International Conference on Advances in Computational Modeling and Simulation

Some Ideas and Progress on the Shape Optimization of Nonlinear Structures

Zhenhan Yao\textsuperscript{a}\textsuperscript{*}, Yingtao Wei\textsuperscript{b}

\textsuperscript{a}Department of Engineering Mechanics, Tsinghua University, Beijing, 100084, China
\textsuperscript{b}Department of Automotive Engineering, Tsinghua University, Beijing, 100084, China

Abstract

For the sensitivity analysis of nonlinear structure with respect to the shape variation, it is formulated based on the geometrical mapping approach, rather than the material derivative approach. The shape variation is regarded as a mapping characterized by the shape variation velocity field, or a fictitious deformation of the continuum, which is not real displacement, and there are no strain and stress corresponding to such fictitious displacement field. Started from the virtual work principle, the sensitivity equations of state variables for nonlinear structure with respect to the shape variation have been formulated, and also the equation for calculating the sensitivity of performances with respect to the shape variation. To enhance the efficiency, the adjoint variable method is applied, wherein the asymmetry of the equation matrix due to the slip contacted case of the frictional contact using Lagrange multiplier method is taken into account. For the gradient-based Kriging method based on the samples determined by the orthogonal maximin Latin hypercube design, a criterion for the best likelihood spatial correlation parameter is suggested, based on the transition from insufficient to excessive control. The criterion is verified using a series of test examples.

© 2011 Published by Elsevier Ltd. Selection and/or peer-review under responsibility of Kunming University of Science and Technology. Open access under CC BY-NC-ND license.

Keywords: shape optimization; nonlinear structure; sensitivity analysis; geometrical mapping approach; gradient-based Kriging method

\textsuperscript{*} Corresponding author. Tel.: +86-10-62785284.
E-mail address: demyzh@tsinghua.edu.cn.
1. Introduction

Structural optimization is one of the important tasks in modern structural design, and it is usually based on the finite element analysis (FEA) and optimization algorithms. For the complex nonlinear structures, such as automotive tires with geometrical, material and contact boundary condition nonlinearities, the FEA for each design sample is time-consuming. Therefore, how to get the optimal design with fewer samples is very important. To reduce the number of samples, the information gained from each sample should be enhanced by using sensitivity analysis (SA). In the optimization algorithms, global algorithms applying different kinds of response surface are more efficient than local searching algorithms, which would be stopped at local minimum rather than global one. Within the response surface approach the Kriging method is more robust than the response surface fitting method, because it avoids to assuming the form of response surface. In the Kriging method, the gradient based Kriging (GBK) method [1] is more suitable than the conventional one for the complex nonlinear structures, because it can reduce the number of samples significantly. For the SA with respect to the shape variation, Choi and Kim have presented so-called material derivative approach (MDA) [2,3]. To enhance the efficiency further, the adjoint variable method (AVM) can be applied.

In this paper, some ideas and progress for the shape optimization of complex nonlinear structures are presented. In Section 2, a geometrical mapping approach (GMA) for the SA in shape optimization is presented. Based on the GMA, the equation system for the sensitivity of variables and that of the object function are formulated in Section 3. In Section 4, a criterion for determining the best likelihood spatial correlation parameter of the GBK method is suggested, and it has been verified by a series of prescribed object functions. Finally, some suggestions for enhancing the reliability of shape optimization are presented as the concluding remarks.

2. Geometrical Mapping Approach

For the shape optimization, the GMA is presented, where the shape variation is regarded as a fictitious deformation of the continuum, or a mapping, characterized by the shape variation velocity (or design velocity) field \( \dot{V}_{ia} \),

\[
\dot{x}_i = v_i + V_{ia} \tau_a = o_x_i + \dot{u}_i, \quad i = 1, 2, 3; \quad \alpha = 1, \ldots, k
\]

where \( o_x_i, x_i \) denote the Lagrange coordinates for the original shape and the shape design corresponding to parameters \( \tau_a \), respectively, \( k \) is the number of shape parameters, and \( \dot{u}_i \) is the fictitious displacement, which is not real displacement, and there are no strain and stress corresponding to such fictitious displacement field. The real displacement fields under loading \( t \) are defined as

\[
\dot{o}_x_i = o_x_i + \dot{u}_i, \quad \dot{x}_i = x_i + \dot{u}_i
\]

for the original shape and the shape design \( \tau \), where \( \dot{o}_x_i, \dot{x}_i \) are Euler coordinates, and \( \dot{u}_i, \dot{u}_i \) are real displacement fields. Under the identical load parameter, the relationship between the displacements of the corresponding mapping points can be expressed as

\[
\dot{u}_i = \dot{u}_i + \dot{u}_{i,\alpha} \tau_a
\]

where the subscript \( \alpha \) denotes \( \partial u / \partial \tau_a \), which means the change rate, or the sensitivity, of variable for the corresponding mapping points during the shape variation, and takes the value at \( \tau_\beta = 0, \beta = 1, \ldots, k \).
Besides Eq. (1) and Eq. (3), another fundamental equation of the GMA is that for the sensitivity of displacement gradients,

\[
\frac{\partial}{\partial \tau_a} \left( \frac{\partial u_i}{\partial x_j} \right)_{\tau=0} = \frac{\partial}{\partial \tau_a} \left( \frac{\partial u_i}{\partial x_j} \right)_{\tau=0} \frac{\partial^2 u_i}{\partial x_k^2} \left( \frac{\partial^2 u_i}{\partial x_k^2} \right)_{\tau=0} + \frac{\partial}{\partial \tau_a} \left( \frac{\partial u_i}{\partial x_j} \right)_{\tau=0} \frac{\partial^2 u_i}{\partial x_k^2} \left( \frac{\partial^2 u_i}{\partial x_k^2} \right)_{\tau=0}
\]

The MDA presented in literature also based on the mapping

\[
x_i = x + \tau \mathbf{V}
\]

where the shape parameter is regarded analogous with the time, \( x, \mathbf{V} \) denote the Euler coordinates of a material point at time \( \tau \) and time 0 respectively, and \( \mathbf{V} = \partial x_i / \partial \tau \). In the MDA, the time rate of change of displacement following the material point can be formulated as

\[
\dot{z} = z' + \mathbf{V} \cdot \nabla z
\]

where \( z, z', \nabla z \) stand for the material derivative, partial derivative with respect to time, and the spatial derivative with respect to the Euler coordinates respectively. For the material derivative of \( \nabla z \),

\[
(\nabla z)' = (\nabla z)' + \mathbf{V} \cdot \nabla (\nabla z) = \nabla z' + \mathbf{V} \cdot \nabla (\nabla z) = \nabla (z - V \cdot \nabla z) + \mathbf{V} \cdot \nabla (\nabla z) = \nabla \dot{z} - \nabla \mathbf{V} \cdot \nabla z
\]

where \( \nabla \) stands for the spatial derivative with respect to the Euler coordinates.

It seems the resulted equation from Eq. (4) and Eq. (7) are identical, but the formulations are different: Lagrangian in Eq. (4) and Eulerian in Eq. (7). For the strain and stress fields in structural optimization the Lagrangian formulation should be applied. Therefore the formulation based on the GMA is more consistent, and the derivation will have clearer physical meaning.

3. Sensitivity Analysis

For the SA of complex nonlinear structure with geometric, material and contact nonlinearities, the formulation can be stated from the virtual work principle for modified shape design:

\[
\int_{\Omega} \delta u_i \epsilon_i = \int_{\Omega} \delta \mu_i \mu_i + \int_{\Omega} \rho \delta E_i \mu_i + \int_{\Omega} C_{LM}^M
\]

In this equation, \( C_{LM}^M \) is the contact boundary term in Lagrangian multiplier approach,

\[
C_{LM}^M = \int_{\Omega} (\lambda \delta u_i \mu_i + \lambda \delta \mu_i \mu_i + \lambda \delta \mu_i \mu_i) dS
\]

where \( \lambda \) is the Lagrange multiplier and \( \Omega \) is the domain of the structure. The Lagrange multiplier follows the virtual work principle:

\[
\int_{\Omega} \lambda \delta u_i \mu_i dS = 0
\]
where \( \lambda_n \), \( \lambda_s \), \( \lambda_l \) denote the Lagrangian multipliers, \( g_n \) is the normal gap for the design \( \tau \) without loading, \( S_t \) stands for the traction-given part of the boundary, \( S^a_t \), \( S^a_l \) the stick and the slide part of contacted boundary. For simplicity the structure is assumed to be contacted with a rigid plane. It should be mentioned that the division of contacted boundary is load and shape design dependent.

For the shape optimization problem, the original shape corresponding to \( \tau = 0 \) is taken as the referential configuration, and then Eq. (8) can be rewritten in the referential configuration as

\[
\int_{S^0} \lambda_S \delta \mu_t |J| dV = \int_{S^0} \lambda_S \delta \mu_t (dS/d\mu_S) dV + \int_{S^0} \rho \lambda_S \delta \mu_t |J| dV
\]

\[
+ \int_{S^0} \lambda_S \delta \mu_t (dS/d\mu_S) dS
\]

\[
+ \int_{S^0} \lambda_S \delta \mu_t (dS/d\mu_S) dS
\]

\[
+ \int_{S^0} \lambda_S \delta \mu_t (dS/d\mu_S) dS + \int_{S^0} \lambda_S \delta \mu_t (dS/d\mu_S) dS
\]

\[
+ \int_{S^0} \lambda_S \delta \mu_t (dS/d\mu_S) dS (10)
\]

Because the virtual displacement is geometrically admissible, arbitrary and arbitrary small deviation of the actual displacement, the virtual displacement for corresponding mapping point of different shape design is identically denoted by \( \delta \mu_t \). For the variation of sensitivity of displacement gradient we have

\[
\delta_\mu (u_{\tau}, V_{\tau}) = \left. \frac{\partial}{\partial \tau} \delta (u_{\tau}, V_{\tau}) \right|_{\tau = 0} = -\delta \mu_t \circ V_{\tau} \alpha, \beta
\]

(11)

Finally the equation system for the sensitivity of displacement \( \delta u^\alpha \) and the sensitivity of Lagrangian multiplier \( \delta \lambda^\alpha \) can be derived, which can be written in matrix form as

\[
(0K + 0N + 0G) \delta u^\alpha = 0g^\alpha + 0F^\alpha + t0F^\alpha - 0C0G \delta \lambda^\alpha
\]

(12)

The matrices in the left side of the first equation is the tangential stiffness matrix, including linear stiffness matrix \( 0K \), nonlinear stiffness matrix \( 0N \) and geometrical stiffness matrix \( 0G \), these matrices are identical with those in nonlinear FEA. The matrices \( 0C, 0G \) are identical with those in nonlinear FEA of contact problem using Lagrangian multiplier approach. \( 0g^\alpha \), \( 0F^\alpha \) are change rate of the external load vector and contact load vector, \( 0F^\alpha \) stands for the fictitious load corresponding to the shape variation characterized by the design velocity field. The fictitious load vector \( 0F^\alpha \) can be written as

\[
0F^\alpha = -\int_{S^0} \delta V_{\tau} \circ (B^T \lambda_B + 0B^T \lambda_B) V_{\tau} dV + \int_{S^0} \delta V_{\tau} \circ (B^T \lambda_B + 0B^T \lambda_B) V_{\tau} dV
\]

\[
+ \int_{S^0} \delta S_{\tau} \circ (B^T \lambda_B + 0B^T \lambda_B) V_{\tau} dV + \int_{S^0} \delta S_{\tau} \circ (B^T \lambda_B + 0B^T \lambda_B) V_{\tau} dV
\]

\[
+ \int_{S^0} \delta V_{\tau} \circ (B^T \lambda_B + 0B^T \lambda_B) V_{\tau} dV + \int_{S^0} \delta S_{\tau} \circ (B^T \lambda_B + 0B^T \lambda_B) V_{\tau} dV
\]

(13)

Because of the length limitation, the detailed formulae will be presented in a separated paper.
Furthermore, the equation for the object function and its sensitivity can be derived as

\[ \psi_t = \int_V f(t, u_1(x), t, u_2(x)) \, dV \approx \frac{\partial \psi}{\partial \mu} \, \mu^* + \psi^* \tau \]  

(14)

\[ \psi^* = \frac{\partial \psi}{\partial \mu} \, \mu^* + \psi^* \tau \]  

(15)

where, if the HEX8 elements are applied,

\[ \frac{\partial \psi}{\partial \mu} \approx \sum_{e} \int_{V_e} \left( \frac{\partial f}{\partial u} \right) \left( \sum_{m=1}^{n} N_m^e(\xi) \right) \, dV \]  

(16)

\[ \psi^* = \int_{V_e} f(t, u_1(x), t, u_2(x)) \, dV \]  

(17)

For solving the sensitivity of object function, the AVM can be applied, the adjoint equation is written as

\[ \frac{\partial \psi}{\partial \mu} = A^T \psi^* + B^T \psi^* + C^T \psi^* + D^T \psi^* \]  

(18)

where the matrix of contact part is asymmetric. The first equation can be solved with algorithm for symmetric system at first, then substitute into the second and solved with Gaussian elimination method, finally back substitute to obtain the final solution. The sensitivity of object function can be computed as

\[ \psi^* = A^T \psi^* + B^T \psi^* + C^T \psi^* + D^T \psi^* \]  

(19)

4. Gradient Based Kriging Method

Kriging method is developed firstly in geology based on assuming continued mineralization between measured values, and it can avoid any assumption of response function. Based on the SA the GBK can reduce the number of design samples significantly.

GBK model is a surrogated model, and the approximate response function \( \hat{y}(x) \) can be formulated as

\[ \hat{y}(x) = f^T(x) \beta + z(x) \]  

(20)

where \( f^T(x) \) is the polynomial regression function, which usually can be assumed to be 1, \( \beta \) is the regression coefficient, and \( z(x) \) is a stationary Gaussian random function with zero mean. The response \( y \) at a point \( x \) and the measured data at all samples \( Y \) are submitted to a multivariate normal distribution

\[ \begin{bmatrix} y \\ Y \end{bmatrix} \sim N_{m+n \times 1} \begin{bmatrix} f^T \\ F \end{bmatrix} \beta, \sigma^2 \begin{bmatrix} 1 & r^T \\ r & R \end{bmatrix} \]  

(21)
The measured data including the response and $n$ gradients at $m$ sample points, the first part of the multivariate normal distribution is the mean, and the second part is the variance including the spatial correlation matrix, in which

\begin{align*}
R_{ij} & = \prod_{k=1}^{n} e^{-\theta_k (x_i^k - x_j^k)^2}, \\
\hat{R}_{ik} & = 2\theta_k (x_i^k - x_j^k) \prod_{k=1}^{n} e^{-\theta_k (x_i^k - x_j^k)^2} \\
R_{ij}^{(i)} & = \prod_{k=1}^{n} e^{-\theta_k (x_i^k - x_j^k)^2}, \\
\hat{R}_{ik}^{(i)} & = 2\theta_k (x_i^k - x_j^k) \prod_{k=1}^{n} e^{-\theta_k (x_i^k - x_j^k)^2} \\
R_{ijk}^{(i,i)} & = -4\theta_1 \theta_2 (x_i^1 - x_j^1) (x_i^2 - x_j^2) \prod_{k=1}^{n} e^{-\theta_k (x_i^k - x_j^k)^2} \\
R_{ij}^{(i,i)} & = 2\theta_1 (x_i^1 - x_j^1) \prod_{k=1}^{n} e^{-\theta_k (x_i^k - x_j^k)^2}
\end{align*}

(22)

where $\theta_k$, $k = 1, 2, \ldots, n$ are spatial correlation parameter for each design variable, and $i, j = 1, 2, \ldots, m$ denote different design samples.

Minimizing the mean square error with unbiased constraint, the linear prediction for the surrogate approximate response surface, namely the Kriging surface, can be obtained,

\begin{equation}
\hat{y}(x) = f^T(x)\beta + r^T(x)R^{-1}(Y - F\beta), \quad \beta = (F^T R^{-1} F)^{-1} F^T R^{-1} Y(X)
\end{equation}

The key issue in the Kriging and GBK method is how to determine the maximum likelihood spatial correlation parameter. The criterion presented in literature is

\begin{equation}
\phi(\hat{\theta}) = \sigma^2(\hat{\theta})|R(\hat{\theta})|^{1/n} = \min_{\theta}\left\{\frac{1}{n} (Y - F\hat{\beta})^T R^{-1} (Y - F\hat{\beta}) | R(\theta) |^{1/n}\right\} = \min_{\theta} \phi(\theta)
\end{equation}

But it is not successful in authors’ case studies.

Based on the sample points determined by Latin hypercube design, especially using the orthogonal maximin Latin hypercube design (OMLHD) algorithm [4], by projecting an $n$-point design on to any design variable, one will get $n$ different levels for that variable. The OMLHD minimizes the pairwise correlations as well as maximize the inter-site distances of the sample points. In this way the whole design space is divided into $n$ nearly equal size subspaces, each one mainly controlled by one sample.

According to a series of test examples with prescribed objective function, one can observe: as the spatial correlation parameter decreases, the surrogate response surface controlled by the observation data from the insufficient control to the excessive control. The transition is corresponding to the deviation of the calculated response function value from the observation data. The maximum likelihood spatial correlation parameter is near this transition. Therefore a criterion is suggested as

\begin{equation}
\hat{\theta} = \min_{\theta} \left\{\frac{1}{m} \sum_{i=1}^{n} (\hat{y}_{i(i)}(\theta) - y_{i(i)})^2 < 1.0 \times 10^{-7}\right\}
\end{equation}

(25)

where $\hat{y}_{i(i)}$, $\theta_{i(i)}$ and $y_{i(i)}$, $\theta_{i(i)}$ are calculated response function and observed response function for all design samples respectively.
The suggested criterion has been verified with a series of numerical examples with prescribed response function. It is observed: the number of samples greater than 1.5 times of the number of design variables is enough, if the response function is simple power functions, or trigonometric functions \( \sin \) and \( \cos \) in the range of \( \pi \) and without random error; if the response function is the trigonometric functions \( \sin \) and \( \cos \) in the range of \( 2\pi \), number of samples greater than 3 times of the number of design variables is required. With random error less than 10%, the GBK can still be applied, sometimes more samples are required.

Fig. 1 shows the projection of all grid point of the Kriging response surface onto the plane of each design variable and the response function, where the obtained response surface using 5 design samples for 3 design variables is satisfactory.

Because of the space limitation, more details and more verification will be presented in separated paper.

For large scale problems, for example with 10 design variables and 15 design samples, the number of grid points of the Kriging surface will be \( 15^{10} \), to calculated the Kriging response function for all grid points is time-consuming, and more effective algorithm for searching the optimal design point should be applied.

5. Concluding Remarks

Two of the key issues for the shape optimization of complex nonlinear structure are presented in this paper. One is for the SA with respect to the shape design, the GMA is presented, which has clearer physical meaning than so called MDA. On this basis the equation system for the sensitivity of displacement is derived from the virtual work equation, and then the sensitivity of performance can be obtained by the AVM. The second is for the GBK method, a criterion for the determination of maximum likelihood spatial correlation parameter is presented, which is based on the samples determined by the OMLHD, and searching for the transition from insufficient control to successive control. This criterion has been verified by a series of test examples.

The shape optimization of complex nonlinear structure should be based on the FEA and SA, or numerical experiments. The physical experiments are characterized with random error, which usually can be reduced significantly by repeated measurements. The numerical experiments also have error, including the error of modeling, the discretization error and calculating error, which cannot be reduced by repeated computation. On the other hand, the numerical examples using GBK shows that although it is very efficient for the observation data of accurate response function, it will be inefficient for the data with considerable error. Only if the numerical error was limited in an admissible range, the optimization using GBK would be efficient, sometimes with more design samples than for the case without error. Therefore, to ensure the accuracy of the FEA and SA is very important.
To ensure the accuracy of the FEA and SA, first of all is to ensure the accuracy of the formulation. Therefore the GMA is applied, and the Lagrange multiplier approach is applied for the contact analysis. Furthermore, the reasonable mesh should be adopted for each shape design sample, different mesh for different shape is reasonable; design velocity field should also be determined for each shape design sample, corresponding to small variation of the design parameter. Otherwise the shape optimization will lose the reliability.

More details on the SA by GMA and the optimization using GBK method with the presented criterion for determination of the maximum likelihood spatial correlation parameter, and the practical engineering applications, will be presented in separated papers.

Acknowledgements

This study is supported by the Manufacture Française des Pneumatiques Michelin, and this support is gratefully acknowledged.

References

[1] Xuan Y, Xiang JH, Zhang WH, Zhang YL. Gradient-based Kriging approximate model and its application research to optimization design. *Sci China E: Tech Sci*, 2009; 52: 1117-1124.

[2] Choi KK, Kim NH. *Structural Sensitivity Analysis and Optimization 1: Linear Systems*. New York: Springer; 2005.

[3] Choi KK, Kim NH. *Structural Sensitivity Analysis and Optimization 2: Nonlinear Systems and Applications*. New York: Springer; 2005.

[4] Joseph VR, Hung Y. Orthogonal-maximin Latin hypercube designs. *Statistica Sinica*, 2008; 18: 171-186.