High Order Orthogonal Designs of Experiments for Metamodeling, Identification and Optimization of Composite Material Properties

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***Abstract* − In this paper the method of penalized high order Legendre polynomials and specific designs of experiments for model building on the basis of numerical or physical experiments is proposed. The generalized thin-plate energy functional is used for penalization of the least square functional. The optimal choice of smoothing parameter (penalization coefficient) is implemented using the cross-validation method. Special axial-symmetrical and 90 degree rotational symmetrical D-optimal experimental designs are obtained using the direct constrained optimization method. The method was tested for known optimization test problems with 2–5 variables and showed prediction accuracy comparable with kriging.**

***Keywords* − Designs of experiments, Legendre polynomials, orthogonal designs, penalized least squares, thin-plate potential energy.**

I. Introduction

Metamodeling, also known as surrogate modeling, is becoming more and more frequently used for multidisciplinary optimization. Many commercial CAE software packages include metamodeling tools. The metamodels are built on the basis of numerical and physical experiments. For the design of numerical experiments different Latin hypercube experimental designs are mostly used. The quality of metamodels is measured with prediction accuracy – the possibility of accurate prediction of response values at input value sets not used by model building. The best prediction accuracy today is obtained by nonparametric approximation methods: kriging, radial basis functions, locally weighted polynomials, polynomial neural networks, multivariate adaptive regression splines. But all these methods often have unsatisfactory reliability – sometimes they may give very accurate models and sometimes worse models. Therefore the traditional response surface method, based on second order polynomial approximations, has not lost its popularity for more than 50 years after its first application. Global polynomial approximations have a significant advantage – they may be used in any universal mathematical software, created for special aims and not containing a metamodel building subsystem like fast simulation software tools [1]−[3]. This paper is an extended and corrected version of paper [4] presented at the 11th World Congress on Computational Mechanics (WCCM XI), Barcelona, Spain, 2014.

II. Multivariate Polynomials and Penalized Least Squares

A. Multivariate Polynomials and Orthogonality

Here we will build approximations in m-dimensional rectangular domains. Without loss of generality the so called coded domain – a unit cube $[-1, 1]^m$ can be used, because simple linear transformation transforms any rectangular domain into a unit hypercube [5], [6]. The full single argument polynomial of degree d contains $d + 1$ terms. The number of terms L in full multivariate degree d polynomial is $L = (d + m)!/d!/m!$

Two types of orthogonality properties are applied to both single argument functions and multivariate functions. In mathematics, two functions f and g are called orthogonal if their inner product is zero. The first type of inner product is integral over the domain Ω:

$$\langle f, g\rangle = \int_D w(x) \cdot f(x) \cdot g(x), \tag{1}$$

where $w(x)$ is the weight function. We will call two functions f and g integrally orthogonal over domain Ω, with respect to weight function $w(x)$ if −

$$\int_\Omega w(x) \cdot f(x) \cdot g(x) = 0. \tag{2}$$

If we have a set of values of scalar or m-dimensional input variables $\boldsymbol{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\}$, then the inner product can be realized in the form of a sum over the set:

$$\langle f, g\rangle = \sum_{i=1}^{n} w(\boldsymbol{x}_i) \cdot f(\boldsymbol{x}_i) \cdot g(\boldsymbol{x}_i) \tag{3}$$

and two functions f and g will be orthogonal over the set $\boldsymbol{D}$ with respect to weight function $w(x)$ if

$$\sum_{i=1}^{n} w(\boldsymbol{x}_i) \cdot f(\boldsymbol{x}_i) \cdot g(\boldsymbol{x}_i) = 0. \tag{4}$$

It should be mentioned that, if functions are integrally orthogonal with respect to the constant weighting function, then the inner product over uniformly distributed points divided by number of points converges to zero when the number of points is increased.

The classic Legendre polynomials $P_i(x)$ are orthogonal in the interval $[-1, 1]$ with respect to the constant weight function $w(x) \equiv 1$ [7]. The first and second kind Chebyshev polynomials are

often used in the approximation practice [8], but they have weighting functions $w(x) = 1/\sqrt{1-x^2}$ and $w(x) = \sqrt{1-x^2}$, respectively. This means that the border regions are classified as more important for the first kind and the central region as more important for the second kind of Chebyshev polynomials.

Discrete Legendre polynomials [1],[9],[10] are orthogonal on the set of n equidistant points for single variable polynomials of degree $d \le n-1$, but the number of points in the set grows exponentially with the number of variables and the use of discrete orthogonal polynomials for $m > 4$ and $d > 3$ seems unpractical.

The property of orthogonality gives the possibility of optimal selection of significant terms in the approximation polynomial function. If all terms of regression function are orthogonal on the set of experimental points, then the least-squares method (LSM) gives the diagonal moment matrix and the coefficient for each term can be calculated independently from others (see [11]). Unlike the singe variable case, the use of multivariate orthogonal polynomials is far less frequent since the number of terms in multivariate high order polynomials increases very rapidly, which makes their application difficult with a degree greater than 3 [8].

The first single variable Legendre polynomials are:

$$P_0(x) = 1,\ P_1(x) = x,\ P_2(x) = \frac{1}{2}(3x^2-1),$$
$$P_3(x) = \frac{1}{2}(5x^3-3x),\ P_4(x) = \frac{1}{8}(35x^4-30x^2+3).$$

The Euclid norms of Legendre polynomials are:

$$\|P_i(x)\| = \sqrt{\int_{-1}^{1} P_i^2(x)\mathrm{d}x} = \sqrt{\frac{2}{2i+1}}. \quad (5)$$

We will introduce the following notation for terms of multivariate Legendre polynomials. The simple multivariate polynomial notation uses coefficients β_i for i-th term and a matrix of integer numbers $e_{i,j}$ – (i =1,..., L, j =1,…, m) – exponents for each variable in the i-th term. Here m – number of arguments (factors) or dimension of argument $\boldsymbol{x} \in \mathbb{R}^m$ and L – the total number of terms in the polynomial. The multivariate Legendre polynomials will be in the form:

$$F(x_1, x_2, \dots, x_m) = \sum_{k=1}^{L} \beta_k \prod_{l=1}^{m} P_{e_{kl}}(x_l). \quad (6)$$

Thus each term of multivariate Legendre polynomial is a product of m single variable Legendre polynomials from particular components. The degree of a term is equal to the sum of the exponents of the variables that appear in it. The degree of polynomial d is equal to the maximum value of polynomial terms. Different terms are integrally orthogonal in the unit hypercube $[-1, 1]^m$.

Here, unlike with the reduction approach [8], [12], we will use mainly full polynomials. The matrices of exponents for different m and d can be generated with a simple computer program. For example, the transpose exponent matrix for two-variable second order polynomial is:

$$E^T = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 & 2 \\ 0 & 1 & 0 & 1 & 2 & 0 \end{bmatrix}. \quad (7)$$

The exponential growth of number of full polynomial terms L along with the number of model parameters (coefficients $\boldsymbol{\beta}$) quickly exceeds the number of data samples, making the estimation of model parameters with the conventional least squares method impossible.

Conventional multivariate polynomial approximation needs more sample points than the number of polynomial terms [13]. For example, a 15-th degree polynomial of three variables has 816 terms, which is much more than the number of experimental runs used in metamodel building practice. One approach for overcoming this problem is the reduction of the number of polynomial terms using different criteria for their adding and elimination [12].

B. Energy Functional and Penalized Least Squares

Instead of reduction of polynomials we will use the penalized least squares approach, which is often used in nonparametric spline and radial basis function methods [14], [15]. For uniformity and simplicity we will always use the unit cube $[-1, 1]^m \in \mathbb{R}^m$ as experimental region $\boldsymbol{\Omega}$ of independent variables (factors).

All approximation methods for the model on the basis of sample data obtained by physical or numerical experiments are, in a way, a compromise between the capacity of the model to precisely approximate the given data (mean square error) and the simplicity of the model. The simplicity of the model may be variously measured, for example, as the number of fitting parameters in regression function or number of terms in finite Taylor or Fourier series. In statistics the measure of simplicity of the model is often associated with smoothness of the obtained approximate model function $\hat{y}(\boldsymbol{x})$. One popular smoothness measurement is the generalization of thin-plate deformation potential energy [14], [16].

The approximation $\hat{y}(x)$ according to the penalized least squares method can be obtained by minimizing total potential energy in the class Φ of applicable functions. The total potential energy can be obtained by adding the thin-plate potential energy multiplied by positive constant factor λ to the usual sum of squared residuals:

$$\hat{y}(x) = \underset{y \in \Phi}{\operatorname{argmin}} \sum_{i=1}^{n} (y(x_i) - y_i)^2 + \lambda \int_{-1}^{1} \left(\frac{\partial^2 y}{\partial x^2}\right) dx. \quad (8)$$

Similarly, for two variable cases the well-known thin-plate smoothing approximation is obtained by using strain energy of plate from isotropic and homogeneous material:

$$U_{\mathrm{defl}} = \frac{D}{2} \iint_{\Omega} \left\{ \left(\frac{\partial^2 w}{\partial x_1^2} + \frac{\partial^2 w}{\partial x_2^2}\right)^2 - 2(1-\upsilon)\left[\frac{\partial^2 w}{\partial x_1^2} \cdot \frac{\partial^2 w}{\partial x_2^2} - \left(\frac{\partial^2 w}{\partial x_1\, \partial x_2}\right)^2\right]\right\} dx_1 dx_2, \quad (9)$$

where $w(x_1, x_2)$ – lateral deflection of plate middle plane at the point $w(x_1, x_2)$, D – flexural rigidity of plate which depends on plate thickness and modulus of elasticity in tension and

compression, here a constant value $D = 2$ will be used, and ν – Poisson's ratio.

In the thin-plate energy functional for data smoothing a zero value is always used for the Poisson's ratio, so the energy functional for two variables becomes [17]:

$$U_{\text{defl}} = \frac{D}{2}\iint_{\Omega}\left\{\left(\frac{\partial^2 w}{\partial x_1^2}\right)^2 + \left(\frac{\partial^2 w}{\partial x_2^2}\right)^2 + 2\left(\frac{\partial^2 w}{\partial x_1\,\partial x_2}\right)^2\right\}dx_1 dx_2. \quad (10)$$

For the generalization of the thin-plate energy functional to the m-dimensional case the integral of highest derivative squares is proposed, but in actual nonparametric multivariate spline approximation of the approximation function is obtained by minimization of functional with second order partial derivatives. Thus, for a given smoothing parameter λ, the generalized thin-plate energy penalized least square method is a solution of the minimization problem [14], [16], [18]:

$$\hat{y}(x) = \underset{y\in\Phi}{\operatorname{argmin}}\sum_{i=1}^{n}(y(x_i) - y_i)^2 + \\ +\lambda\int_{\Omega}\sum_{i=1}^{m}\sum_{j=1}^{m}\left(\frac{\partial^2 y}{\partial x_i\,\partial x_j}\right)^2 dx_1 dx_2 \ldots dx_m. \quad (11)$$

III. Penalized Least Squares Method for High Order Multivariate Legendre Polynomials

Using the class of multivariate Legendre polynomials (6) we must find the column vector $\widehat{\boldsymbol{\beta}}$, which minimizes the penalized least squares functional:

$$\hat{\beta} = \underset{\beta\in\mathbb{R}^L}{\operatorname{argmin}}\left\{\sum_{i=1}^{n}\left(\sum_{l=1}^{L}\beta_l\prod\nolimits_{j=1}^{m}P_{e_{l,j}}(w_{ij}) - y_i\right)^2 + \right. \\ \left. +\lambda\int_{\Omega}\sum_{i=1}^{m}\sum_{j=1}^{m}\left[\frac{\partial^2}{\partial x_i\,\partial x_j}\left(\sum_{l=1}^{L}\beta_l\prod_{j=1}^{m}P_{e_{l,j}}(x_j)\right)\right]^2 \mathrm{d}x_1\mathrm{d}x_2\ldots\mathrm{d}x_m\right\}, \quad (12)$$

where $\boldsymbol{w}_i$ – column vector of points of experimental design (sample points in the experimental area) and y_i – measured or calculated response function values at the i-th sample point, i = 1, 2,…, n. The first part of the functional is the conventional sum of squares of LSM; the second part is the smoothness penalization term.

The thin-plate energy functional is a nonnegative definite quadratic form from an L-dimensional column vector of coefficients β with a symmetrical constant $L \times L$ matrix Q.

We will denote the L-dimensional regression vector function, consisting from all terms of polynomial function from input factors – m-dimensional vector $\boldsymbol{x}$ as:

$$z^T(x) = [f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots, f_l(\boldsymbol{x})] \quad (13)$$

and the matrix of regressors $\boldsymbol{X}$ is the $n \times L$ matrix of polynomial terms at sample points:

$$X_{i,l} = \prod_{j=1}^{m}P_{e_{l,j}}(w_{i,j}),\ (i = 1, 2,\ldots, n,\ l=1, 2,\ldots, L). \quad (14)$$

Therefore the penalized least squares functional in matrix form is:

$$\boldsymbol{y}^{\mathrm{T}}\boldsymbol{y} - \boldsymbol{y}^{\mathrm{T}}\boldsymbol{X}\boldsymbol{\beta} - \boldsymbol{\beta}^{\mathrm{T}}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{y} + \boldsymbol{\beta}^{\mathrm{T}}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\lambda}\boldsymbol{\beta}^{\mathrm{T}}\boldsymbol{Q}\boldsymbol{\beta}, \quad (15)$$

where the elements of matrix $\boldsymbol{Q}$ are the second order derivatives of energy function:

$$Q_{ij} = \frac{\partial^2}{\partial\beta_i\,\partial\beta_j}\left(\int_D\sum_{i=1}^{m}\sum_{j=1}^{m}\left(\frac{\partial^2 F}{\partial x_i\,\partial x_j}\right)^2 dx_1 dx_2\ldots dx_m\right). \quad (16)$$

Using (6, 16) we obtain expressions for calculating the thin-plate energy matrix elements:

$$Q_{rq} = \sum_{i=1}^{m}\left[\int_{-1}^{1}P''_{e_{qi}}(x_i)P''_{e_{ri}}(x_i)dx_i \times \prod_{\substack{l=1\\ l\neq i}}^{m}\int_{-1}^{1}P_{e_{ql}}(x_l)P_{e_{rl}}(x_l)dx_l\right] + \\ +2\sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\left\{\int_{-1}^{1}P'_{e_{qi}}(x_i)P'_{e_{ri}}(x_i)dx_i \times \right. \\ \left. \int_{-1}^{1}P'_{e_{rj}}(x_j)P'_{e_{qj}}(x_j)dx_j \times \prod_{\substack{l=1\\ l\neq i,\ l\neq j}}^{m}\int_{-1}^{1}P_{e_{ql}}(x_l)P_{e_{rl}}(x_l)dx_l\right\}. \quad (17)$$

The direct expressions for elements of matrix $\boldsymbol{Q}$ are quite awkward for analytical integration, because the number of terms in them is proportional to the number of combination pairs of variables, i.e. $m(m-1)/2$. But the definite integrals of products with first and second derivatives can be calculated precisely using Gauss-Legendre quadrature. The matrices for any number of dimensions m and polynomial degree can be calculated and saved for use in approximations.

These matrices are relatively sparse, because the $Q_{i,j}$ is always zero if any sum of exponents $p_{i,k} + p_{j,k}$ is an odd number. The matrices are definitely nonnegative, because the potential energy of deformation cannot be negative physically. Matrices have zeroes in the rows and columns corresponding to the constant and linear terms of the polynomial.

After the derivation of the LSM functional we obtain the system of linear algebraic equations for finding the fitting coefficients $\boldsymbol{\beta}$:

$$(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X} + \boldsymbol{\lambda}\boldsymbol{Q})\boldsymbol{\beta} - \boldsymbol{X}^{\mathrm{T}}\boldsymbol{y} = 0. \quad (18)$$

The matrix of the system is symmetrical and positive-definite (if the submatrix of linear terms of $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ is a full range matrix), therefore the system can be solved using Cholesky decomposition or any iterative methods [19]. For high order polynomials ($d > 10$) and number of variables $m > 5$, the size of the matrix will be very large and solving the system will be time-consuming.

A. The Optimal Choice of Smoothing Parameter λ

We use the conventional leave-one out or k-fold cross validation for choosing the optimal value of the smoothing parameter. In tests with known analytical response functions this method gave satisfactory but not excellent results. In most cases the result was slightly under-smoothed (λ value less than optimal).

B. The Optimal Selection of Significant Terms

First it should be noted that the use of orthogonal polynomials instead of conventional multivariate polynomials is advisable only when insignificant terms are eliminated. Full Legendre or Chebyshev polynomials (with all possible terms up to degree d included) give exactly the same approximation as conventional polynomials. Here we propose the use of cross-validation criterion for the decision to eliminate or keep the term with small Euclid norm. Some authors [8] use the F criterion and confidence interval calculations, but this approach is not fully correct for determined computer experiments.

IV. Designs of Experiments

When using classical response surface methodology with second order polynomial approximations the central composite designs (CCD) are most frequently used [5], [6]. The space filling designs (first introduced in [20] and later named Latin hypercubes (LH) [21]) can be used as well and allow the possibility to use other approximation methods, including nonparametric.

CCDs have a relatively small number of points (experimental runs) and good prediction accuracy with minimal prediction variance. With special choice of star point distance CCDs have the rotatability property [5], [6], [23], which means that the prediction variance is equal for all points at equal distance from the center point in coded space $[-1, 1]^m$.

Unfortunately, all these good properties are valid only with fundamental assumptions about the physical model. First – the true response must be exactly second order polynomial function. Second – the variance of the measured response is constant and does not depend on input variables. Third – the rotatability property requires implementing experiments outside the experimental domain of interest, which may be impossible physically. If the true responses are not a polynomial, they often can be approximated with acceptable accuracy in the domain of interest. For example, the $\sin(3x)$ function can be approximated with a third order polynomial in the interval $[-1, 1]$, but by adding two points outside the interval ($x = -1.41$ and $x = 1.41$) the error of approximation becomes inacceptable.

Although the terms of the regression function (multivariate Legendre polynomials) are integrally orthogonal, they are not orthogonal on any set of experimental design points, especially if the number of points is not much larger than total number of possible terms. In this case the optimal selection of significant terms may be a problem. Therefore a new class of experimental designs for use with orthogonal Legendre polynomials was created.

The experimental designs for high order multivariate Legendre polynomial approximations (up to $d = 7$) were obtained using the direct optimization method [2]. The following constraints were used: 1) all experimental points are located in the unit cube $[-1, 1]^m$, 2) designs have central symmetry, axial symmetry and 90° rotation symmetry properties, 3) designs are invariant to the permutation of input variables, 4) designs have given replications of canter point, 5) designs are orthogonal – all non-diagonal elements of information matrix X^TX are equal to zero, 5) designs are D-optimal – the determinant of matrix X^TX must have maximum possible value in consideration of given constraints. The tables of optimized designs for $m = 2, 3, 4, 5$ and $p = 2, 3, 4, 5, 6, 7$ are published in the home page of the Institute of Mechanics of RTU: http://www.mmd.rtu.lv/zpla.htm.

The symmetry properties given above mean that all projections of new designs are equal, just as they are for CCDs. This was achieved by using special groups of symmetric points. For example, a four factor design consists of:

1) n_c center points (0, 0, 0, 0);

2) n_{32} groups each containing 32 points of all permutations of type $(0, \pm a, \pm a, \pm a)$;

3) n_{24} groups each containing 24 points of all permutations of type $(0, 0, \pm a, \pm a)$;

4) n_{16} groups each containing 16 points of all permutations of type $(\pm a, \pm a, \pm a, \pm a)$;

5) n_8 groups each containing 8 points of all permutations of type $(\pm a, \pm a, \pm a, \pm a)$.

Using only one group type 4) with $a = 1$, one group type 5) with $a = 2$ and 6 center points the classical rotatable 30-point CCD design will be obtained. But the orthogonality property for 3rd or 4th degree polynomials requires more experimental points. Using the design optimization software, the 89-point four factor 3rd order orthogonal design was obtained, see Fig. 1. This design consists of two groups of type 3), two groups of type 4), one group of type 5) and one center point.

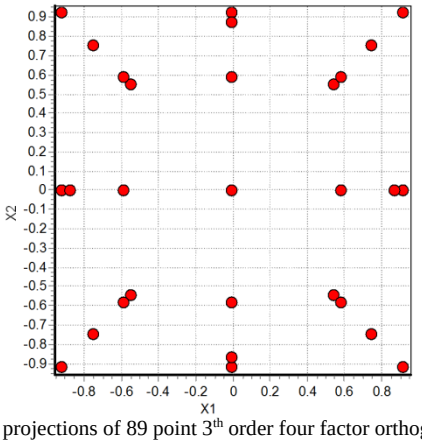

Fig. 1. 2D projections of 89 point 3th order four factor orthogonal design.

A. Testing standard error of predicted response and rotatability of new designs

If the measured responses include some noise caused by errors of input factors by the physical characteristics of the experimental object or process or by registration of responses, then the estimated coefficients of approximate model have variance, even though the used regression function is adequate [5], [22]. The main approximation quality measure is the mean prediction error MSE:

$$\mathrm{MSE}(\hat{y}) = \sqrt{\frac{1}{D}\int_D (\hat{y}(\boldsymbol{x}) - y(\boldsymbol{x}))^2 dx}. \qquad (19)$$

This measure can be calculated only if the exact response function $y(\boldsymbol{x})$ is known. In practice the prediction error is estimated using the root mean square error (RMSE) criterion, which is calculated in additional experimental points (test points) and is not used in the building of approximation, see (28).

Instead of the expensive use of additional experimental runs, the cross-validation method is often used [2], [5].

Of course, one can expect that less variance of estimated approximation coefficients gives less prediction error of the approximate model. This principle is implemented by the criterion of *D*-optimality, which seeks to minimize the product of variance of all approximation coefficients by maximizing the determinant of the moment matrix [5], [6].

Under the usual assumptions about independent and identically distributed errors of registered responses, and, of course, with the assumption of constant error variance σ^2 we have:

$$\mathrm{Var}[\hat{y}(\boldsymbol{x})] = \boldsymbol{z}^{\mathrm{T}}(\boldsymbol{x})(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{z}(\boldsymbol{x})\sigma^2. \quad (20)$$

As a result, the estimated standard error of $\hat{y}(\boldsymbol{x})$ is given by:

$$\mathrm{STD}(\hat{y}(\boldsymbol{x}) = s\sqrt{\boldsymbol{z}^{\mathrm{T}}(\boldsymbol{x})(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{z}(\boldsymbol{x})}, \quad (21)$$

where s is the estimate of σ – square root of the mean square error of the fitted response surface:

$$s = \sqrt{\sum_{i=1}^{n}\frac{(y_i-\hat{y}_i)^2}{n-L}} \quad (22)$$

Some authors use the scaled prediction variance for comparing designs with different number of runs [5]:

$$v(x) = \frac{n\mathrm{Var}[\hat{y}(x)]}{\sigma^2} = \boldsymbol{z}^{\mathrm{T}}(\boldsymbol{x})(\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{z}(\boldsymbol{x})n. \quad (23)$$

The *G*-optimality criterion seeks to minimize the maximum value of $v(\boldsymbol{x})$ in the domain of interest. Another criterion for measuring prediction accuracy is the mean prediction standard deviation, which can be calculated as integral of prediction variance divided by the volume of the domain. For the coded area unit cube $\Omega = [-1, 1]^m$ the mean variance of prediction will be:

$$\sigma^2_{\mathrm{total}} = 2^{-m}\int_{\Omega}\sigma^2_{\mathrm{err}}d\boldsymbol{x} = 2^{-m}\sigma^2\sum_{i=1}^{n}\int_{\Omega}\left(\sum_{j=1}^{l}R_{ji}z_j(\boldsymbol{x})\right)^2 d\boldsymbol{x}, \quad (24)$$

where:

$$\boldsymbol{R} = (\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathrm{T}}. \quad (25)$$

This criterion can be calculated analytically for Legendre polynomials or with the Monte Carlo method for non-orthogonal functions and non-orthogonal experimental designs.

The Euclid norms of polynomial terms are products of single variable Legendre polynomial norms (5):

$$\|z_i\| = \prod_{j=1}^{m}\left\|P_{e_{i,j}}\right\| = \prod_{j=1}^{m}\frac{1}{2e_{i,j}+1}, \quad (26)$$

and the mean variance of predicted response can be calculated simply:

$$\sigma^2_{\mathrm{total}} = 2^{-m}\sigma^2\sum_{j=1}^{L}\left\|z_j\right\|^2\sum_{i=1}^{n}R^2_{ji}. \quad (27)$$

The rotatability measure can be estimated visually, analyzing scatterplots of dependence of the response variance or standard deviation on the distance from the center of domain.

Fig. 2 and Fig. 3 show the contour plots of scaled prediction variance *v* and the scatterplots of standard deviation for the 89 point 3rd order orthogonal design. Fig. 4 and Fig. 5 show the same characteristics for the 89 point 3rd order design from [23]. The mean standard error of prediction for the first design is 0.643, for the second design it is 1.463

The new designs are not exactly rotatable, but the scatterplots of the prediction variance show good stability property.

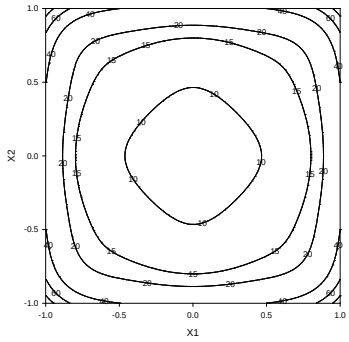

Fig. 2. Contour plot of scaled prediction variance for 89 point 4-factor orthogonal design, right – scatterplot of standard deviation of predicted response versus distance from the center.

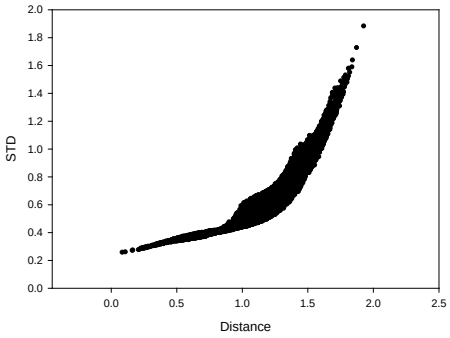

Fig. 3. Scatterplot of standard deviation of predicted response versus distance from the center for 89 point 4-factor orthogonal design.

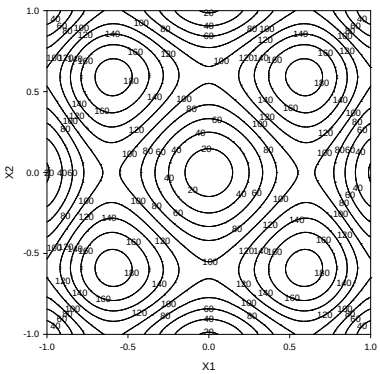

Fig. 4. Contour plot of scaled prediction variance for 89 point design [23].

V. Approximation and Optimization Tests

A. Testing for Common Optimization Test Problems

Analytical function tests included Rosenbrock's valley, Griewangk's function, Goldstein-Price's function, six-hump camel back function, as well as three-argument Wendelberger

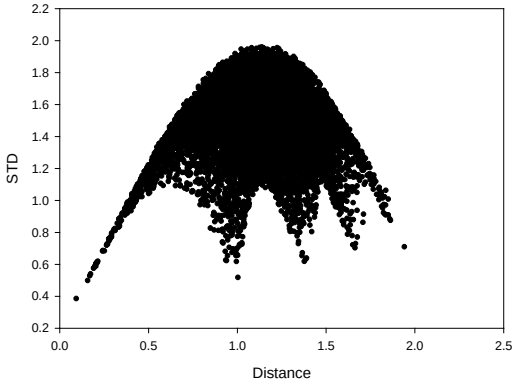

Fig. 5. Scatterplot of standard deviation of predicted response versus distance from the center for 89 point 4-factor design [23].

function [24], 1-7 argument test function from [2]. To compare different test results all experimental areas were linearly scaled to the unit cube $[-1, 1]^m$.

The accuracy of approximation for tests with known response functions f_{test} was measured with the relative average prediction error σ_{test} in additional confirmation points not used in model building:

$$\sigma_{\text{test}} = 100\% \frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(f_{\text{test}}(z_i) - \hat{f}_{\text{test}}(z_i)\right)^2}}{\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(f_{\text{test}}(z_i) - \overline{f}_{\text{test}}\right)^2}} =$$

$$= 100\% \sqrt{\frac{\text{mean square error}}{\text{variance}}}, \qquad (28)$$

where z_i – confirmation points (i=1,…, N), $\hat{f}_{test}(w_i)$ – approximated value of test function, $\overline{f}_{\text{test}}$ – average value of test function in confirmation points. 100000 uniformly randomly selected confirmation points (Latin hypercube sample) in region of interest were used.

B. Testing Results for Analytical Functions

Some of the classic optimization test functions of 2-3 variables are polynomials (Rosenbrocks function, Goldstein-Price function, Himmelblau function) and it goes without saying that high order polynomial approximation for such functions has advantages over other methods. This fact was confirmed in tests.

The summary of other tests is briefly described in the following text. The prediction accuracy of proposed high order polynomial approximation is comparable with the prediction accuracy of nonparametric kriging method and locally weighted polynomials for the case of determined responses without noise. In most cases kriging approximations are slightly better, but for a low number of sample points kriging sometimes can give unacceptable results, which hardly ever happens with parametric approximations. For middle-level Gaussian noise (5–10 % of standard deviation of response from its mean) penalized high order polynomials almost always have less prediction error than kriging and locally weighted polynomials.

C. Testing for Practical Optimization Test Problems

The effectiveness of the penalized Legendre polynomial approximation method and newly created orthogonal high order designs was confirmed by solving several practical optimization problems. For lack of space, we will only mention one – identification of composite material elastic parameters using the vibration method [25]. The 89 point 4-factor orthogonal design gave significantly better approximations for the dependence of specimen eigenfrequencies on the elastic modulus than the previously used 100–200 point Latin hypercube designs.

VI. Conclusion

The new orthogonal high order experimental designs demonstrated good effectiveness for the use with the penalized Legendre polynomial approximation method. They allow simple elimination of insignificant terms and using a number of experimental runs less than the number of terms in full multivariate polynomials.

By testing the proposed method on different common test problems and practical optimization problems for 2-5 input variables, a mean prediction error was obtained that is comparable with the approximation error of nonparametric kriging and second-third order locally weighted polynomials. In the case of responses with 5–10 % Gaussian noise (measured relative to the standard deviation of response from its mean) the proposed method showed noticeably better results than other methods. The cross-validation method for choosing the smoothing factor value has known issues and did not always give optimal λ values, similarly as with the choice of kriging hyperparameters. Due to rapidly rising workload, the method in its proposed form is not suited for models with number of input variables $m > 10$. The model building is the most difficult and time consuming process, but the use of the created parametric metamodels is very simple and they can be implemented in any optimization software.

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Jānis Auziņš. Augstas kārtas ortogonālie eksperimentu plāni kompozītu materiālu īpašību metamodelēšanai, identifikācijai un optimizācijai.

Rakstā tiek piedāvāta sodīto augstas kārtas Ležandra polinomu metode un speciāli eksperimentu plāni matemātisko modeļu veidošanai uz skaitlisko un naturālo eksperimentu bāzes. Daudzargumentu ortogonālo Ležandra polinomu pielietojums ļauj relatīvi vienkārši izslēgt maznozīmīgus polinomu locekļus no polinomiālajiem modeļiem. Vispārinātā plānas plates potenciālā enerģija tiek lietota kā soda sastāvdaļa mazāko kvadrātu funkcionālim. Izgludināšanas parametra (soda koeficienta) optimālā vērtība tiek iegūta ar krosvalidācijas metodi. Ar tiešās optimizācijas metodi iegūti D-optimāli, aksiāli un 90° rotācijas simetriski eksperimentu plāni. Piedāvātā metode realizēta datorprogrammā *EDAOpt*, kura tiek attīstīta un lietota Rīgas Tehniskajā universitātē jau vairāk nekā 15 gadus. Metode pārbaudīta vispārlietotajām optimizācijas testa funkcijām ar 2-5 mainīgajiem un praktiskiem kompozītmateriālu īpašību identifikācijas uzdevumiem. Ar piedāvāto metodi izveidotu modeļu prognozes precizitāte ir apmēram vienāda ar kriginga metodes precizitāti. Uzdevumiem ar nenoteiktību, kuri satur parametru izkliedes, metode dod augstāku prognozes precizitāti, kas ir ļoti būtiski jaunu kompozītmateriālu eksperimentālajos pētījumos.