Metamodel building on the basis of globally weighted high order polynomials

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Traditionally the metamodels for multidisciplinary optimization are built using global polynomial approximations (mainly second order) and nonparametric methods: kriging, radial basis functions, locally weighted polynomials. The main problem by using of nonparametric approximations is the choice of optimal smoothing parameters. The mostly used leave-one-out cross validation often gives undersmoothed result. The use of high order global polynomials needs large number of experimental points and often gives wrong prediction in corner points of research area. Here we propose the global polynomial approximations in which the compromise between the two quality criterions are used: sum of squared residuals and global smoothness of response function. Both of them are analogues of potential energy. First – residual sum of squares is simply total potential energy of linear springs placed between experimental points and the response surface. The second criterion U is analogue of beam and plate bending potential energy:

$$U = \int_D \sum_{i=1}^{m} \sum_{j=1}^{m} \left(\frac{\partial^2 F}{\partial x_i \partial x_j} \right)^2 dx_1 dx_2 \dots dx_m \tag{1}$$

where F is the polynomial regression function, x_1, x_2,…,x_m are the input variables (factors), D is the experimental region scaled to m-dimensional cube $[-1,1]^m$.
If $m = 1$, the expression (1) gives potential energy of beam bending, $m = 2$ gives potential energy of plate bending. For $m > 3$ expression (1) represent the generalization of m-dimensional surface bending potential energy.
The number of terms in k-th degree polynomial of m variables with coefficients β_I is

$$L = \frac{(k+1)(k+2)\cdots(k+m)}{m!} \tag{2}$$

The potential energy of generalized surface bending according to polynomial function can be calculated as quadratic form with constant matrix Q

$$U = \boldsymbol{\beta}^{\mathrm{T}} \boldsymbol{Q} \boldsymbol{\beta} \tag{3}$$

The values of matrix $\boldsymbol{Q}$ elements in the case of polynomials can be calculated by analytical integration of the parts of expression (1).
The potential energy of residuals, used in classical least square method is

$$P = \boldsymbol{\beta}^{\mathrm{T}} \boldsymbol{M} \boldsymbol{\beta} - 2\boldsymbol{\beta}^{\mathrm{T}} \boldsymbol{R}^{\mathrm{T}} \boldsymbol{y} + \boldsymbol{y}^{\mathrm{T}} \boldsymbol{y} \tag{4}$$

where $\boldsymbol{R}$ is the matrix of regression term values in experimental points an $\boldsymbol{y}$ is the column of measured responses and $\boldsymbol{M} = \boldsymbol{R}^{\mathrm{T}} \boldsymbol{R}$.
The total potential energy, which must be minimized for obtaining of best weighted polynomial fit is

$$P + U = \boldsymbol{\beta}^{\mathrm{T}} \boldsymbol{M} \boldsymbol{\beta} - 2\boldsymbol{\beta}^{\mathrm{T}} \boldsymbol{R}^{\mathrm{T}} \boldsymbol{y} + \boldsymbol{y}^{\mathrm{T}} \boldsymbol{y} + \alpha \boldsymbol{\beta}^{\mathrm{T}} \boldsymbol{Q} \boldsymbol{\beta} \tag{5}$$

The coefficient α controls the smoothing of approximation function and the optimal value for this coefficient can be found by leave-one-out crossvalidation. In the case $\alpha = 0$ we obtain the traditional least square method. Interesting property of the proposed method is the fact, that the number of experimental points can be less than the number of terms in the regression function.

The weighted global polynomial approximation method was tested for several classical test problems and some structural design metamodeling benchmarks, for example design of GF/PP sandwich panel for transport application.
The metamodel prediction accuracy was comparamble with that of nonparametric kriging and locally weighted polynomials. For systems without stochastic error of responses the kriging was the best, for middle level noise best was the proposed method and for systems with large noise components locally weighted polynomials gave the best prediction accuracy.