

RESPONSE SURFACE METHODS FOR STOCHASTIC STRUCTURAL OPTIMIZATION

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Abstract.*Response surface models are frequently chosen to reduce computational cost for structural optimization problems. These methods are also very popular for structural reliability analysis. It is therefore not surprising that response surface models are very attractive for reliability-based structural optimization. The paper discusses strategies to obtain a suitable response surface model, to assess its quality concerning prediction, and to use the response surface mode to identify important and unimportant variables. Selected mathematical and structural examples illustrate the applicability of the presented approach.*

1 INTRODUCTION

Due to the ever increasing demand on performance and cost-efficacy of structures, the need for numerical tools to optimize such structures in the design process has become very strong. The computational demand arising from optimization methods is quite heavy, and it is even more increasing since various stochastic uncertainties have to be taken into account in the design optimization process (see e.g.¹).

The sources of uncertainties in structural optimization may arise from several sources:

- Design variables (e.g. manufacturing tolerances)
- Objective function (e.g. tolerances, external factors)
- Constraints (e.g. tolerances, external factors)

These sources are indicated in Fig. 1. For structural safety issues, the main concern are uncertainties in the constraints. This usually comes from the uncertainties in the loads (e.g. wind or earthquakes). The traditional design approach to take these unavoidable uncertainties into account is the introduction of so-called *safety margins* (cf. Fig. 2). One of the major issues in establishing design procedures in code format is the appropriate (and in a sense optimal) definition of the safety margins.



Figure 1: Uncertainties in Optimization



Figure 2: Safety Margin in Optimization

2 RESPONSE SURFACE MODELS

2.1 Mathematical Formulation

The mathematical formulation for response surfaces is closely related to linear regression and interpolation modeling. A response surface model is based on linear regression if its functional form is linear in the unknown parameters p_k , i.e.

$$\eta(\mathbf{x}) = \sum_{k=1}^{n} p_k f_k(\mathbf{x})$$

A regression model is constructed from a sequence of input values \mathbf{x}_i , $i = 1 \dots m$ and corresponding model output values y_i , $i = 1 \dots m$. The set of parameters p_k can be determined by solving the least squares problem

$$S^{2} = \sum_{i=1}^{m} \left[y_{i} - \sum_{k=1}^{n} p_{k} f_{k}(\mathbf{x}_{i}) \right]^{2} \rightarrow \text{Min.!}$$

If the number of parameters n is equal to the number of data pairs m, then the regression model becomes an interpolation model.

Global functions are functions not localizing in certain areas (such as polynomials). Simple examples are linear polynomial function

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$$\eta_l(\mathbf{x}) = p_0 + \sum_{k=1}^n p_k x_k$$

and the quadratic model

$$\eta_q(\mathbf{x}) = p_0 + \sum_{k=1}^n p_k x_k + \sum_{k=1}^n \sum_{j=1}^n p_{kj} x_k x_j$$

Localized models represent the response in specific regions, such as radial basis functions³

$$\eta_r(\mathbf{x}) = \sum_{k=1}^n p_k \, \phi_k(\mathbf{x}, \mathbf{x}_k)$$

in which $\phi_k(\mathbf{y}) = \phi_k(||\mathbf{y}||) = \phi_k(r)$ are functions depending only on the magnitude of the vector argument and \mathbf{x}_k are the localization points of the RBF functions. If the localization points coincide with the data points, then this model is interpolating. Otherwise it is a linear regression model. A typical example are thin plate splines for which the radial dependence is modeled as

$$\phi(r) = r^2 \log r$$

2.2Design of Experiments (DoE)

In order to establish the response surface, a set of support points is needed. These points should satisfy the following requirements:

- Explore range of variables by numerical experiments
- Cover range of all variables as uniformly as possible
- Keep number of experiments small

An intuitive approach would be to divide each variable into M small intervals and cover all possible combinations of variables x_i ; i = 1 ... n. This is a so-called *factorial design*. It can easily be seen that the total number N of support points equals $N = M^n$. This curse of dimensionality (exponential growth with dimension n) makes factorial designs virtually infeasible for complex problems.



Figure 3: Design of experiments (DOE), left: Factorial design, center: Monte Carlo Sampling, right:Latin Hypercube Sampling

Fig. 3 compares factorial design with Monte Carlo sampling and Latin Hypercube sampling.For practical applications, Latin Hypercube sampling (or similar methods based on low-discrepancy numerical sequences) provide a good compromise between accuracy and computational efficacy.

2.3Quality of metamodel

Since the metamodel aims at predicting the behavior of a complex system in terms of very simple mathematical functions, it is of vital importance to ensure sufficient predictive quality of this metamodel. A first and simple quality measure is the coefficient of determination (CoD, R^2). This quantity measures the correlation between the actual data *Y* and the model predictions *Z*:

$$R^{2} = \left(\frac{\mathbf{E}[(Y - \overline{Y}) \cdot (Z - \overline{Z})]}{\sigma_{Y}\sigma_{Z}}\right)^{2} = \rho_{YZ}^{2}; \ Z = \sum_{i=1}^{n} p_{i} g_{i}(X)$$

One well-known problem with this measure is that the R^2 -value may be high due to overfitting (which eventually leads to bad prediction behavior). If an additional test data set T is available, then a true measure for the prediction quality can be computed, which is herein called *Coefficient of Quality* (CoQ)

$$\operatorname{CoQ} = \left(\frac{\mathbf{E}[(T-\overline{T}) \cdot (Z_T - \overline{Z}_T)]}{\sigma_T \sigma_{Z_T}}\right)^2 = \rho_{TZ_T}^2; \ Z_T = \sum_{i=1}^n p_i g_i(X_T); \ 0 \le \operatorname{CoQ} \le 1$$

In practical application it is useful to randomly split data into training set/test set and repeat the computation of the CoQ several times to obtain a stable statistical estimator of CoQ. This strategy allows to assess the variability of the CoQ at the same time such that confidence intervals can be provided.

It should be noted that the CoQ is a global measure based on a correlation coefficient and should not be misconstrued as a valid measure for local errors of the response surface model.

2.4Importance measures

One very important type of information for optimization is the knowledge which variables are likely to have most influence on the objective function and/or constraints. Therefore importance measures are necessary. There are several possibilities, the most simple one is based on linear correlations. It turns out that this is suitable only for almost linear models. Here it is suggested to systematically investigate the dependence of the CoQ on the inclusion/exclusion of individual variables. The procedure can be summarized as follows:

- Compute the CoQ for full model (all input variables)
- Remove input variable x_k from regression models, compute CoQ_k for the reduced model and compute the drop in the $\text{CoQ} \Delta_k = \text{CoQ} \text{CoQ}_k$
- Compute the normalized importance measure $I_k = \frac{\Delta_k}{\Sigma \Delta_k} \text{CoQ}$ Positive importance measures I_k indicate that variable x_k is important, negative measure indicate that this variable should be removed from the model. The sum of all importance measures equals the CoQ: $\sum_{k=1}^{n} I_k = \text{CoQ}$.

If a variable with negative importance has been removed from the model, then the CoQ should increase. When the process of elimination is repeated until there are no more variables with negative importance, then this quite naturally leads to the Metamodel of Optimal Quality (MOQ). For numerical evaluation, these concepts are implemented in the software package slangTNG⁴.

2.5Examples

As a first example we consider a 3-dimensional test function given as⁵

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$$g = \sin x_1 + 7\sin^2 x_2 + 0.1x_3^4 \sin x_1$$

All variables are uniformly distributed in the range $[-\pi, \pi]$. This highly nonlinear function has been used in⁵ to demonstrate the use of Sobol indices for global sensitivity analysis. Based on a Latin Hypercube sampling with 500 samples, the Thin Plate Spline model yields a CoQ = 0.954 and importance measures $I_1 = 0.416$, $I_2 = 0.366$ and $I_3 = 0.185$. In order to compare these results to those given in⁵, both importance measures were normalized to a sum of 1. The comparison is shown in Table 1. The agreement is excellent.

Variable	Normalized Importance (CoQ)	Normalized Importance ⁵
<i>x</i> ₁	0.436	0.449
x_2	0.383	0.357
<i>x</i> ₃	0.185	0.194

Table 1: Relative importances using CoQ compared to exact results

We then consider a 6-dimensional test function given as

$$g = 0.5x_1 + x_2 + 0.5x_1x_2 + 5\sin x_3 + 0.2x_4 + 0.1x_5$$

All variables are in the range $[-\pi, \pi]$, the 6th variable x_6 does not appear in the function. A DOE with 100 samples (using Latin Hypercube Sampling) has been established, and the corresponding function values were computed. For the computation of the CoQ, the samples were split into training set and test set (30 times repeated random splitting with 67 samples for training set and 33 samples for the test set). Again, the response surface model chosen was Thin Plate Spline interpolation over the training set.

Table 2 shows the linear correlations between the input variables and the function values together with the importance measures I_k and the effect of successive elimination of variables with smallest importance on the CoQ.

ρ	$I_{k}^{(1)}$	$I_{k}^{(2)}$	$I_{k}^{(3)}$	$I_k^{(4)}$	$I_{k}^{(5)}$
0.07	0.13	0.11	0.11	0.11	n.a.
0.52	0.30	0.33	0.25	0.25	0.19
0.58	0.37	0.41	0.55	0.57	0.64
0.06	-0.01	-0.07	-0.08	n.a.	n.a.
0.14	-0.06	-0.08	n.a.	n.a.	n.a.
0.03	-0.06	n.a.	n.a.	n.a.	n.a.
CoQ	0.61	0.73	0.83	0.92	0.81
$\sigma_{\rm CoO}$	0.11	0.08	0.07	0.02	0.07

Table 2: Importance measures for different order models

The results show that the MOQ contains only the variables x_1 , x_2 , and x_3 . For this reduced model the CoQ reaches a value of CoQ = 0.92. The analysis has been repeated with a larger sample size of the DOE, i.e. 500 samples. The changes in the prediction quality and in the relative importance of the variables are shown in Table 3. It can be seen that the CoQ increases clearly. The relative importances of the variables did not change substantially, but the MOQ now also includes the variable x_4 .

CoQ	0.918	0.964	0.986	0.985	0.822
$\sigma_{\rm CoO}$	0.010	0.006	0.002	0.002	0.021

Table 3: CoQ for different order models, DOE with 500 samples

Generally it should be stated that as the sample size increases more and more, then also the MOQ should contain more and more relatively unimportant variables.

3 APPLICATION TO STRUCTURAL OPTIMIZATION

3.1 Deterministic Problem

In order to study the applicability of the concept as presented to a structural optimization problem consider a frame under static loads as shown in Fig. 4. The structure is a linear elastic plane frame under two static loads H and V. It is represented by a simple finite element model using the software slangTNG⁴, possible loss of stability (buckling) is accounted for in the analysis. The objective is to minimize the structural mass subject to the constraints:

- Horizontal deflection $u < u_0$
- Vertical deflection $w < w_0$
- Buckling load factor applied to the nominal loads $\lambda \ge \lambda_0$



Figure 4: Frame structure with horizontal and vertical load

The material parameters are E = 210 GPa and $\rho = 7850$ kg/m³. The loads are H = 100 kN and V = 117 kN, the allowable deflections are $u_0 = 0.05$ m and $w_0 = 0.05$ m. The lower limit on the buckling load factor is $\lambda_0 = 2.5$.

Carrying out an optimization run with the standard gradient-based optimizer CONMIN⁶ results in optimal cross sections $d_1 = 0.082$ m, $d_2 = 0.069$ m, $d_3 = 0.137$ m, $d_4 = 0.152$ m. In this solution all constraints are active, i.e. the solution is located on the boundary of the feasible domain. The total structural mass is m = 1388 kg. This result was achieved with 100 FE analyses.

3.2 Stochastic Problem

It is now assumed that the loads acting on the structure are independent random variables with mean values $\overline{H} = 100$ kN, $\overline{V} = 117$ kN and coefficients of variation of 5%. Apparently, the

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constraints cannot be satisfied deterministically. Therefore the constraints now have to be satisfied with a prescribed reliability levels $\beta_u = \beta_w = 3$ for the displacements and $\beta_{\lambda} = 4$ for the buckling load factor. Two approaches are considered, the first one being the method of safety factors. This simply upscales the deterministic optimum cross sections such that all probabilistic constraints are satisfied. With a few repeated FE analysis this leads to a design with mass m = 1706 kg (increase of 23% as compared to the deterministic problem).

The second approach is stochastic optimization (RBDO). Here the probabilistic constraints are directly included into the optimization process. The probabilities of constraint violation computed by FORM⁷. This very straightforward approach requires about 35.000 structural analyses. The number is so large because FORM internally solves another optimization problem. The optimal cross sections are determined to be $d_1 = 0.081$ m, $d_2 = 0.076$ m, $d_3 = 0.150$ m, $d_4 = 0.171$ m. The structural mass m = 1657 kg (19% increase as compared to the deterministic problem, and 4% less than the upscaling solution).

3.3 Adaptive Response Surface Method (ARSM)

The stochastic optimization requires a representation of the objective and the constraints as a function of both the design variables (i.e. the cross section widths d_k) and the stochastic variables (i.e. the loads V and H). Hence the response surfaces depend on 6 variables. Since initially it is not clear in general where in the design space the optimum will be located, an initial DOE with a very wide range for the variables is analyzed. Based on the response surface derived from this DOE an optimal solution is found. The DOE is then repeated by recentering around the optimum design and narrowing its range. The process is schematically shown in Fig. 5.



Figure 5: Adaptive response surface method, re-centering and narrowing of DOE

For the present example, an initial DOE with 256 structural analyses was established. All constraint functions were approximated by Metamodels of Optimal Quality and the stochastic optimization was carried out. The DOE was then re-centered around the optimum and its range narrowed by a factor of 0.7. This was repeated giving totally 4 iterations. The optimal design after these 4 iterations was $d_1 = 0.083$ m, $d_2 = 0.078$ m, $d_3 = 0.144$ m, $d_4 = 0.172$ m with a total structural mass of m = 1665 kg. This result is not feasible because Constraint 1 is slightly violated. This violation is due to local errors inherent in the response surface approximation. It turns out that upscaling this solution by only 0.2% satisfies all constraints, and the structural mass becomes m = 1673 kg. Compared to the deterministic solution, this is an increase of 20.5%. Considering the computational demand it is seen that compared to full

stochastic analysis computation is reduced by a factor of 35. This is a very substantial gain in computational efficacy. Of course, even when using ARSM, the stochastic analysis is substantially more expensive than the deterministic analysis, in this case by a factor of 10. When comparing the designs from the full stochastic design optimization and the optimization based on the ARSM there is no visible difference, the structural mass m differs by 1.5%. Therefore it may be concluded that the response surface method is a tool which can help to carry out stochastic structural optimization in a fast an reasonably accurate way.

4 CONCLUSIONS

Stochastic structural optimization avoids highly specialized designs and therefore reduces imperfection sensitivity. It naturally includes statistical uncertainties into the design optimization process. Furthermore, it allows the inclusion of quality control measures (manufacturing, maintenance) into the design process. It is, however, computationally very expensive unless based on approximations such as response surface models.

The paper developed a strategy to assess the quality of response surface models (the coefficient of quality, CoQ) and to identify important and unimportant design and stochastic variables. Based on this CoQ, metamodels of optimal quality (MOQ) can be established and utilized for structural optimization. Combining this with an adaptive method to successively refine the MOQ one can achieve excellent stochastic optimization results with moderate computational effort.

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