined and the probability of improvement is maximized across the whole domain of x. The improvement is achieved when $y_{\min}$ is greater than the uncertain output Y, thus $I = \max(y_{\min} - Y, 0)$ and the probability of improvement $P[I(x)]$ is according to Forrester et al. (2008)

$$P[I(x)] = \frac{1}{s\sqrt{2\pi}} \int_{-\infty}^{0} \frac{(I - \hat{y}(x))^2}{2s^2} \mathrm{d}I \,. \tag{2}$$

New support points are sequentially added into the maximum value of $P[I(x)]$ until the $P[I(x)]$ approximates zero. $P[I(x)]$ shows the location of the maximum improvement but not its amount. The better criterion is therefore the expected improvement function.

Maximizing the expected improvement function (EIF) (Jones et al., 1998) is based on the idea of the probability of improvement. EIF is an expected value of $P[I(x)]$ defined as

$$E[I(x)] = (y_{\min} - \hat{y})\Phi\left(\frac{y_{\min} - \hat{y}}{s}\right) + s\phi\left(\frac{y_{\min} - \hat{y}}{s}\right). \tag{3}$$

The maximum value of EIF localizes the next point that should be added into the surrogate model to make it more accurate. Proposed EIF makes a balance between a local and a global search. The local search is focused on an improvement of the local minimum vicinity and the global search concentrates primarily on unknown areas exploration where the standard error of the predictor has the maximum value. This approach is sequential and maximization of EIF is done repeatedly until the maximum of EIF is greater than some prescribed value. The Branch and Bound method used in Jones et al. (1998) for the maximization is however quite often too expensive to run to final convergence (Bichon et al., 2008). The complete global optimization algorithm is called Efficient Global Optimization (EGO).

Goal seeking searches for an input (a goal) that corresponds to a specific predefined function value. It is based on the maximization of the conditional log-likelihood function by varying inputs and Kriging model parameters; see Forrester et al. (2008) for more details.

2.2.2. Updates for meta-models replacing constraints functions in RBDO

Bichon et al. (2008) use an adaptive update of Kriging together with an adaptive importance sampling (AIS). An update of a meta-model is inspired by Jones et al. (1998). Instead of EIF, *Expected Feasibility function* (EFF) is utilized. Since an improvement of the meta-model is not used for global minimization but for the reliability assessment, the bound dividing the domain into the safe and the failure region has to be more accurate. An equality constraint for a reliability assessment is defined as $G(\mathbf{u}) = \bar{z}$ where $\bar{z}$ is a threshold value. EFF is therefore integrated over a region $\bar{z} \pm \varepsilon$. Efficient Global Reliability Analysis (EGRA) first generates a small number of support points (at least to define the quadratic polynomial) and computes true function values in those support points for building the Gaussian process model. Those samples are recommended to cover the design space uniformly over the bounds $\pm 5\sigma$. The point that maximizes the EFF is located by DIRECT algorithm and the true function is calculated. EFF is maximized and support points are added into the meta-model repeatedly until the stopping criterion in the form of the prescribed maximum EFF value is not fulfilled.

Active Kriging + Monte Carlo Simulation (Echard et al., 2011) creates and updates a meta-model only on a generated Monte Carlo (MC) population and not on any other points. At the beginning, few support points are chosen from the whole MC population by e.g. k-means clustering. Subsequently, support points for an update are obtained by minimizing the so-called *Learning function* on whole MC population, which is the ratio of an absolute value of a predicted value by a meta-model to Kriging variance. Since the MC population is generated only for one combination of design variables, this method in its unmodified version works only for reliability assessment. Nevertheless, several options are available to extend it for RBDO. First, a new meta-model can be trained for each combination of design variables proposed by RBD optimizer, however, this approach can be quite time consuming. Second, a meta-model is kept for all design variables combinations and just new points from new MC populations are added to make the meta-model more precise across the whole design space. Third, the MC population can be widen just for the meta-model improvement purposes.

Meta-model independent update for RBDO not utilizing the feature of the ability to forecast a predictor error is not very often used. Myšáková et al. (2013) use a multi-objective optimization for locating additional support points regardless of the meta-model type. There are two criteria: first, a new support point should be near the limit state that is carried out by minimizing the quadrate of the surrogate limit state function. Second, to bring the maximum new information, the point should be far from other points as quantified by MiniMax metric. The final Pareto-front is clustered and the best points are added to DoE to update the meta-model. This routine is run sequentially until the stopping criterion is fulfilled.

3. Conclusions

For a meta-model updating, it is necessary to distinguish what is a purpose of the meta-model. The reliability assessment requires an improvement mainly in the vicinity of the most probable point. In the reliability-based design optimization, the meta-model can replace an objective function or the constraints in the both forms of equality or inequality. In case of an objective function approximation, the global optimum should be located and updated. Constraints meta-models require an improvement in the defined contour dividing the space into the feasible (or safe) and non-feasible (or failure) domain. If Monte Carlo or variance reduction techniques (e.g. Importance sampling or Subset simulation) are utilized for a reliability assessment for each combination of design variables in the RBDO procedure, the meta-model replacing the true limit state function is more essential unless the objective function is very time consuming. A meta-model is one of very few options to solve the problem. However, the outcome is highly dependent on the meta-model ability to describe the given problem. Any time, an issue of over-fitting and/or over-simplification can occur and the quality of the used meta-model must be therefore continuously checked. For comparative studies of meta-models' performance under multiple modelling criteria, see e.g. Jin et al. (2001).

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References

Bichon, B. et al. (2008) Efficient global reliability analysis for nonlinear implicit performance functions. AIAA journal, 46, 10, pp. 2459-2468.

Bucher, C., Bourgund, U. (1990) A fast and efficient response surface approach for structural reliability problems. Structural safety, 7, 1, pp. 57-66.

Dubourg, V. (2011) Adaptive surrogate models for reliability analysis and reliability-based design optimization. PhD thesis, Université Blaise Pascal, Clermont-Ferrand, France.

Echard, B., Gayton, N., Lemaire, M. (2011) AK-MCS: An active learning reliability method combining Kriging and Monte Carlo simulation. Structural Safety, 33, 2, pp. 145-154.

Forrester, A., Sóbester, A., Keane, A. (2008) Engineering design via surrogate modelling: a practical guide. John Wiley & Sons.

Jin, R., Chen, W., Simpson, T. W. (2001) Comparative studies of metamodelling techniques under multiple modelling criteria. Structural and multidisciplinary optimization, 23, pp. 1-13.

Jones, D. R. (2001) A taxonomy of global optimization methods based on response surfaces. Journal of global optimization, 21, 4, pp. 345-383.

Jones, D. R., Schonlau, M., Welch, W. J. (1998) Efficient global optimization of expensive black-box functions. Journal of Global optimization, 13, 4, pp. 455-492.

Kushner, H. J. (1964) A new method of locating the maximum point of an arbitrary multipeak curve in the presence of noise. Journal of Basic Engineering, 86, 97, pp. 97-106.

Myšáková, E., Pospíšilová, A., Lepš, M. (2013) Multiobjective adaptive updating of surrogate models, In: Proc. 19th Int. Conf. Engineering Mechanics, Inst. of Thermomechanics, Academy of Sciences of the Czech Republic.