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МЕТАМОДЕЛИ ЗА МУЛТИДИСЦИПЛИНАРНА ОПТИМИЗАЦИЯ НА БЛА

ПЛАМЕН РОГЛЕВ, ДИМО ЗАФИРОВ

Резюме: *Приложението на програмни продукти за симулация и анализ с висока вярност при концептуалното и предварителното проектиране на летателни апарати среща трудности заради високата „изчислителна цена" и наличието на „цифров шум". Това ограничава ефективността им като инструменти за оптимизация. За преодоляването на тези проблеми могат да се използват метамодели. Направен е преглед на няколко метода за създаване на метамодели, които могат да намерят приложение при мултидисциплинарната оптимизация и на начините за оценката им. Метамодели построени с използване на полиноми от втора и трета степен, кригинг и радиални базисни функции са приложени за симулиране на разпределението на подемната сила по разпереността на крилото и е направено сравнение на тяхната вярност.*

Ключови думи: *метамодели, повърхност на отклика, кригинг, радиални базисни функции*

METAMODELS FOR MULTIDISCIPLINARY DESIGN OPTIMIZATION OF UAV

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Abstract: *The application of high-fidelity simulation and analysis tools in conceptual and preliminary aircraft design faces difficulties as high computational price and numerical noise. This limits their performance as optimization instruments. Metamodels might be used to overcome these problems. Several methods for building metamodels that can be applied in multidisciplinary design optimization and their assessment are reviewed. Polynomial metamodels of third and second order, kriging and radial basis functions metamodels are implemented to simulate the lift distribution along the span of a wing and their fidelity is compared.*

Key words: *metamodel, response surface, kriging, radial basis functions*

1. Introduction

The preliminary aircraft design is a multidisciplinary activity which requires an extensive exploration of all of the possible variants and configurations. It is necessary to study the whole of the design space in order to obtain knowledge about the relations between the design variables and the aircraft performance. So the industry has given considerable attention to multidisciplinary design optimization (MDO) as manufacturers try to reduce the time-to-market and competitiveness of new products. The benefits of MDO are obvious but methods for its implementation are less well defined and the computational challenges facing researchers are big. This has brought the need for new design

methodologies, especially in the case of unconventional airplane configurations. The widely used design practices that rely on semi-empirical equations based on statistical data derived from existing aircraft are not representative of this new design space and cannot be used. This obviates the need to introduce physics based models. There is a tendency towards the use of high fidelity analysis methods (Navier-Stokes fluid flow and FEM structural analyses) as early as possible in the design process where the increased accuracy can most significantly influence the design. However, their high computational price limits the scope to which the high fidelity analyses may be applied in the early stages of the aircraft design process. And the computational cost is further increased when they are directly used for automated optimization. The presence of numerical noise in realistic engineering simulations often makes ineffective the use of gradient-based optimization methods. Numerical noise is a result of incomplete convergence of iterative processes, round-off errors or the discrete representation of continuous physical phenomena. To overcome this, global optimization techniques (most often evolutionary methods) are used. But they further increase computational cost, as they require a large number of iterations. To cope with the problem the use of metamodels has been introduced.

The metamodel or "model of a model" is an abstraction of the model representing its properties in a computationally efficient way. It is an approximate representation (**y***=**f***(**x**)) of the objective function (**y**=**f**(**x**)). The meta-model provides filtering of the numerical noise of high fidelity models in the optimization process. It offers a means for rapid design space exploration and more importantly, visualization of the design search space and the influence of the design parameters. This improves the man-machine interoperation and alleviates the "black box effect" of the design software.

The meta-model is based on a set of results that are obtained with the high-fidelity aircraft design simulation. For this purpose, sampling of the multi-dimensional design domain is done by design of experiments (DoE) methods.

2. Methods

There exist several meta-model building methods like polynomial regression, kriging, regression splines, radial basis functions (RBF) and Artificial Neural Networks (ANN).

The two most used model classes in the analyses are the polynomial models and the kriging model. It should be noted that kriging and RBF models are interpolating models, i.e. they are exact in the given data points, whereas polynomial models and ANN are approximating models. There exist various statistical verification methods by which the quality (or 'representativeness') of the different meta-models can be assessed and the most suitable method can be selected. These methods consider a subset of the data set, called verification points, in which the error of the prediction (**y**-**y***) is evaluated for a fit that is made for the data set without the verification points.

2.1 Polynomials

One commonly used and relatively simple class of meta-models are the polynomial regression models, which are also often referred to as response surface models (RSM). The coefficients of the polynomial regression model are usually determined according to a least-squares procedure. RSM was originally developed to build models from experimental results and then started to be used for the modelling of numerical experiments. The difference is in the type of error generated by the response. In physical experiments, inaccuracy is due, to measurement errors while, in computer experiments, numerical noise is present. In RSM, the errors are assumed to be random.

Polynomial regression models provide global representation of the data, i.e. one regression function is used for the whole domain. Polynomial functions of different orders can be used. The linear regression model is the first order polynomial. Most often a second order polynomial is used. Higher order models can also be built. But with higher orders polynomials there exists risk of so called over-fitting of the data. In that case the polynomial follows the data closely and it captures local oscillations, but it does not properly describe the global behaviour of the data. So the reliability of polynomial models for extrapolation is very poor, especially for high order polynomial models.

The second order polynomial regression models take the following form:

$$y^* = \beta_0 + \sum_{i=1}^{N} \beta_i x_i + \sum_{i=1}^{N} \beta_{ii} x_i^2 + \sum_{i=1}^{N} \sum_{j=1}^{N} \beta_{ij} x_i x_j \quad (1)$$

where N is the number of design variables, and β_i; β_{ii}; β_{ij} are the regression coefficients determined by the linear regression (the model y^* is linear in the coefficients) of the polynomial model. The minimum number of points necessary is *(N+1) (N+2)/2*. This means that the cost of computation goes up quadratically with the number of dimensions of optimization.

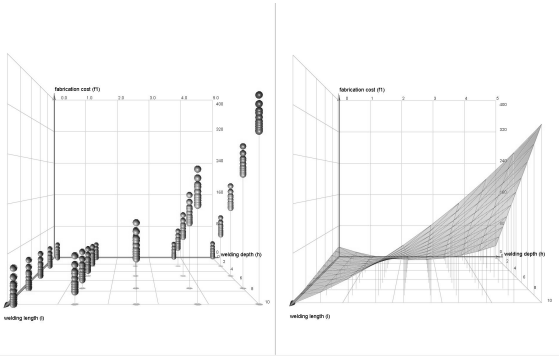

Fig. 1. *Designed experiments with full factorial design (left), response surface with second-degree polynomial (right)*

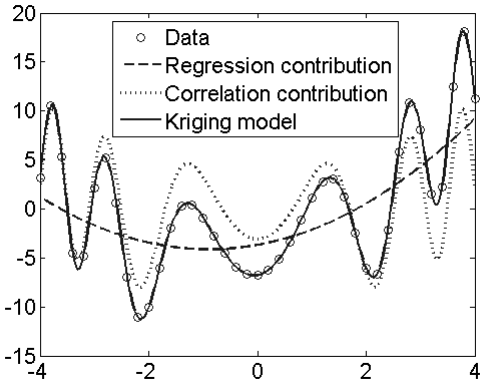

Fig. 2. *Plot of a simple kriging approximation and the different contributions to the model*

2.2 Kriging

Kriging models originated from geo-statistics. They are named after the South African geologist Danie G. Krige. They found their way into modeling of data coming from computationally expensive simulations during the last decade. The kriging model combines a global regression model and local refinements into one interpolation. The global model is a generalized regression model to which a local model is added using a correlation function to couple points in the data set that are in the vicinity of each other. (Fig. 2).

A kriging model approximates the original relationship by

$$y^*(\mathbf{x}) = P(\mathbf{x}, \boldsymbol{\beta}) + Z(\mathbf{x}) + \varepsilon \qquad (2)$$

where $P(\mathbf{x}, \boldsymbol{\beta})$ is a polynomial with free parameters $\boldsymbol{\beta}$ as defined in Equation (1) for the polynomial regression. $Z(\mathbf{x})$ is the realization of a stationary, normally distributed Gaussian random process with mean zero, variance σ^2 and non-zero covariance. The term ε describes solely the approximation error (bias) since random errors are excluded in this formulation. The expression $P(\mathbf{x}, \boldsymbol{\beta})$ provides a global trend for the meta-model behaviour as in the standard response surface approach. The general case, in which the choice of $P(\mathbf{x}, \boldsymbol{\beta})$ is not restricted, is called **universal kriging**. In many applications, the function P is used in the simplest possible way - $P(\mathbf{x}, \boldsymbol{\beta}) = \beta$ (often called **ordinary kriging**). The second part $Z(\mathbf{x})$ assures the interpolation of the observations y at the sampling points $\mathbf{x}^i$ as it creates a localized deviation from the polynomial part of the model. As a result, the output of the kriging model at the sampling points equals the original observations and there are no residuals at the sampling points.

The Gaussian random process is characterized by the covariance matrix of $Z(\mathbf{v})$ defined as:

$$\mathrm{Cov}\,(Z(\mathbf{x}^k), Z(\mathbf{x}^l)) = \sigma^2 \mathbf{R} \qquad (3)$$

A correlation function has to fulfil the requirements $R(\mathbf{x}^k\mathbf{x}^l) = R(\mathbf{x}^l\mathbf{x}^k)$ and $R(\mathbf{x}^k, \mathbf{x}^k) = 1$, respectively, such that the resulting correlation matrix $\mathbf{R}$ is symmetric and its diagonal entries are all equal to one. There are many different formulations meeting these requirements. Usually functions of the form

$$R(\mathbf{x}^k \mathbf{x}^l) = \prod_{i=1}^{n} R_i(x_i^k x_i^l) \qquad (4)$$

are used. Suitable one-dimensional correlation function is the *Gaussian correlation function:*

$$R(x^k x^l) = \exp(-\theta(x^k - x^l)^2) \qquad (5)$$

where θ is a scaling parameter for the correlation function. Although kriging models provide interpolating through the data points, independent of the values for the θ_j parameters, the shape of the model depends on these θ_j parameters. If all θ_j are large, then the overall model will be approximating the regression model with local spikes around the available data points, whereas for small θ_j the model will interpolate more smoothly through the data points.

Because the typical linear regression used to model the behaviour of the mean is a second order polynomial regression, the minimum number of points required in kriging metamodel is still *(N + 1) (N + 2)/2;*

2.3 Artificial Neural Networks

Artificial neural networks are composed of *nodes* (also called *units*) which correspond to the neurons in human brain. The structure of ANNs is characterized by layers as depicted in Figure 3. Each ANN has one input layer and one output layer whose nodes accept input or produce output, respectively. Additionally, the ANN can have one or more hidden layers which contain intermediate variables

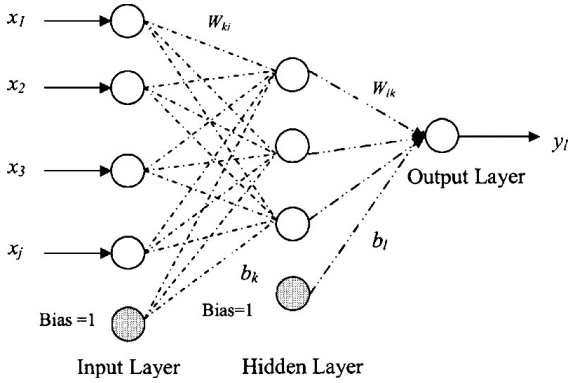

Fig. 3. *Artificial Neural Network*

Depending on the configuration of the connections between the individual units, there are two different types of ANNs: **feedforward networks** and **recurrent networks**. In feedforward ANNs, the output of one node is only passed on to nodes in subsequent layers, and in recurrent ANNs, the output of one node can also be used as input for nodes on the same layer or on preceding layers.

The individual nodes *i* of an artificial neural network accept only one-dimensional input and transform it into output o_i by the so-called **activation function** h_i. The scalar input value of a node *i*, which is termed **net input** and symbolized by net_i, is defined as weighted sum over output values o_j of all nodes *j* that are anterior and directly connected to unit *i*.

$$net_i = \sum_{j=1}^{n} w_{ij} o_j \tag{6}$$

When non-linear activation functions are used in he nodes in the hidden layer non-linear input-output relations can be modeled. Building an ANN, i.e., computing the optimal weights, requires a training for which in general many input-output combinations are needed. As a general rule of thumb, the minimum number of data points required is often computed as three times the number of connections in the network - *3((Nin+1)Nh+ (Nh+1)Nout))*. Moreover the difficulties with using ANNs as metamodels for time-consuming computer simulations include the large variety of possible variants for their structure and the complex implications on their behaviour. This usually rules out ANNs as suitable metamodels for problems that are expensive to analyze. Additionally the training of ANNs usually relies on gradient-based optimization techniques, which only ensure convergence to local minima. Hence, in order to find the global minimum of the error function, the learning phase should be initiated from different starting points. As a consequence, establishing an ANN as useful and reliable metamodel entails a significant computational effort.

2.4 **Radial Basis Functions**

The Radial Basis Function (RBF) method is an interpolating method on all data points. In this method so-called radial basis functions are centered on the input data points. The RBF metamodel is composed of a polynomial part $P(\mathbf{x}, \boldsymbol{\beta})$ and a sum over of radial functions f whose independent variable is the Euclidean distance between prediction point and respective sampling point. Although the radial basis function can have almost any radial symmetric form, they are normally Gaussian functions:

$$f(\mathbf{x},\mathbf{c}) = \exp(- \theta \|x - c\|^2) \tag{7}$$

where **c** is the centre of the radial basis function, $x - c$ is the Euclidean distance from **x** to and **c**, and θ is a parameter, chosen in advance, that determines the width of the RBF.

The predictive model based on the data pairs $\{(\mathbf{x}^1,y^1),\ldots,(\mathbf{x}^n,y^n)\}$ is then:

$$y(\mathbf{x}) = P(\mathbf{x},\beta) + \sum_{j=1}^{n} w_j e^{-\theta \|x - x^j\|^2} \tag{8}$$

In this way it is similar to the kriging method.

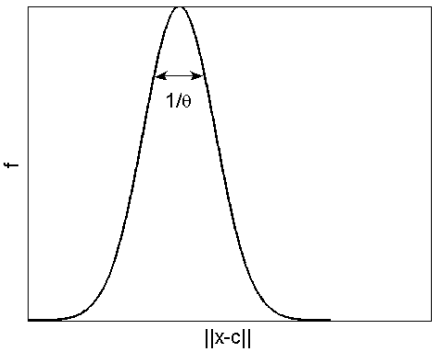

Fig. 4. *Sketch of a radial basis function*

2.5 Assessments of meta-models

In order to select the best method for the task most important is the capability of the metamodel to generalize well over the total input space. For assessment of this capability there are different methods. The following are presented in [4]:

1. Validation by an independent data set that was not used for the model
2. Leave-one-out cross validation
3. P-fold cross validation

In the first method the available data is split into two sets. With the first set the meta-model is built, while the approximation error on the second set is

considered. A drawback of this method is that the comparison of the methods is only done in selected points and thus this method has only local validity and is not very robust. On the other hand, the advantage is that the fitting and validation are only done once which results in a better efficiency.

In the second method, the leave-one-out cross validation, each single data point is used in turn for validation while a meta-model is built with the other N-1 data points. While now global quality measure is obtained, the drawback of this method is that all considered fitting methods have to be applied and validated N times, which is computationally expensive.

The third method, the p-fold cross validation method, provides a global coverage of the estimated error while keeping computation time low. In this method the data set is split into p disjoint subsets of about equal size. While one subset is kept as validation set the models are built using the rest of the data. Notice that when p=N this methods is equal to the leave-one-out method. However when N is large a pfold cross validation with a moderate p value can be a computationally efficient alternative to leave one-out cross validation with regard to obtaining a global fit quality measure.

2.6 Application of metamodels

Polynomial metamodels have been widely used in methodologies for MDO of aircraft. Quadratic polynomial representation is commonly assumed since it has been proved to yield good results as pointed by Mavris [2].

Giunta[1] has performed a preliminary investigation into the use of polynomial and kriging metamodels for the optimization of a high-speed commercial transport aircraft. He explored a 5 and a 10 variables design problems and found that both modelling approaches yield similar results. He points that while the kriging interpolating techniques will reproduce experimental error in observed data (or numerical noise in computer generated data), the kriging methods have some attractive modelling properties. However the errors calculated using both types of metamodels are not significantly different.

Simpson in [3] compared second order polynomial and ordinary kriging metamodels in 3 examples each with 3 variables. Validation was done by an independent data set that was not used for the models. Maximum absolute error, mean absolute error and the root of mean squared error were calculated and compared. The kriging metamodels, despite using a constant term for the global model, are slightly more accurate than the polynomial metamodels.

3. Metamodels of the lift distribution along the span of a wing

In order to asses the fidelity of the methods proposed for the building of metamodels four different ones were created with QstatLab software. The particular application that was chosen was the distribution of the coefficient of lift Cl along the span of the wing in accordance to the angle of sweep of the wing. The model data used is shown on Fig.5.

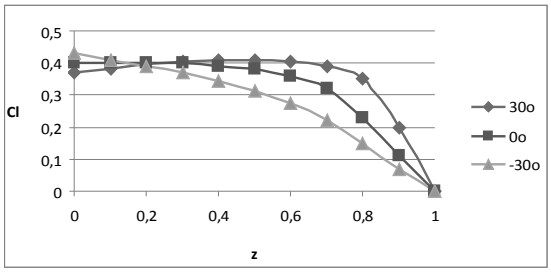

Fig.5. *Model data for the distribution of Cl along the span for three sweep angles*

A total of 33 data points were used, 11 for each angle of sweep(-30^o; 0^o; 30^o). Of them 27 were used for the construction of the metamodels and 6 other were used to evaluate their fidelity

3.1 Third order polynomial metamodel

The response surface created with a third order polynomial metamodel is presented on Figure 6.

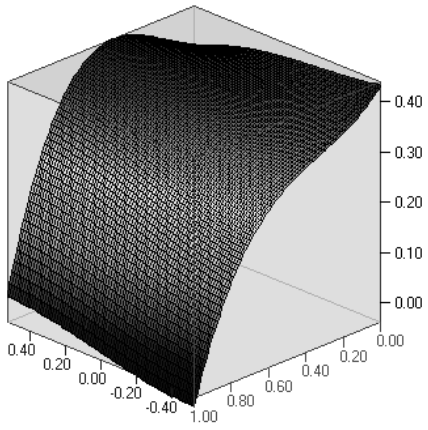

Fig.6. *Third order Polynomial metamodel*

3.2 Second order polynomial metamodel

The response surface created with a second order polynomial metamodel is presented on Figure 7.

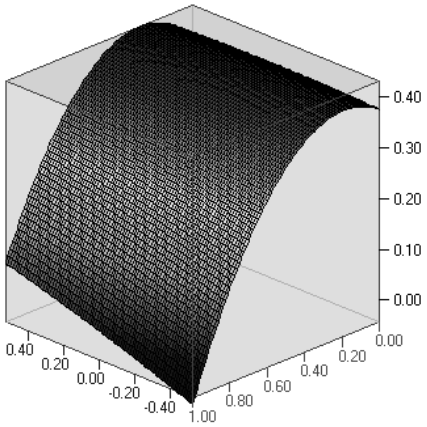

Fig.7*. Second order polynomial metamodel*

3.3 Kriging metamodel

On Figure. 8 the kriging metamodel is shown. For its creation ordinary kriging method was used.

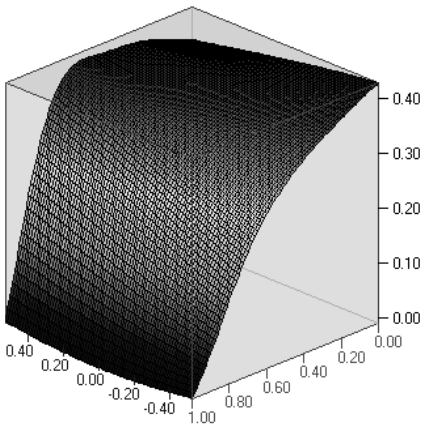

Fig. 8. *Kriging metamodel*

3.4 Radial basis function metamodel

On Figure. 9 the RBF metamodel is shown. For its creation a cubic spline RBF was used.

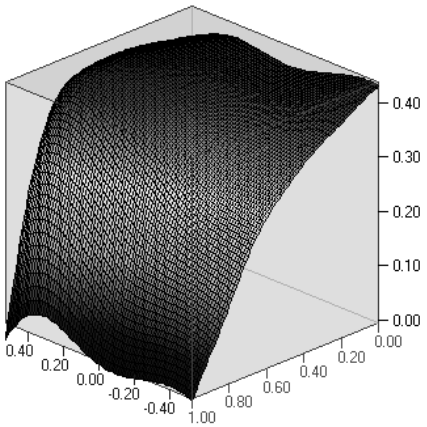

Fig. 9. *RBF metamodel*

3.5 Evaluation of the metamodels

The evaluation was done by an independent data set that was not used for the creation of the metamodels. The maximum absolute error and the root of mean squared error for the different methods are presented in Table 1.

Table 1

Type of metamodel	**Maximum absolute error**	**Root of mean squared error**
Third order polynomial	0,0554	0,0244
Second order polynomial	0,0886	0,0395
Kriging	0,0286	0,0121
RBF	0,0371	0,0168

4. Conclusions

The kriging method provides metamodels that are of highest fidelity. Second is the RBF method. However they both come with increased computational cost. For the conceptual and preliminary design optimization the accuracy of the polynomial metamodels is sufficient. They minimize the influence of numerical noise and experimental errors. Polynomial metamodels provide better visualization of the design search space. Kriging or RBF can be applied at a later stage of design to augment their fidelity.

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