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Accurate displacement derivatives for structural optimization using approximate reanalysis

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Abstract

A unified approach for accurate approximations of displacements and displacement derivatives with respect to design variables is presented. The solution procedure is based on results of a single exact analysis at an initial design. Unlike common approximations of the structural response, the approach presented is not based on calculation of derivatives. Rather, approximations of displacements are used to evaluate displacement derivatives at various modified designs. It is shown that similar computational procedures are employed for evaluating displacements, first- and second-order derivatives of displacements. The procedure presented is suitable for different types of design variables and structures. Numerical results show that accurate approximations of derivatives can be achieved with a small computational effort for designs obtained by very large changes in the initial structure. © 2001 Elsevier Science B.V. All rights reserved.

1. Introduction

The derivatives of the response vector with respect to the system parameters are usually referred to as the sensitivity coefficients. Sensitivity analysis is used to:

- Predict the changes in the system response due to changes in the structure parameters.
- Select a search direction in design optimization problems.
- Construct explicit approximations of the constraint functions in terms of the structure parameters (e.g. first-order Taylor series approximations).
- Generate approximations for the response of a modified system, including approximate reanalysis models.
- Assess the effects of uncertainties in the structure properties (material properties, geometric parameters and other parameters of the computational model) on the system response.

It has been noted [1] that a predominant contributor to the cost and time of the optimization of large structural systems is the calculation of first-order derivatives. Moreover, calculation of the latter derivatives for a given design involves structural analysis of the design. As a consequence, there has been much interest in efficient computation procedures for sensitivity analysis. Early and recent developments in methods for sensitivity analysis are discussed in [1–4]. Efficient evaluation of approximate first-order derivatives by various sensitivity analysis methods has been demonstrated in a previous study [5].

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Methods of sensitivity analysis can be divided into the following classes:

(a) Analytical methods which are widely used and often demonstrate good performance. However, implementation of these methods is difficult in some problems, such as shape optimization, where analytical derivatives of the stiffness matrix are not easy to obtain.

(b) "Semi-analytical", or "quasi-analytical" methods, based on finite-difference evaluation of the right-hand-side vector, the so-called "pseudo load". These methods combine ease-of-implementation and computational efficiency, therefore they have been implemented in several finite element programs. However, the errors associated with the finite difference approximation of the right-hand side vector can be substantial [6,7].

(c) Finite-difference methods are the easiest to implement and therefore they are quite popular. For a problem with n design variables, finite difference derivative calculations repeat the analysis for $(n+1)$ different stiffness matrices. This procedure is usually not efficient compared to analytical and semi-analytical methods. The large number of analyses associated with finite difference calculations can be avoided by employing approximate reanalysis methods.

The two general methods used for calculating the sensitivity of the system response are:

- The direct method, based on the implicit differentiation of the analysis equations that describe the system response with respect to the desired parameters, and the solution of the resulting sensitivity equations.
- The adjoint-variable method, where an adjoint physical system is introduced whose solution permits the rapid evaluation of the desired sensitivity coefficients.

In this paper, analytical derivatives by direct differentiation are considered.

Calculation of second-order derivatives of the response functions is needed in various applications. Some of the most powerful optimization algorithms involve calculation of the matrix of second derivatives or its approximation. The quality of some explicit approximations of the constraint functions, such as the Taylor series, could be significantly improved by considering second-order terms. However, the computational effort involved in calculating the matrix of second derivatives might be prohibitive. To reduce this effort, some methods use only the diagonal elements of the latter matrix.

In a typical optimization process it is necessary to evaluate the response for numerous modified designs. Only for some of the designs it is necessary also to evaluate the response derivatives. In cases where results of exact analysis for the modified design are available, calculation of exact response derivatives is straightforward and an approximate procedure is usually not needed. The approach presented herein is intended for problems where results of exact analysis for the modified design are not available and exact calculation of derivatives for the latter design involves many calculations.

Effective solution techniques for structural analysis and sensitivity analysis are essential in the optimization of large-scale structures. To reduce the computational effort, extensive studies on explicit approximations of the structural behavior in terms of the design variables have been made in recent years. High quality approximations of the structural response have been developed, but most approximations that are adequately accurate for the response are not sufficiently accurate for the response derivatives.

The combined approximations (CA) approach developed recently is most suitable for efficient-accurate evaluation of the structural response at various modified designs [8–11]. The solution process is based on results of a single exact analysis of an initial design, and it is suitable also for large changes in the design variables. The approximations are easy to implement and they are suitable for different types of design variables and structures. Unlike common approximations of the structural response, the CA approach is not based on calculation of derivatives. Rather, it will be shown in this paper that the response approximations can be used to evaluate the response derivatives.

2. Problem formulation

A unified approach for accurate approximations of displacements and displacement derivatives at various modified designs is presented in this paper. The problem under consideration can be stated as follows. Given an initial design and the corresponding stiffness matrix $\mathbf{K}^*$ the resulting displacements $\mathbf{r}^*$ are computed by the equilibrium analysis equations

$$\mathbf{K}^*\mathbf{r}^* = \mathbf{R}^*, \tag{1}$$

where $\mathbf{R}^*$ is the initial load vector. It is assumed that the stiffness matrix $\mathbf{K}^*$ is given from the initial analysis in the decomposed form

$$\mathbf{K}^* = \mathbf{U}^{*\mathrm{T}}\mathbf{U}^*, \tag{2}$$

where $\mathbf{U}^*$ is an upper triangular matrix. That is, calculation of the displacements by Eq. (1) involves forward and backward substitutions. Once the displacements $\mathbf{r}^*$ are evaluated, the stresses can readily be determined by the stress–displacement relations.

Assume a change in the design so that the modified stiffness matrix is given by

$$\mathbf{K} = \mathbf{K}^* + \Delta\mathbf{K}, \tag{3}$$

where $\Delta\mathbf{K}$ is the change in the stiffness matrix due to the change in the design. The object is to find accurate approximations of displacements $\mathbf{r}$ and displacement derivatives $\partial\mathbf{r}/\partial\alpha$, $\partial^2\mathbf{r}/\partial\alpha^2$ with respect to a design variable α, for various modified designs, without solving the sets of modified equations. The latter equations are given below.

(a) The modified analysis equations are

$$\mathbf{K}\mathbf{r} = (\mathbf{K}^* + \Delta\mathbf{K})\mathbf{r} = \mathbf{R}. \tag{4}$$

(b) The modified first-order derivative equations are obtained by direct differentiation of Eq. (4) with respect to a design variable α. In many problems it is assumed that the load vector is independent of the design variables, that is $\partial\mathbf{R}/\partial\alpha = \mathbf{0}$. For simplicity of presentation this assumption will be considered here, but the approach presented is suitable for the more general case where the elements of the load vector are functions of the design variables. Differentiating equation (4) with respect to α and rearranging gives the first-order derivative equations at the modified design

$$\mathbf{K}\frac{\partial\mathbf{r}}{\partial\alpha} = -\frac{\partial\mathbf{K}}{\partial\alpha}\mathbf{r}. \tag{5}$$

The direct approach involves solution of Eq. (5) for $\partial\mathbf{r}/\partial a$ and then taking the desired component of the vector. For multiple design variables, Eq. (5) must be solved repeatedly for each variable. In cases where the decomposed form of Eq. (2) is available for matrix $\mathbf{K}$, calculation of $\partial\mathbf{r}/\partial\alpha$ involves only forward and backward substitutions. However, in the present formulation exact analysis has been done only at the initial design, therefore the decomposed form of Eq. (2) is available only for the initial stiffness matrix $\mathbf{K}^*$.

(c) The modified second-order derivative equations are obtained by differentiating Eq. (5) with respect to α and rearranging

$$\mathbf{K}\frac{\partial^2\mathbf{r}}{\partial\alpha^2} = -\frac{\partial^2\mathbf{K}}{\partial\alpha^2}\mathbf{r} - 2\frac{\partial\mathbf{K}}{\partial\alpha}\frac{\partial\mathbf{r}}{\partial\alpha}. \tag{6}$$

Again, since exact analysis has been carried out only at the initial design, the decomposed form of Eq. (2) is not available for the modified stiffness matrix $\mathbf{K}$.

In the present formulation, the design variables may represent members' cross-sections, coordinates of joints or structural shape. The elements of the stiffness matrix are not restricted to certain forms and can be general functions of the design variables. Once the displacement derivatives are evaluated, the stress derivatives can be readily determined by explicit differentiation of the stress–displacement relations.

Approximate expressions for evaluating displacements, first-order derivatives and second-order derivatives of displacements at a modified design are derived subsequently in Section 3. A computational procedure and numerical results are demonstrated in Section 4. It will be shown that similar computational procedures are used for evaluating the various quantities. The numerical results demonstrate that accurate approximations of derivatives can be achieved with a small computational effort for designs obtained by very large changes in the initial structure.

3. Evaluation of modified displacements derivatives

3.1. Modified displacements

For completeness of presentation, evaluation of modified displacements by the CA method is briefly described in this section. A detailed presentation of the solution process is given elsewhere [11]. Given the initial stiffness matrix $\mathbf{K}^*$ in the decomposed form of Eq. (2) and the initial displacements $\mathbf{r}_1 = \mathbf{r}^*$, calculation of the modified displacements $\mathbf{r}$ for any given change $\Delta\mathbf{K}$ in the stiffness matrix involves the following steps:

(a) The modified stiffness matrix $\mathbf{K}$ is first introduced [Eq. (3)]. Since $\mathbf{K}^*$ is already given, this step involves only calculation of $\Delta\mathbf{K}$.

(b) The basis vectors $\mathbf{r}_i$ are calculated by the following recurrence relation:

$$\mathbf{r}_i = -\mathbf{K}^{*-1}\Delta\mathbf{K}\mathbf{r}_{i-l} = -\mathbf{B}\mathbf{r}_{i-l} \quad (i = 2, 3, \ldots, s), \tag{7}$$

in which s is the number of vectors considered and matrix $\mathbf{B}$ is defined by

$$\mathbf{B} \equiv \mathbf{K}^{*-1}\Delta\mathbf{K}. \tag{8}$$

A small number of basis vectors (2–3 vectors) is often adequate to achieve sufficient accuracy [8–11]. In addition, calculation of the basis vectors by Eq. (7) involves only forward and backward substitutions, in cases where $\mathbf{K}^*$ is available in the form of Eq. (2) from initial analysis of the structure. The vector $\mathbf{r}_2$, for example, is calculated by

$$\mathbf{K}^*\mathbf{r}_2 = -\Delta\mathbf{K}\mathbf{r}_1. \tag{9}$$

We first solve for the vector of unknowns $\mathbf{t}$ by the forward substitution

$$\mathbf{U}^{*\mathrm{T}}\mathbf{t} = -\Delta\mathbf{K}\mathbf{r}_1. \tag{10}$$

The vector $\mathbf{r}_2$ is then calculated by the backward substitution

$$\mathbf{U}^*\mathbf{r}_2 = \mathbf{t}. \tag{11}$$

Similarly, $\mathbf{r}_3$ is calculated by

$$\mathbf{K}^*\mathbf{r}_3 = -\Delta\mathbf{K}\mathbf{r}_2. \tag{12}$$

(c) The reduced matrix $\mathbf{K}_\mathrm{R}$ and the reduced vector $\mathbf{R}_\mathrm{R}$ are calculated by

$$\mathbf{K}_\mathrm{R} = \mathbf{r}_\mathrm{B}^\mathrm{T}\mathbf{K}\mathbf{r}_\mathrm{B}, \quad \mathbf{R}_\mathrm{R} = \mathbf{r}_\mathrm{B}^\mathrm{T}\mathbf{R}. \tag{13}$$

(d) The vector of unknown coefficients $\mathbf{y}$ is calculated by solving the set of $(s \times s)$ equations

$$\underset{s\times s}{\mathbf{K}_\mathrm{R}}\,\underset{s\times 1}{\mathbf{y}} = \underset{s\times 1}{\mathbf{R}_\mathrm{R}}. \tag{14}$$

The reduced set of simultaneous equations (14) can be transformed into uncoupled form. This topic will be discussed later in Section 3.

(e) The modified displacements $\mathbf{r}$ are evaluated by

$$\mathbf{r} = y_1\mathbf{r}_1 + y_2\mathbf{r}_2 + \cdots + y_s\mathbf{r}_s = \mathbf{r}_\mathrm{B}\mathbf{y}, \tag{15}$$

where $\mathbf{r}_\mathrm{B}$ is the matrix of the basis vectors, defined as

$$\underset{m\times s}{\mathbf{r}_\mathrm{B}} = \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_s. \tag{16}$$

In the procedure presented, the computed terms of the binomial series expansion are used as high quality basis vectors in reduced basis approximations. The unknown coefficients of the reduced basis expression can be readily determined by solving a reduced set of the analysis equations. The efficiency and the accuracy of the results achieved by the CA method have been demonstrated in previous studies [8–11]. It will be shown subsequently how the expressions presented above are used to evaluate first- and second-order derivatives of the displacement functions by similar solution procedures.

3.2. Modified first-order derivatives

Given the expressions developed in the previous section, evaluation of the first-order derivatives $\partial\mathbf{r}/\partial\alpha$ at the modified design $\mathbf{K} = \mathbf{K}^* + \Delta\mathbf{K}$ involves the following steps:

(a) The matrix of derivatives $\partial\mathbf{K}/\partial\alpha$ is determined. The elements of the stiffness matrix $\mathbf{K}$ are usually explicit function of the design variables, therefore the derivatives $\partial\mathbf{K}/\partial\alpha$ are readily available. For example, in the common case where the elements of matrix $\Delta\mathbf{K}$ are linear functions of the variable α, the modified stiffness matrix [Eq. (3)] can be expressed as

$$\mathbf{K} = \mathbf{K}^* + \alpha\Delta\mathbf{K}^*, \tag{17}$$

in which the elements of matrix $\Delta\mathbf{K}^*$ are constant. The matrix of derivatives $\partial\mathbf{K}/\partial\alpha$ in this case is simply equal to $\Delta\mathbf{K}^*$.

(b) The matrix of derivatives of basis vectors $\partial\mathbf{r}_B/\partial\alpha$ is determined. Since the elements of $\mathbf{r}_1$ are independent of the changes in the design, the derivatives $\partial\mathbf{r}_1/\partial\alpha$ are equal to zero. The remaining derivative vectors $\partial\mathbf{r}_i/\partial\alpha$ depend on $\Delta\mathbf{K}$ and can be calculated by differentiation of Eq. (7). Rearranging the latter equation to read

$$\mathbf{K}^*\mathbf{r}_i = -\Delta\mathbf{K}\mathbf{r}_{i-1} \quad (i = 2, 3, \ldots, s), \tag{18}$$

and differentiation with respect to α yields

$$\mathbf{K}^*(\partial\mathbf{r}_i/\partial\alpha) = -(\partial\Delta\mathbf{K}/\partial\alpha)\mathbf{r}_{i-1} - \Delta\mathbf{K}(\partial\mathbf{r}_{i-1}/\partial\alpha). \tag{19}$$

Evidently, the derivatives $\partial\mathbf{r}_i/\partial\alpha$ depend on the expressions of the basis vectors $\mathbf{r}_i$. Consider again the common case where the elements of matrix $\Delta\mathbf{K}$ are linear functions of the variable α [Eq. (17)]. Defining the vectors of constant elements $\mathbf{r}_1^*, \mathbf{r}_2^*, \mathbf{r}_3^*$

$$\mathbf{r}_1^* = \mathbf{r}^*, \quad \mathbf{r}_2^* = -\mathbf{K}^{*-1}\Delta\mathbf{K}^*\mathbf{r}_1^*, \quad \mathbf{r}_3^* = -\mathbf{K}^{*-1}\Delta\mathbf{K}^*\mathbf{r}_2^*\ldots, \tag{20}$$

then we have from Eq. (18)

$$\mathbf{r}_1 = \mathbf{r}_1^*, \quad \mathbf{r}_2 = \alpha\mathbf{r}_2^*, \quad \mathbf{r}_3 = \alpha^2\mathbf{r}_3^*\ldots \tag{21}$$

Once the vectors of Eq. (20) have been calculated by forward and backward substitutions, calculation of the basis vectors by Eq. (21) for various α values is trivial. The resulting matrix $\mathbf{r}_B$ [Eq. (16)] is given by

$$\mathbf{r}_B = \mathbf{r}_1^*, \alpha\mathbf{r}_2^*, \alpha^2\mathbf{r}_3^*, \ldots, \tag{22}$$

and the corresponding matrix $\partial\mathbf{r}_B/\partial\alpha$ is

$$\frac{\partial\mathbf{r}_B}{\partial\alpha} = \mathbf{0}, \mathbf{r}_2^*, 2\alpha\mathbf{r}_3^*, \ldots \tag{23}$$

(c) The matrix $\partial\mathbf{K}_R/\partial\alpha$ and the vector $\partial\mathbf{R}_R/\partial\alpha$ are calculated by differentiating Eq. (13)

$$\begin{aligned}\frac{\partial\mathbf{K}_R}{\partial\alpha} &= \frac{\partial\mathbf{r}_B}{\partial\alpha}^{\mathrm{T}}\mathbf{K}\mathbf{r}_B + \mathbf{r}_B^{\mathrm{T}}\frac{\partial\mathbf{K}}{\partial\alpha}\mathbf{r}_B + \mathbf{r}_B^{\mathrm{T}}\mathbf{K}\frac{\partial\mathbf{r}_B}{\partial\alpha},\\ \frac{\partial\mathbf{R}_R}{\partial\alpha} &= \frac{\partial\mathbf{r}_B}{\partial\alpha}^{\mathrm{T}}\mathbf{R}.\end{aligned} \tag{24}$$

(d) The vector of unknowns $\partial\mathbf{y}/\partial\alpha$ is calculated by solving the set of $(s \times s)$ equations, obtained by differentiating Eq. (14) and rearranging

$$\mathbf{K}_\mathrm{R}\frac{\partial \mathbf{y}}{\partial \alpha} = \frac{\partial \mathbf{R}_\mathrm{R}}{\partial \alpha} - \frac{\partial \mathbf{K}_\mathrm{R}}{\partial \alpha}\mathbf{y}. \tag{25}$$

(e) The approximate displacement derivatives are evaluated by differentiating the approximate displacement expression (15)

$$\frac{\partial \mathbf{r}}{\partial \alpha} = \frac{\partial \mathbf{r}_\mathrm{B}}{\partial \alpha}\mathbf{y} + \mathbf{r}_\mathrm{B}\frac{\partial \mathbf{y}}{\partial \alpha}. \tag{26}$$

It can be observed that the numerical procedures for evaluating the approximate displacements and displacement derivatives are similar.

3.3. Modified second-order derivatives

Higher-order derivatives can be evaluated in a way similar to that described above. In this section, calculation of approximate second-order derivatives is demonstrated. Given the expressions developed in previous sections, evaluation of the above derivatives for the modified design $\mathbf{K} = \mathbf{K}^* + \Delta\mathbf{K}$ involves the following steps:

(a) The matrix of derivatives $\partial^2\mathbf{K}/\partial\alpha^2$ is first determined. As noted earlier, the elements of the stiffness matrix $\mathbf{K}$ are usually explicit function of the design variables, therefore the derivatives $\partial^2\mathbf{K}/\partial\alpha^2$ are readily available. For example, in the common case, where the elements of matrix $\Delta\mathbf{K}$ are linear functions of the variable α, the stiffness matrix is expressed in the form of Eq. (17). Since the elements of matrix $\Delta\mathbf{K}^*$ are constant

$$\partial^2\mathbf{K}/\partial\alpha^2 = \mathbf{0}. \tag{27}$$

(b) The matrix of derivatives $\partial^2\mathbf{r}_\mathrm{B}/\partial\alpha^2$ is determined. In the case where the elements of matrix $\Delta\mathbf{K}$ are linear functions of the variable α, differentiation of Eq. (23) with respect to α gives

$$\frac{\partial^2 \mathbf{r}_\mathrm{B}}{\partial \alpha^2} = \mathbf{0}, \mathbf{0}, 2\mathbf{r}_3^*, \ldots \tag{28}$$

(c) The matrix $\partial^2\mathbf{K}_\mathrm{R}/\partial\alpha^2$ and the vector $\partial^2\mathbf{R}_\mathrm{R}/\partial\alpha^2$ of second-order derivatives are calculated by differentiation of Eq. (24)

$$\begin{aligned}\frac{\partial^2 \mathbf{K}_\mathrm{R}}{\partial \alpha^2} &= \frac{\partial^2 \mathbf{r}_\mathrm{B}^\mathrm{T}}{\partial \alpha^2}\mathbf{K}\mathbf{r}_\mathrm{B} + \mathbf{r}_\mathrm{B}^\mathrm{T}\frac{\partial^2 \mathbf{K}}{\partial \alpha^2}\mathbf{r}_\mathrm{B} + \mathbf{r}_\mathrm{B}^\mathrm{T}\mathbf{K}\frac{\partial^2 \mathbf{r}_\mathrm{B}}{\partial \alpha^2} + 2\left(\frac{\partial \mathbf{r}_\mathrm{B}^\mathrm{T}}{\partial \alpha}\frac{\partial \mathbf{K}}{\partial \alpha}\mathbf{r}_\mathrm{B} + \frac{\partial \mathbf{r}_\mathrm{B}^\mathrm{T}}{\partial \alpha}\mathbf{K}\frac{\partial \mathbf{r}_\mathrm{B}}{\partial \alpha} + \mathbf{r}_\mathrm{B}^\mathrm{T}\frac{\partial \mathbf{K}}{\partial \alpha}\frac{\partial \mathbf{r}_\mathrm{B}}{\partial \alpha}\right),\\ \frac{\partial^2 \mathbf{R}_\mathrm{R}}{\partial \alpha^2} &= \frac{\partial^2 \mathbf{r}_\mathrm{B}^\mathrm{T}}{\partial \alpha^2}\mathbf{R}.\end{aligned} \tag{29}$$

(d) The vector of unknowns $\partial^2\mathbf{y}/\partial\alpha^2$ is calculated by solving the set of $(s \times s)$ simultaneous equations, obtained by differentiating Eq. (25) and rearranging

$$\mathbf{K}_\mathrm{R}\frac{\partial^2 \mathbf{y}}{\partial \alpha^2} = \frac{\partial^2 \mathbf{R}_\mathrm{R}}{\partial \alpha^2} - \frac{\partial^2 \mathbf{K}_\mathrm{R}}{\partial \alpha^2}\mathbf{y} - 2\frac{\partial \mathbf{K}_\mathrm{R}}{\partial \alpha}\frac{\partial \mathbf{y}}{\partial \alpha}. \tag{30}$$

(e) The second-order derivatives of the displacements are calculated by differentiating Eq. (26)

$$\frac{\partial^2 \mathbf{r}}{\partial \alpha^2} = \frac{\partial^2 \mathbf{r}_\mathrm{B}}{\partial \alpha^2}\mathbf{y} + 2\frac{\partial \mathbf{r}_\mathrm{B}}{\partial \alpha}\frac{\partial \mathbf{y}}{\partial \alpha} + \mathbf{r}_\mathrm{B}\frac{\partial^2 \mathbf{y}}{\partial \alpha^2}. \tag{31}$$

4. Computational considerations

4.1. Solution procedure

The presentation of Section 3 shows that similar algebraic operations are involved in calculations of displacements, first- and second-order derivatives of displacements for modified designs. In this section, a

Table 1
Summary of algebraic operations

Step	Response	1st derivatives	2nd derivatives
a. Introduce coefficient matrix	$\mathbf{K}$	$\partial\mathbf{K}/\partial\alpha$	$\partial^2\mathbf{K}/\partial\alpha^2$
b. Introduce basis vectors	$\mathbf{r}_B$	$\partial\mathbf{r}_B/\partial\alpha$	$\partial^2\mathbf{r}_B/\partial\alpha^2$
c. Introduce reduced quantities	$\mathbf{K}_R$, $\mathbf{R}_R$	$\partial\mathbf{K}_R/\partial\alpha$, $\partial\mathbf{R}_R/\partial\alpha$	$\partial^2\mathbf{K}_R/\partial\alpha^2, \partial^2\mathbf{R}_R/\partial\alpha^2$
d. Calculate reduced unknowns	$\mathbf{y}$	$\partial\mathbf{y}/\partial\alpha$	$\partial^2\mathbf{y}/\partial\alpha^2$
e. Calculate final unknowns	$\mathbf{r}$	$\partial\mathbf{r}/\partial\alpha$	$\partial^2\mathbf{r}/\partial\alpha^2$

computational procedure that emphasizes this similarity is introduced. All operations related to the above three computational tasks will be considered at each step of the solution process. The solution procedure involves the following steps (summary of the operations is given in Table 1).

(a) The matrices of coefficients are introduced:
- The modified stiffness matrix $\mathbf{K}$ [Eq. (3)].
- The matrix of first-order derivatives $\partial\mathbf{K}/\partial\alpha$.
- The matrix of second-order derivatives $\partial^2\mathbf{K}/\partial\alpha^2$.

The amount of calculations depends on the nature of the $\mathbf{K}$ and on the number of changed elements. It has been noted that, since $\mathbf{K}^*$ is already given, introduction of $\mathbf{K}$ involves only calculation of $\Delta\mathbf{K}$. In the common case, where the elements of matrix $\Delta\mathbf{K}$ are linear functions of the variable α, the matrix of derivatives $\partial\mathbf{K}/\partial\alpha$ is simply equal to $\Delta\mathbf{K}^*$ [see Eq. (17)] and the elements of matrix $\partial^2\mathbf{K}/\partial\alpha^2$ equal zero [Eq. (27)].

(b) The matrices of basis vectors are introduced:
- The matrix of basis vectors $\mathbf{r}_B$ [Eq. (16)].
- The matrix of first-order derivatives $\partial\mathbf{r}_B/\partial\alpha$.
- The matrix of second-order derivatives $\partial^2\mathbf{r}_B/\partial\alpha^2$.

Most of the computational efforts are invested in calculation of the basis vectors $\mathbf{r}_B$. Since this operation involves only forward and backward substitutions, this effort is significantly reduced. It has been noted [12] that calculation of each basis vectors requires 2% of the CPU time required for complete reanalysis. In addition, previous experience has shown that a small number of vectors is often sufficient to achieve accurate results. In certain cases, repeated calculation of the matrices of basis vectors involves almost no computational effort. In the common case of approximations along a line, repeated calculation of the matrices $\mathbf{r}_B$, $\partial\mathbf{r}_B/\partial\alpha$ and $\partial^2\mathbf{r}_B/\partial\alpha^2$ is trivial [Eqs. (22), (23), (28)].

(c) The reduced matrices and vectors are introduced:
- The reduced matrix $\mathbf{K}_R$ and the reduced vector $\mathbf{R}_R$ [Eq. (13)].
- The matrix $\partial\mathbf{K}_R/\partial\alpha$ and the vector $\partial\mathbf{R}_R/\partial\alpha$ [Eqs. (24)].
- The matrix $\partial^2\mathbf{K}_R/\partial\alpha^2$ and the vector $\partial^2\mathbf{R}_R/\partial\alpha^2$ [Eq. (29)].

(d) The reduced unknown vectors are calculated:
- The coefficients vector $\mathbf{y}$ [Eq. (14)].
- The vector $\partial\mathbf{y}/\partial\alpha$ [Eq. (25)].
- The vector $\partial^2\mathbf{y}/\partial\alpha^2$ [Eq. (30)].

It is instructive to note that in each of the above calculations the same matrix of coefficients $\mathbf{K}_R$ is considered and only the right-hand side vector is different.

(e) The final unknown vectors are calculated:
- The displacements vector $\mathbf{r}$ [Eq. (15)].
- The first-order derivatives vector $\partial\mathbf{r}/\partial\alpha$ [Eq. (26)].
- The second-order derivatives vector $\partial^2\mathbf{r}/\partial\alpha^2$ [Eq. (31)].

Most of the operations in the above procedure are straightforward and involve a small computational effort. In a recent study [13] it has been found that solution of nonlinear analysis problems by the CA method required 30–35% of the CPU time needed by conventional nonlinear analysis. For linear reanalysis, evaluation of the displacements by the CA method may involve only 20–25% of the CPU time.

4.2. Accuracy of the approximations

The accuracy of the derivatives depends on the accuracy of the approximate displacements. To improve the accuracy of the latter, an uncoupled set of new basis vectors can be introduced, using a Gram–Schmidt orthogonalization and normalization method [11,13]. For any assumed number of basis vectors, the results obtained by considering either the original set of basis vectors or the new set of uncoupled basis vectors are identical. The advantage in using the latter vectors is that all expressions for evaluating the displacements become explicit functions of the design variables and it is not necessary to solve the reduced set of simultaneous equations (14). Consequently, additional vectors can be considered without modifying the calculations that were carried out already and the errors involved in the approximations can readily be evaluated. In addition, the uncoupled system is more well-conditioned and possible ill-conditioning is avoided.

The set of new basis vectors $\mathbf{V}_i$ $(i = 1, \ldots, s)$ is determined by the original ones $\mathbf{r}_i$ from [11]

$$\mathbf{V}_1 = \left|\mathbf{r}_1^{\mathrm{T}}\mathbf{K}\mathbf{r}_1\right|^{-1/2}\mathbf{r}_1, \tag{32}$$

$$\begin{aligned} \overline{\mathbf{V}}_i &= \mathbf{r}_i - \sum_{j=1}^{i-1}\left(\mathbf{r}_i^{\mathrm{T}}\mathbf{K}\mathbf{V}_j\right)\mathbf{V}_j, \\ \mathbf{V}_i &= \left|\overline{\mathbf{V}}_i^{\mathrm{T}}\mathbf{K}\overline{\mathbf{V}}_i\right|^{-1/2}\overline{\mathbf{V}}_i, \quad i = 2, \ldots, s, \end{aligned} \tag{33}$$

where $\overline{\mathbf{V}}_i$ and $\mathbf{V}_i$ are the ith non-normalized and normalized vectors, respectively. Defining the matrix $\mathbf{V}_{\mathrm{B}}$ of new basis vectors and the vector $\mathbf{z}$ of new coefficients, the reduced system of Eq. (14) becomes uncoupled and the final displacements are given by the explicit expression

$$\mathbf{r} = \mathbf{V}_{\mathrm{B}}\mathbf{z} = \mathbf{V}_{\mathrm{B}}\left(\mathbf{V}_{\mathrm{B}}^{\mathrm{T}}\mathbf{R}\right). \tag{34}$$

The accuracy of the results for a specific number s of basis vectors can be evaluated by the sth term of the approximate displacements expression [Eq. (34)]

$$\mathbf{r}^{(s)} = \mathbf{V}_s\left(\mathbf{V}_s^{\mathrm{T}}\mathbf{R}\right). \tag{35}$$

If the solution process converges, the size of the elements of the vector $\mathbf{r}^{(s)}$ in Eq. (35) can be used as a convergence criterion, namely

$$E_r = \frac{\|\mathbf{r}^{(s)}\|}{\|\sum_{i=1}^{s}\mathbf{r}^{(i)}\|} = \frac{\|\mathbf{V}_s(\mathbf{V}_s^{\mathrm{T}}\mathbf{R})\|}{\|\sum_{i=1}^{s}\mathbf{V}_i(\mathbf{V}_i^{\mathrm{T}}\mathbf{R})\|} \leqslant E_r^{\mathrm{U}}, \tag{36}$$

where E_r^{U} is a small number and $\| \; \|$ is the Euclidean norm. In cases where the accuracy of the approximations is inadequate, additional basis vectors may be considered.

4.3. Numerical results

The example presented below demonstrates the accuracy of the approximations achieved for very large changes in the design. Consider the classic ten-bar truss problem shown in Fig. 1 with a single loading condition of two concentrated loads. The design variables are the members' cross-sectional areas, the initial cross-sections equal unity, the modulus of elasticity is $E = 30{,}000$, and the eight analysis unknowns are the horizontal and vertical displacements at joints 1, 2, 3 and 4, respectively. The stress constraints are $-25.0 \leqslant \sigma \leqslant 25.0$, and the minimum size constraints are $0.001 \leqslant \mathbf{X}$. Assuming the weight as an objective function, the resulting optimal design is

$$\mathbf{X}_{\mathrm{opt}}^{\mathrm{T}} = \{8.0, 0.001, 8.0, 4.0, 0.001, 0.001, 5.667, 5.667, 5.667, 0.001\}.$$

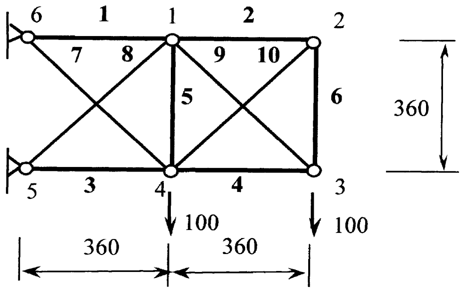

Fig. 1. Ten-bar truss.

The line from the initial design to the optimal design is given by

$$\mathbf{X} = \mathbf{X}^* + \alpha\Delta\mathbf{X}^*,$$

where $\Delta\mathbf{X}^*$ is defined as

$$\Delta\mathbf{X}^{*\mathrm{T}} = \{7.0, -0.999, 7.0, 3.0, -0.999, -0.999, 4.667, 4.667, 4.667, -0.999\}.$$

For $\alpha = 1.0$ (the optimum) the change in the design is very large: members 1 and 3 are increased by 700%, member 4 is increased by 300%, members 7–9 are increased by 467%, and the topology is changed by eliminating members 2, 5, 6, 10, and joint 2 (displacements 3 and 4).

Assuming that results of exact analysis are available for the initial design, evaluation of the displacements, the first- and the second-derivatives with respect to α will be illustrated for $\alpha = 0.5, 0.75$, and 1.0. The corresponding modified cross-sections are summarized in Table 2.

The results given in Tables 3–6 for various numbers of assumed basis vectors show that 2–3 basis vectors provide good accuracy. Yet, the accuracy is improved by considering additional vectors. As noted earlier, the accuracy of the displacement derivatives depends on the accuracy of the approximate displacements. The error percentage obtained for the displacements and displacement derivatives are summarized in Table 5. It can be observed that there is no significant change in errors between $\alpha = 0.5$ and 0.75. In addition, the errors in the displacements and in the displacement derivatives are of the same order of magnitude. In Table 6, the second-order derivatives have not been calculated for $\alpha = 1.0$, since at this point, joint 2 is practically eliminated.

Table 2
Cross-sections of elements for modified designs $\alpha = 0.5$, 0.75, and 1.0

Element	Cross-sections		
	$\alpha = 0.5$	$\alpha = 0.75$	$\alpha = 1.0$
1	4.500	6.250	8.000
2	0.501	0.251	0.001
3	4.500	6.250	8.000
4	2.500	3.250	4.000
5	0.501	0.251	0.001
6	0.501	0.251	0.001
7	3.334	4.500	5.667
8	3.334	4.500	5.667
9	3.334	4.500	5.667
10	0.501	0.251	0.001

Table 3
Approximate displacements and displacements derivatives for $\alpha = 0.5$

Number of basis vectors	2	3	4	5	Exact
Displacements	0.50	0.52	0.52	0.52	0.52
	1.53	1.46	1.48	1.49	1.49
	0.71	0.76	0.77	0.77	0.77
	3.56	3.63	3.64	3.65	3.65
	−0.89	−0.98	−0.99	−0.98	−0.98
	3.77	3.87	3.89	3.90	3.90
	−0.54	−0.55	−0.55	−0.55	−0.55
	1.71	1.64	1.62	1.62	1.62
1st derivatives	−0.80	−0.81	−0.80	−0.79	−0.79
	−2.16	−2.16	−2.11	−2.09	−2.09
	−1.05	−1.04	−1.02	−1.01	−1.01
	−4.96	−4.93	−4.91	−4.89	−4.89
	1.24	1.23	1.21	1.24	1.24
	−5.21	−5.17	−5.13	−5.10	−5.10
	0.85	0.85	0.86	0.87	0.86
	−2.37	−2.36	−2.39	−2.42	−2.42
2nd derivatives	2.55	2.52	2.51	2.52	2.52
	6.17	6.35	6.29	6.34	6.34
	3.11	2.99	2.97	3.00	3.00
	14.02	13.79	13.78	13.81	13.81
	−3.52	−3.28	−3.27	−3.27	−3.27
	14.58	14.26	14.23	14.29	14.30
	−2.67	−2.64	−2.65	−2.64	−2.64
	6.66	6.82	6.86	6.81	6.81

Table 4
Approximate displacements and displacements derivatives for $\alpha = 0.75$

Number of basis vectors	2	3	4	5	Exact
Displacements	0.36	0.37	0.37	0.38	0.38
	1.13	1.07	1.10	1.11	1.11
	0.52	0.56	0.58	0.59	0.59
	2.64	2.72	2.73	2.74	2.74
	−0.66	−0.75	−0.76	−0.74	−0.74
	2.81	2.91	2.94	2.95	2.95
	−0.38	−0.40	−0.39	−0.39	−0.39
	1.27	1.21	1.18	1.17	1.17
1st derivatives	−0.41	−0.42	−0.41	−0.40	−0.40
	−1.17	−1.15	−1.12	−1.09	−1.09
	−0.56	−0.57	−0.55	−0.53	−0.53
	−2.71	−2.72	−2.70	−2.67	−2.67
	0.68	0.70	0.68	0.71	0.71
	−2.86	−2.87	−2.84	−2.80	−2.80
	0.44	0.44	0.45	0.46	0.46
	−1.30	−1.27	−1.30	−1.34	−1.34
2nd derivatives	0.94	0.94	0.93	0.94	0.94
	2.46	2.48	2.44	2.50	2.50
	1.20	1.18	1.16	1.20	1.21
	5.62	5.55	5.54	5.58	5.58
	−1.41	−1.36	−1.34	−1.35	−1.35
	5.89	5.80	5.77	5.84	5.84
	−0.99	−0.99	−1.00	−0.98	−0.98
	2.68	2.70	2.73	2.67	2.67

Table 5
Errors (%) in displacements and displacements derivatives for modified designs

Modified design	$\alpha = 0.5$		$\alpha = 0.75$	
Number of basis vectors	2	3	2	3
Displacements	4.2	0.8	6.1	1.9
	−2.9	1.8	−2.1	3.8
	7.5	1.8	11.3	4.0
	2.3	0.4	3.6	0.9
	8.6	−0.2	10.8	−0.5
	3.1	0.6	4.8	1.4
	2.2	−0.9	1.8	−2.0
	−5.4	−1.3	−8.4	−3.1
1st derivatives	−0.8	−1.4	−1.2	−3.1
	−3.1	−2.9	−7.9	−5.9
	−4.1	−3.6	−5.9	−8.0
	−1.4	−0.8	−1.6	−1.8
	−0.5	0.6	3.8	1.1
	−2.1	−1.3	−2.4	−2.8
	1.9	1.4	4.3	2.7
	2.2	2.5	3.0	4.8
2nd derivatives	−1.1	0.1	0.6	0.6
	2.6	−0.1	1.9	0.9
	−3.5	0.4	0.3	2.2
	−1.5	0.2	−0.9	0.4
	−7.5	−0.1	−4.3	−0.3
	−2.0	0.2	−0.9	0.7
	−1.1	0.0	−0.5	−0.5
	2.1	−0.2	−0.4	−1.1

Table 6
Approximate displacements and displacements derivatives for $\alpha = 1.0$

Number of basis vectors	2	3	4	5	Exact
Displacements	0.28	0.29	0.29	0.30	0.30
	0.90	0.84	0.88	0.90	0.90
	0.41	0.45	0.47	0.49	0.49*
	2.10	2.17	2.19	2.21	2.21*
	−0.53	−0.61	−0.62	−0.60	−0.60
	2.24	2.34	2.37	2.40	2.40
	−0.30	−0.31	−0.31	−0.30	−0.30
	1.01	0.95	0.93	0.90	0.90
1st derivatives	0.25	0.25	0.25	0.24	0.24
	0.74	0.72	0.69	0.64	0.64
	*	*	*	*	*
	*	*	*	*	*
	0.43	0.46	0.44	0.47	0.47
	1.81	1.84	1.81	1.74	1.74
	0.26	0.27	0.27	0.29	0.29
	0.82	0.80	0.81	0.87	0.88

* Joint 2 is practically eliminated.

5. Concluding remarks

Calculation of the derivatives of the response vector with respect to the system parameters is often necessary in the solution of structural optimization problems. The response derivatives are used to predict the changes in the system response due to changes in the design variables, to select search directions during the optimization process and to generate approximations for the response of a modified system. In a typical structural optimization process it is necessary to evaluate the response for numerous modified designs. For some of these designs it is necessary also to evaluate the response derivatives.

In this paper a unified approach for accurate approximations of displacements and displacement derivatives with respect to design variables was presented. It has been shown that the CA method developed recently is most suitable for this purpose. Unlike common approximations of the structural response, the approach presented is not based on calculation of derivatives. Rather, approximations of modified displacements are used to evaluate the modified displacement derivatives.

Similar computational procedures are employed for evaluating displacements, first- and second-order derivatives of displacements. Numerical results show that accurate approximations of derivatives can be achieved with a small computational effort for designs obtained by very large changes in the initial structure. In the example presented, small errors have been obtained by considering only 2–3 basis vectors. In other problems, the accuracy can be improved as necessary by considering more basis vectors.

The approximations presented are based on results of a single exact analysis of an initial design. The computational procedure is easy to implement, suitable for different types of design variables and structures and can be used with a general finite element system.

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