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HIGH ORDER ORTHOGONAL DESIGNS OF EXPERIMENTS FOR METAMODELING, IDENTIFICATION AND OPTIMIZATION OF MECHANICAL SYSTEMS

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The penalized least squares method that uses the thin-plate potential energy functional for smoothing polynomial approximations of experimental data is a well-known approach [4]. Thus for a given smoothing parameter λ, the generalized thin-plate energy penalized least square method requires a solution of the minimization problem:

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

where the first part of the functional is the conventional sum of squared residuals and the second part represents the potential energy of thin plate, whose bending corresponds to response function y, and $\boldsymbol{x}_i$, $i = 1,2,\ldots,n$ is the set of m experimental input factors (designs of experiments), y_i, $i = 1,2,\ldots, n$ are the registered response values in experimental runs [2]. In the present work this method will be used for multivariate Legendre polynomials and a special class of orthogonal D-optimal experimental designs will be introduced.

All approximations are constructed in coded area – unit cube $\boldsymbol{\Omega} = [-1,1]^m$, where m is the number of input variables (factors). Multivariate Legendre polynomials are sum of terms, in which all terms are products of univariate Legendre polynomials. Full p-th order Legendre polynomial contains all terms for which the sum of degrees of univariate components $\le p$. The use of full multivariate Legendre polynomials for approximation gives no advantage compared to full degree conventional polynomials, because the best fitting function will be the same. But the integral orthogonality of terms of Legendre polynomials allows to estimate the significance of individual terms and to eliminate unnecessary terms from the regression function [2]. The vector of fitting coefficients of Legendre polynomials $\boldsymbol{\beta}$ can be obtained by Least Squares Method:

$$\boldsymbol{\beta} = (\boldsymbol{X}'\boldsymbol{X} + \boldsymbol{\lambda Q})^{-1}\boldsymbol{X}'\boldsymbol{y}, \tag{2}$$

where $\boldsymbol{X}$ is the model matrix (values of all terms of regression function in all points of experimental design [3]), the apostrophe means transpose, $\boldsymbol{Q}$ is the constant symmetrical and positively defined matrix of thin-plate potential energy. The values of matrix $\boldsymbol{Q}$ elements depend only on the number of variables *m* and degree of polynomial *p*. The use of Legendre polynomials simplifies the calculation of penalty matrices. For the cases $p = 2$ and $p = 3$ the penalty matrix $\boldsymbol{Q}$ is diagonal. For normalized Legendre polynomials the absolute value of coefficient β_i is proportional to the significance *of i*-th term of regression function. For the choice of number of eliminated terms and the value of smoothing parameter λ the cross-validation method can be used [2].

The terms of Legendre polynomials are integrally orthogonal in the unit cube $[-1,1]^m$, but they are not orthogonal on the sample of experimental points. Therefore, the use of orthogonal experimental designs for better elimination of insignificant terms is preferred. The experimental designs for high order multivariate Legendre polynomial approximations (up to p =7) were obtained using the direct optimization method [1]. The following constraints are used: 1) all experimental points are located in the unit cube $[-1,1]^m$, 2) designs have central symmetry, axial symmetry and 90 degree rotation symmetry properties, 3) designs are invariant to the permutation of input variables, 4) designs have given replications of centre point, 5) designs are orthogonal – all non-diagonal elements of information matrix $\boldsymbol{X'X}$ are equal to zero, 5) designs are *D*-optimal – the determinant of matrix $\boldsymbol{X'X}$ 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 Machine and Mechanism Dynamics lab of RTU. Designs are not precisely rotatable, but the scatterplots of the prediction variance show good stability property.

The method was tested for known optimization test problems with 2-5 variables and showed prediction accuracy comparable with kriging. For the noisy responses the proposed approach gives a better prediction accuracy of the approximate model. The usability of the method is demonstrated by several practical optimization problems, including vibration-based identification of material elasticity parameters and inverse metamodeling with highly correlated inputs.

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