自動微分法を用いた機械構造物の感度解析

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機械構造物の高精度化、高機能化に伴い、構造設計の最適化問題などが研究されてきている。機械構造物の設計改善や最適設計を実施する上で設計変数に対する種々の評価特性の感度解析は重要である。特に幾何学非線形や材料非線形のある構造物などでは（例えば、弾塑性問題）、高階の微分係数を利用した感度解析が有効である。従来からの高階の微分係数を利用した感度解析の研究は、２階の微分係数を求めてテーラー展開を利用して行われてきた。しかし、それらの研究は、定式化の段階であり、実際に機械構造物に適用して、高階の微分係数を利用した感度解析の有効性ついて論じていない。

本報では、自動微分法を利用した有限要素法の感度解析コードを機械構造物に適用して、高階の微分係数を用いた感度解析の有効性について述べる。

Sensitivity Analysis of Machine Structure Using an Automatic Differentiation

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To design optimal mechanical structures, design sensitivity analysis technique using higher order derivatives is important. However, usual techniques for computing the derivatives,for example numerical differential method , are very hard to apply to real scale structures. To overcome the problem, we study a new approach for the higher order sensitivity analysis of the finite element method using an automatic differentiation method.

This paper reports some experiments on the design sensitivity analysis of mechanical structures using higher order partial derivatives.

Keywords :　Sensitivity Analysis, Automatic Differentiation, Optimal Design, FEM

1 Introduction

The importance of the sensitivity analysis using the finite element method (FEM) has been recognized to get higher precision and higher functionalities of mechanical structures in the structural design optimization(Haftka et al 1986a; Brebbia et al 1989; Eschenauer et al 1990). For example, to evaluate dynamical characteristics of structures, we use the modal analysis techniques(Ozaki 1988). The optimal mechanical design has been studied by the sensitivity analysis using the method. The traditional sensitivity analysis methods are such methods as a direct differential method, adjoint variable method, and numerical differential method(Adelman et al 1986; Haftka et al 1989). Those techniques for the sensitivity analysis(Haftka et al 1989; Kleiber and Hisada 1993) require numerically computed partial derivatives of the objective functions(Vanderplaats 1984). Jacobian or Hessian matrices are used to compute optimal values by Newton- or quasi-Newton algorithms(Evtushenko 1985; Ratschek et al 1988). However, there are several problems for the computation: (1) truncation and rounding errors become large when numerically executing the sensitivity analyses, (2) much computation time is required to compute higher order derivatives to get optimal solutions, and (3) it is difficult to develop programs for computing higher order derivatives of a function with very many variables(e.g., Vanhonacker 1980; Belle 1982; Haug et al 1982; Jawed et al 1984; Haftka et al 1986b; Wanxie et al 1986; Dailey 1989).

To solve the problem, we study a new approach for higher order sensitivity analysis of FEM using an automatic differentiation method(Ozaki 1991; 1992; 1993,Ozaki and Kimura 1994). Our using tool: DAFOR for automatic differentiation method is a pre-processor for usual Fortran compilers(Berz 1989; 1990a). Users of the tool first input their Fortran function programs to compute the values of the functions with very many variables for the FEM structural analysis by an automatic differentiation technique. Next, the tool analyzes the input program and inserts statements to compute higher order partial derivatives of the function. Then, the tool automatically generates a special Fortran program with sensitivity analysis capability. The method of the code generation to compute partial derivatives concerning many variables is attained by the automatic differentiation technique developed by Iri (1984),Roll (1986),Berz (1989; 1990b),Iri and Kubota (1991), and Griewank et al (1991). The unique the feature of automatic differentiation method is that the technique can compute higher order partial derivatives with very high accuracy(Berz 1989). The generated program is free from both truncate and rounding errors(Iri and Kubota 1991; Griewank et al 1991). Therefore, the using the tool, the users can easily carry out sensitivity analysis for optimizing structural design problems.

This paper describes the principles of the automatic differentiation method and reports the computational results of the FEM codes generated by the method applied to a plane truss structure. Dixon et al (1988) theoretically discuss the importance of automatic differentiation techniques for finite element optimization, however, they do not show numerical results of the method. On the other hand, in this paper, we emphasize the theory as well as the experimental results. The results indicate that the technique and the use of sensitivity analysis by FEM generated using an automatic differentiation method are very effective in the sense that (1) unlike usual sensitivity analyses for FEM methods (e.g., Fox et al 1968; Wu and Arora 1986; Haftka et al 1989; Jao and Arora 1992; Kleiber 1993), the generated program can simultaneously compute the values of partial derivatives of a given function with very high accuracy, and that (2) the values of higher partial derivatives computed by the generated program and the one computed by usual re-analysis by the FEM coincide each other.

This paper organized as follows: In section 2, the basic principles of the automatic differentiation method is introduced. In section 3, we have carried out some experiments to apply the automatic differentiation technique to sensitivity analysis. In section 4 , we give some concluding remarks.

2 Basic Principles of Automatic Differentiation

In this section, we will provide the mathematical background of the theory of automatic differentiation method. Automatic Differentiation method are, in general, based on the direct application of the *chain rule* for computing partial derivatives of a composit function of given function with many variables. In the following, we will describe the outline of the mathematical theory based on Berz(1989; 1990a). We will also provide the mathematical background of the theory of automatic differentiation required for the promised study of non-linearities. It is an application of the relatively new field of *Nonstandard Analysis,* which allows the introduction of arbitrarily small quantities, *infinitesimals,* in a rigorous theory of analysis.

2.1 Principle of First Order Partial Derivatives Using an Automatic Differentiation

Consider the vector space R^2 of ordered pairs (a_0,a_1), $a_0,a_1 \in R$,in which an addition and a scalar multiplication are defined in the usual way:

$$(a_0,a_1)+(b_0,b_1)=(a_0+b_0,a_1+b_1) \tag{1}$$

$$t\cdot(a_0,a_1)=(t\cdot a_0,t\cdot a_1) \tag{2}$$

for a_0,a_1 , $b_0,b_1 \in R$. Besides the above addition and scalar multiplication a multiplication between vectors is introduced in the following way :

$$(a_0,a_1)\cdot(b_0,b_1)=(a_0\cdot b_0,a_0\cdot b_1+a_1\cdot b_0) \tag{3}$$

for a_0,a_1 , $b_0,b_1 \in R$. With this definition of a vector multiplication the set of ordered pairs becomes an algebra, denoted by ${}_1D_1$.

Note that the multiplication is the same one would obtain by multiplying $(a_0+a_1\cdot x)$ and $(b_0+b_1\cdot x)$ and keeping terms linear in x.

Similarly, as in the case of complex numbers, one can identify $(a_0,0)$ as the real numberes a_0 . Although as a complex number, (0,1) is a root of -1, here it has another interesting property :

$$(0,1)\cdot(0,1)=(0,0), \tag{4}$$

which follows directly from equation(3). So (0,1) is a root of 0. Such a property suggests thinking of $d=(0,1)$ as something infinitely small ; so small in fact that its square vanishes. Consequently, we call $d=(0,1)$ the differential unit. The first component of the pair (a_0,a_1) is called the real part, and the second component is called the differential part.

It is easy to verify that (1,0) is a neutral element of multiplication, because according to equation(3)

$$(1,0)\cdot(a_0,a_1)=(a_0,a_1)\cdot(1,0)=(a_0,a_1) \tag{5}$$

It turns out that (a_0,a_1) has a multiplicative inverse if and only if a_0 is nonzero ; so ${}_1D_1$ is not a fileld. In case $a_0 \neq 0$ the inverse is

$$(a_0,a_1)^{-1}=(\frac{1}{a_0},-\frac{a_1}{a_0^2}) \tag{6}$$

It is easy to check that in fact $(a_0,a_1)^{-1}\cdot(a_0,a_1)=(1,0)$. The space ${}_1D_1$ is a subspace of the field R^* introduced in *Nonstandard Analysis*. Besides the usual real number, R^* contains a variety of infinitely small and infinitely large quantities. The outstanding result of the theory of Nonstandard Analysis is that differentiation becomes an algebraic problem : a function f is differentiable if and only if for any arbitrary small quantity δ, the real part of the quotient,

$$\frac{f(x+\delta)-f(x)}{\delta}, \tag{7}$$

is independent of the choice of the specific δ. Thus, given any differentiable function f, we can compute its derivatives just by evaluating the formula for a special choice of δ. We choose δ = d = (0,1) and thus obtain

$$f'(x)=\Re\left[\frac{f(x+d)-f(x)}{d}\right] \text{ or}$$
$$f'(x)=\vartheta[f(x+d)-f(x)]=\vartheta[f(x+d)], \tag{8}$$

where $\Re$ denote the real part, and ϑ denotes the differential part. In the last step use has been made of the fact that $f(x)$ has no differential part. Hence differential algebras are useful to compute derivatives directly, without requiring an analytic formula for the derivatives and without the inaccuracies of numerical techniques.

2.2 Principle of Higher Order Partial Derivatives Using an Automatic Differentiation

We define $N(n,v)$ to be the number of monomials in v variables through order n.

We will show that $N(n,v) = \dfrac{(n+v)!}{n!v!} = C(n+v,v)$,

where $C(i,j)$ is the familiar bionomial coefficient. First note that the number of monomials with exact order n equals $N(n,v-1)$ because each monomial of exact order n can be written as a monomial with one variable less times the last variable to such a power that the total power equals n. Thus we have $N(n,v) = N(n-1,v) + N(n,v-1)$: the number of monomials in v variables through order n equals the number of relation is satisfied by $C(n+v,v)$. Since also, obviously, $C(1+1,1) = 2 = N(1,1)$, the formula follows by induction.

Now assume that all these N monomials are arranged in a certain manner order by order. For each monomial M, we call I_M the position of M according to the ordering. Conversely, with M_I we denote the I th monomial of the ordering. Finally, for an I with $M_I = x_1^{i_1} \cdots\cdots x_v^{i_v}$, we define $F_I = i_1! \cdots\cdots i_v!$.

We now define, in addition, a scalar multiplication and a vector multiplication on R^N in the following way :

$$(a_1,\ldots,a_N) + (b_1,\ldots,b_N) = (a_1 + b_1,\ldots,a_N + b_N) \tag{9}$$

$$t \cdot (a_1,\ldots,a_N) = (t \cdot a_1,\ldots,t \cdot a_N) \tag{10}$$

$$(a_1,\ldots,a_N) \cdot (b_1,\ldots,b_N) = (c_1,\ldots,c_N) \tag{11}$$

where the coefficients c_i are defined as follows :

$$c_i = F_i \sum_{\substack{0 \le v,\mu \le N \\ M_v \cdot M_\mu = M_i}} \frac{a_v \cdot b_\mu}{F_v \cdot F_\mu}. \tag{12}$$

To help clarify these definitions, let us look at the case of two variables and second oeder. In this case, we have n = 2 and v =2. There N = C(2+2,2) = 6 monomials in two variables, namely,

$$1, x, y, xx, xy, yy. \tag{13}$$

As an example, using the ordering in equation (13), we have $I_{xy} = 5$ and $M_3 = y$. Using the ordering in equation (13), we obtain for c_1 through c_6 in equation (12) :

$$
\begin{aligned}
c_1 &= a_1 \cdot b_1 \\
c_2 &= a_1 \cdot b_2 + a_2 \cdot b_1 \\
c_3 &= a_1 \cdot b_3 + a_3 \cdot b_1 \\
c_4 &= 2 \cdot (a_1 \cdot b_4/2 + a_2 \cdot b_2 + a_4 \cdot b_1/2) \\
c_5 &= a_1 \cdot b_5 + a_2 \cdot b_3 + a_3 \cdot b_2 + a_5 \cdot b_1 \\
c_6 &= 2 \cdot (a_1 \cdot b_6/2 + a_3 \cdot b_3 + a_6 \cdot b_1/2).
\end{aligned} \tag{14}
$$

On ${}_nD_v$ we introduce a third operation ∂_i :

$$\partial_i(a_1,\dots,a_N) = (c_1,\dots,c_N) \tag{15}$$

with

$$c_i = \begin{cases} 0 & \text{if } M_i \text{ has order n} \\ a_{I(M_i \cdot x_v)} & \text{otherwise} \end{cases} \tag{16}$$

So ∂_v moves the derivatives arround in the vector. Suppose a vector contains the derivatives of the function f ; then applying ∂_v to in one obtains the derivatives of $\frac{\partial f}{\partial x_v}$ through one order less.

Although in ${}_1D_1$, $d = (0,1)$ was an infinitely small quantity, here we have a whole variety of infinitely small quantities with the property t hat high-enough powers of them vanish. We give special names to the ones in components I belonging to first - order mnomials, denoting them by dM_I. In the example of ${}_2D_2$, we have $dx = (0,1,0,0,0,0)$, and $dy = (0,0,1,0,0,0)$. It then follows from the theory of Nonstandard Analysis that instead of equation (8) we obtain

$$f(x+dx, y+dy) = (f, \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial^2 f}{\partial x^2}, \frac{\partial^2 f}{\partial x \partial y}, \frac{\partial^2 f}{\partial y^2})(x,y). \tag{17}$$

In the general case of v variables and order n, after evaluating f in the differential algebra one obtains

$$\frac{\partial^{i_1+i_2+\dots+i_v} f}{\partial x_1^{i_1} \partial x_2^{i_2} \cdots \partial x_v^{i_v}} = c_{I(x_1^{i_1} \cdots x_v^{i_v})} \tag{18}$$

where $I(x_1^{i_1} \cdots\cdots x_v^{i_v})$ is the index of the monomial $(x_1^{i_1} \cdots\cdots x_v^{i_v})$, as defined in the beginning of this section.

3 Sensitivity Analysis on Mechanical Structures using an Automatic Differentiation Technique

We have applied the automatic differentiation method to sensitivity analysis problems with the FEM, which is the most popular in structural analyses. In the case studies described below, automatic differentiation method is used to investigate the sensitivity of design variables of mechanical structures. The automatic differentitation method can be applied to both linear and non-linear equations(Berz 1989 ; Ozaki 1991), if the equations are n-th order differentiable. Moreover, using the method, we can highly accurately compute higher order partial derivatives with many variables.

In the case studies, we have applied the method to two-dimensional linear FEM problems of structural analyses(Ozaki 1989).

3.1 Example : First - and Higher -Order Sensitivity Analysis

The code of sensitivity analysis of FEM using the automatic differentiation has been applied to a plane truss structure. The model is a simple static model shown in Figure 1, by which we simulate a train passing over an iron bridge. It consists of eight nodes and thirteen truss elements. The boundary conditions are that the node 7 and 8 are fixed, and that the nodes 1, 2, and 3 respectively have the loads 10,000kgf, 20,000kgf, and 10,000kgf.

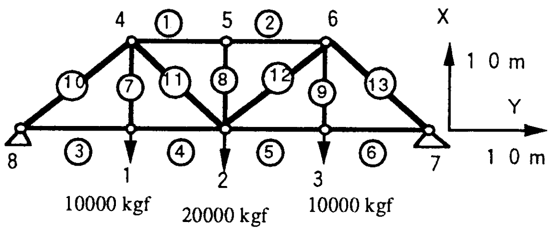

Fig.1. Analytical model for higher order sensitivity analysis

The experiment of the sensitivity analysis are to compute the values of first and higher order partial derivatives and to predict the stress of each element against radius of each element. The object to compute the values of higher order partial derivatives is to indicate effectiveness of Taylor series expansion using coefficient of differential of higher order when the machine structures are large changing design in order to optimize. In particular, the method is very effective when the connection of nonlinearity is existed between object function and design variables. The relation of the stress of each element against radius of each element is non-linear.

The experiment is the sensitivity analysis of the important stress for the fracture mechanics. The sensitivity analysis as to the stress of each element against the radius of each element is executed. The sensitivity as to the stress of each element against radius of the element 1 through 13 is computered. The highest sensitivity of element against radius of each element is the case of radius of element 2. The values of first and higher order partial derivatives as to the stress of element 2 against radius of the element 2 computered as is shown in Table 1.

Table1. Compressive stress sensitivity of element 2 against radius of element 2

	Stress sensitivity of element 2 against radius of element 2 (kgf / mm³)
Value of first order derivatives	1.9099 *10⁻²
Value of second order derivatives	-5.7296 *10⁻³
Value of third order derivatives	2.2918 *10⁻³

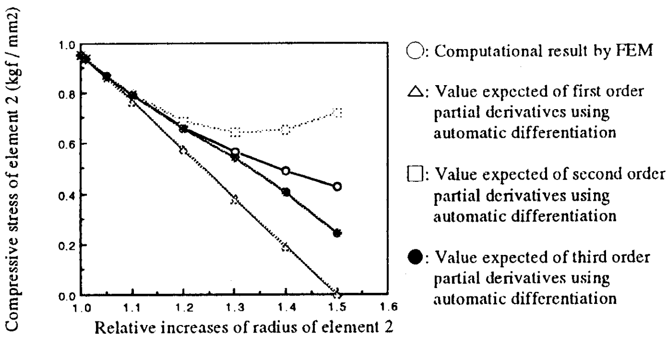

Fig.2. Value expected from high order partial derivatives using automatic differentiation and computational value by FEM

The objective of this analysis is in order to examine the effectiveness of higher order differential coefficient against non-linearity. When we have changed the values of radius of the element 2 to 1 %, 5 %, 10 %, 20 %, 30 %, 40 % , and 50 % inceases, we have gotten the results shown in Figure 2 by computing the compressive stress of element 2 by the higher order partial derivatives obtained using an automatic differentiation. The result of direct re-computation by FEM above the condition is shown in Figure 2. The results of the compressive stress of element 2 predicted by the first order sensitivity analysis using an automatic differentiation and the ones by the direct re-computation by FEM do not concide with each other when the changes of design variables are large, on the other hand the results of the compressive stress of element 2 predicted by the higher order sensitivity analysis and the ones by the direct re-computation by FEM concide with each other even if the changes are so large.

4 Concluding Remarks

Using an automatic differentiation technique, we have observed the following advantages in the analyses.

(1) We can very easily and quickly execute sensitivity analysis of structural design problems.

(2) We can also predict the effects of changing design parameters with high accuracy.

The most remarkable feature of the automatic differentiation method is that the method can simultaneously compute the values of higher order partial derivatives. This results in the following effects in the sensitivity analyses.

(3) Our method becomes superior to the conventional ones using numerical differentiacion , because our method do not raise with rounding error and trancating error in numerical computaitional process of sensitivity analysis.

(4) Our method is very effective when changing quantity of the design parameters become larger the non-linerity.

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