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# APPLICATION OF METAMODEL BASED ON CLASSICAL AND SPACE FILLING EXPERIMENTAL DESIGN IN DESIGN OPTIMIZATION

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**Abstract:** Engineering analysis using computer based simulation is used extensively to predict the performance of a system. Such engineering analyses rely on running expensive and complex computer codes. Statistical techniques such as design of experiments and response surface methodology are widely used to construct approximate models of these costly analysis codes which minimize the computational expense of running computer analyze. These models referred as metamodels, are then used in place of the actual analysis codes to reduce the computational burden of engineering analyses. In this paper, we compare two experimental design methods in terms of their capability to generate better approximations for engineering applications.

**Keywords:** Metamodel, Experimental design, Orthogonal Array, Central Composite Design, Optimization

# INTRODUCTION

Engineers use finite element analysis packages to evaluate the performance of a structure, computational fluid dynamics packages to predict the flow characteristics of a fluid media in or over a domain and Monte Carlo simulation to estimate the reliability of a product. Also traditional engineering design optimization which is the process of identifying the right combination of product parameters is often done manually, time consuming and involves a step by step approach. Approximation methods are widely used to reduce the computational burden of engineering analyses. The use of long running computer simulations in design leads to a fundamental problem when trying to compare and contrast various competing options. It is also not possible to analyze all of the combinations of variables that one would wish. Metamodels, also referred as surrogate models, are a cheaper alternative to costly analysis tools and can significantly reduce the computational time involved.

Metamodeling involves (a) choosing an experimental design for generating data, (b) choosing a model to represent the data, and (c) fitting the model to the observed data. There are several options for each of these steps. In this paper, a methodology of developing metamodel and applying it to the optimization problem is explained. As a case study, the roof slab of a Prototype Fast Breeder Reactor was taken and design optimization was carried out. In this approach, experimental design, metamodels, evolutionary algorithm, and finite element analysis tool are brought together to provide an integrated optimization system. Alexander et. al [1] discussed the recent advances in surrogate based design for global optimization. Simpson et.al [10] has done a survey on the application of metamodels on design. The paper also gives the following recommendations: (i) If many factors(more than 50) must be modeled in a deterministic application, neural networks may be the best choice (ii) If the underlying function to be modeled is deterministic and highly nonlinear in a moderate number of factors (less than 50, say), then kriging may be the best choice despite the added complexity, (ii) In deterministic applications with a few fairly well behaved factors, another option for exploration is using the standard Response surface methodology approach. In Simpson, et al. [9], kriging methods are compared against polynomial regression models for the multidisciplinary design optimization of an aero spike nozzle. Fasihul et al [4] investigated the effects of experimental design on the development of artificial neural networks as simulation metamodels. This paper shows that a modified-Latin Hypercube design, supplemented by domain knowledge, could be an effective and robust method for the development of neural network simulation metamodels. Nestor et.al. [6] discussed the fundamental issues that arise in the SBAO of computationally expensive models such as those found in aerospace systems. The paper mainly focused on the design of experiments based on Latin Hypercube Sampling (LHS) & Orthogonal Arrays (OA) and Surrogate modeling techniques based on polynomial regression

model, kriging and radial basis function. Ruichen et.al [7] compares four popular metamodeling techniques— Polynomial Regression, Multivariate Adaptive Regression Splines, Radial Basis Functions, and Kriging- based on multiple performance criteria using fourteen test problems representing different classes of problems. Giunta, et al. [5] also compare kriging models and polynomial regression models for two 5 and 10 variable test problems. In Varadarajan, et al. [12], Artificial Neural Network (ANN) methods are compared with polynomial regression models for the engine design problem in modeling the nonlinear thermodynamic behavior. In Yang, et al., [14], four approximation methodsenhanced Multivariate Adaptive Regression Splines (MARS), Stepwise Regression, ANN, and the Moving Least Square- are compared for the construction of safety related functions in automotive crash analysis, for a relative small sampling size. Similarly many researchers have compared the various experimental designs and/or metamodeling techniques. Only limited researchers are explained about the application of metamodel in the optimization of complex design problems with more number of variables. This paper explains the methodology of performing experimental design, creating metamodel and applying it to the optimization. The author in their previous work [8] made an attempt with Orthogonal Array (OA) method. In this work, the metamodel was developed using two experimental design methods namely, OA and Central Composite Design (CCD).

#### METHODOLOGY

During the optimization process, the model of the component to be optimized will be called for analysis several times, each time with different geometric parameters. So the model has to be in parametric form, which enables it to change the parameter whenever required. So a parametric model of the component has to be modeled using CAD tool which is compatible with the analysis (CAE) tool. Sensitivity analysis of the component was performed to find the effect of the objective function and the state variables (stress/deformation) on the variation of geometric parameters. The parameters which influence more on the state variables are alone considered for the optimization study. In order to reduce the computation cost and to have a better sampling search in the design space, design of experiments was performed using OA and CCD. For the sampling points, the computer experiment was conducted using ANSYS package and the results are fed to Minitab software to create the metamodel. This metamodel was used in Genetic Algorithm (GA) coding for optimization.

### CASE STUDY

The foremost step in the metamodel based optimization is the development of metamodel. Development of metamodel requires lot of experiments to be carried out to the train the model. Experiments may not be feasible in case of complex problems like our case study and in such situations, simulation will be useful. This method of using computer simulation for developing metamodel is termed as design of computer experiments and is explained in detail in the following chapters.

# Parametric Modeling and finite element analysis

As explained earlier, metamodel development requires lot of simulations, for which parametric model of the structure being optimized is required. The structure considered for the metamodel based optimization is a roof slab of a nuclear reactor. The roof slab acts as a support for various components of the reactor and is shown in Figure 1. The main objective of the optimization is to minimize the total

weight of the roof slab. As the model will be explored during analysis for various combinations of parameters, a parametric model of the roof slab was developed. The variables taken for parametric modeling are various plate thicknesses and height of the roof slab. The parametric model was created using the finite element software ANSYS. The necessary loading conditions (weight of various components on the roof slab) and boundary conditions are applied on the structure and a methodology of analyzing the structure for static loading condition was established.

# Sensitivity analysis

The next step in metamodel based optimization is to predict the decision variables for the roof slab through an investigation of the sensitivity of the objective function on



Figure 1. Parametric model of the roof slab

small increments of these variables. The design variables considered for the sensitivity analysis are H1,  $T_1$ ,  $T_3$ ,  $T_4$ ,  $T_5$  and  $R_1$ . Sensitivity analysis is carried out using ANSYS sweep optimization module and the analysis reveals that deformation is sensitive to the variations in the parameters  $H_1$ , and  $T_1$ , stress is sensitive to the variations in the parameters  $T_1$ ,  $T_3$ ,  $T_4$ ,  $T_5$  and  $R_1$ , and cost of the roof slab is sensitive to the variations in the parameters  $T_1$  and  $T_4$ . So each parameter is contributing to in different aspects and hence all the parameters are taken as design variables for the optimization process.

#### **Experimental Design**

An important issue to metamodeling is to achieve good accuracy of metamodels with a reasonable number of sample points. Experimental design is the sampling plan in design space. The type of experimental design adopted in this work was L 32 OA and CCD, since many researchers have

used these techniques for the design of computer experiments [2, 11, 12]. Minitab software has been used to perform the experimental design. The factor  $H_1$  has four levels and factors  $T_1$ ,  $T_3$ ,  $T_4$ ,  $T_5$  and  $R_1$  have two levels each as given in Table 1.

Metamodeling

Metamodeling, often referred as Response Surface Methodology (RSM), involves (a) choosing an experimental design for generating data, (b) choosing a model to Table 1. Various parameters considered

Factors	Levels							
ractors	1	2	3	4				
H₁(m)	1.6	1.6	-	-				
T <sub>1</sub> (m)	0.015	0.02	0.025	0.03				
T <sub>3</sub> (m)	0.015	0.02	0.025	0.03				
T <u>4</u> (m)	0.015	0.02	0.025	0.03				
T₅(m)	0.015	0.02	0.025	0.03				
R <sub>1</sub> (m)	0.015	0.02	0.025	0.03				

design for generating data, (b) choosing a model to <u>Ri(III)</u> 0.013 0.02 0.023 0.03 represent the data, and (c) fitting the model to the observed data. Detailed description of the RSM is given in Simpson et. al [10]. Based on the experimental design, the computer experiments were conducted for the various combinations of factors at different levels using the OA experimental design. The metamodeling technique used in this study is polynomial regression and has been applied by a number of researchers [2,10,11,13,14] in designing complex engineering systems. The most widely used response surface approximating functions are low-order polynomials. For significant curvature, a second order polynomial which includes all two-factor interactions can be used. A second order polynomial model can be expressed as:

 $\hat{\mathbf{y}} = \mathbf{B}_0 + \mathbf{B}_1 \mathbf{x}_1 + \mathbf{B}_2 \mathbf{x}_2 + \dots + \mathbf{B}_k \mathbf{x}_k + \mathbf{B}_{12} \mathbf{x}_1 \mathbf{x}_2 + \dots + \mathbf{B}_{k-1} \mathbf{k} \mathbf{x}_{k-1} \mathbf{x}_k + \mathbf{B}_{11} \mathbf{x}_1^2 + \mathbf{B}_{22} \mathbf{x}_2^2 + \dots + \mathbf{B}_{kk} \mathbf{x}_k^2$ (1)

The parameters of the polynomial in Equations (1) are usually determined by least squares regression analysis by fitting the response surface approximations to existing data. For the roof slab optimization problem, three metamodels are created to approximate the cost of roof slab, stress developed and deflection using L32 array computer experimentation. In order to validate the metamodel some random experiments ware conducted and compared with the finite element simulation of the actual model. The fitness of the metamodels generated using the two experimental methods are given in Table 2. It can be noted that R<sup>2</sup> values of the metamodel based on CCD is poor compared to that of OA design. The reason is that OA is a space filling design and CCD is a classical design space and by taking replicate design points as shown in Figure 2. Also classical design space. As computer experiments involve mostly systematic error rather than random error, a good experimental design tends to fill the design space. Many researchers also indicated that the use of space filling designs when sampling deterministic computer analyses.



(a) Classical experimental design
 (b) Space filling design
 Figure 2. Classical and Space filling design
 Table 2. Fitness of metamodels

Response parameter	Metamodel	based on OA	Metamodel based on CCD		
	R-Squared value (%)	R-Squared	R-Squared value (%)	R-Squared	
		(Adjusted) value (%)	R Squared value (%)	(Adjusted) value (%)	
Cost	96.4	96.2	78.44	77.76	
Stress	72.0	69.9	82.48	74.86	
Deformation	94.1	93.6	82.2	74.45	

Optimization

The objective of this optimization is to minimize the weight of the roof slab. The method of probabilistic search based on evolutionary algorithms was chosen for the present optimization problem. The real-coded genetic algorithm (RCGA) is developed for obtaining the optimal dimensions of the roof slab of PFBR. The code template developed by Deb [3] was used for this purpose. Certain modifications in the algorithm of this program were necessary to apply it for the present study. RCGA is developed for six input variables and two constraints. Various thicknesses of the roof slab and the height of the roof slab are considered as the design variables for optimization. The state variables in the optimization are maximum stress and maximum deformation. In this study the maximum stress is the material yield strength and maximum deflection is the permissible axial movement of the control plug. Optimization of the roof slab was carried out by this approach and the cost of roof slab is reduced by 46% by OA approach and 41.4% by CCD approach. Table 3 shows the design and state variables after

optimization. The table also compares the results optimization using the metamodels developed by OA and CCD. The optimized roof slab is also checked for its design adequacy under static and dynamic conditions in Finite Element package ANSYS.

Optimized	Experimental Design method	H1 (m)	T1 (mm)	T3 (mm)	T4 (mm)	T5 (mm)	R1 (mm)	COST ( in Cores)	Stress (MPa)	Deformation (m)
	OA	1.6	15	15	15	15	15	7.58	92.4	0.0037
	CCD	1.7	20	20	15	15	15	8.37	87.2	0.0033
Existing	-	1.8	30	30	30	30	30	14.3	82.7	0.0024

Table 3. Results of optimization process

#### ••• CONCLUSION

Traditional solution methods for optimizing complex real life engineering problems can be very expensive and often results in sub-optimal solutions. In this paper, an approach to develop metamodel for complex real time problem is presented. As a case study, a roof slab for which design optimization has to be carried out is considered. A metamodel based optimization approach is presented to address expensive computational cost of large FE runs using meta-models. With the proposed strategy of performing computer experiments, creating metamodel and the application of evolutionary algorithms, this optimization methodology can easily be adopted to more complex structural problems.

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