

Geometric nonlinear sensitivity analysis for nonparametric shape optimization with non-zero prescribed displacements

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1. Abstract

The large number of design variables in nonparametric shape optimization brings a challenging demand for efficient and accurate sensitivity evaluation methods. It is even more critical when nonlinearities are taken into account. The ultimate future goal is to use these methods in large scale industrial shape optimization problems that present nonlinear properties.

This paper investigates geometric nonlinear sensitivity analysis with non-zero prescribed displacements, which is a common setup for many industrial structural nonlinear problems. Firstly, the analytical sensitivity formula is derived in discrete form, with which no further discretization steps are needed for implementation. Since the number of design variables is much larger than the number of responses, the adjoint approach is utilized.

Secondly, a straightforward semi-analytical procedure is presented to calculate the sensitivities with finite element codes. In general commercial FEA codes, the stiffness matrix information may not be accessible, reaction force results is thus utilized to replace the direct evaluation and retrieve of stiffness matrix. The reaction forces could be obtained efficiently through nonlinear analysis on element level models under prescribed displacements of the equilibrium point.

Lastly, the procedure is demonstrated with a benchmark cantilever beam example. And the accuracy problem of the results is presented. The results show that the truncation error due to the rigid rotation of elements also appears in nonlinear sensitivity analysis. The techniques to correct the error are briefly discussed.

2. Keywords: geometric nonlinear sensitivity analysis, prescribed displacement, nonparametric shape optimization, adjoint method

3. Introduction

Nonparametric shape optimization takes nodal coordinates as design variables, which provides the largest possible design space. However, the large number of design variables requires a method for highly efficient sensitivity evaluation.

Linear static sensitivity analysis in structural optimization has been well studied and summarized since decades of years ago [1-3]. The most common ways to obtain sensitivities are global finite difference method, continuum or variational method and discrete (semi-)analytical method. The implementation of global finite difference scheme is straightforward. However, it suffers from errors when perturbation size is too large or too small, and also from large computational costs for repeated time-consuming structural analysis. The continuum derivative method first differentiates on the variational equation of the system and thereafter discretizes the formula. It is of high accuracy but requires more mathematical understanding of continuum equations. The discrete method differentiates directly on discretized governing equations of finite element systems, where semi-analytical approximation is widely used to replace the analytical derivative of system quantities.

The serious accuracy problem along with the semi-analytical approach has been observed [4, 5]. It is recognized to be associated with the rigid body rotation of elements [4, 6]. During the past twenty years, “exact” and “refined” semi-analytical methods have been developed [7-10], which successfully eliminates this type of error.

Sensitivity analysis for different types of nonlinearities has also been widely investigated. Variational forms of sensitivity considering geometric nonlinearity, critical load factor, hyperelastic material, elastoplastic problems, contact problem and dynamic problems have been systematically presented [11]. Specially, variational form of geometric nonlinearity under prescribed displacements is presented [12]. Discrete form of geometric nonlinear sensitivity analysis under mechanical force loads has been derived [13], and an implementation with a general finite element code MARC is realized [14]. Examples of discrete method for limit load, material nonlinearity and the combination of geometric and material nonlinearity are also presented [15-19].

In this paper, the geometric nonlinear sensitivity analysis for shape optimization is investigated, where the structure is loaded with non-zero prescribed displacements. The discrete semi-analytical adjoint method is employed. In section 4, the analytical sensitivity formula with adjoint approach and a straightforward semi-analytical analysis procedure are presented. In section 5, the procedure is demonstrated with a benchmark

example. The accuracy problem is presented and corresponding correction methods are also discussed.

4. Geometric nonlinear sensitivity analysis with non-zero prescribed displacements

4.1. Secant and tangent stiffness matrix in nonlinear analysis

Generally, the governing equation of a finite element system is:

$$\mathbf{K} \cdot \mathbf{U} = \mathbf{F} \quad (1)$$

, where \mathbf{U} is the nodal displacement vector, \mathbf{K} is the stiffness matrix, and \mathbf{F} is the external force vector. When nonlinearity presents, the stiffness matrix \mathbf{K} is of nonlinear relationships with \mathbf{U} , and Eq.(1) becomes:

$$\mathbf{K}_S(\mathbf{U}) \cdot \mathbf{U} = \mathbf{F} \quad (2)$$

, where \mathbf{K}_S is the so-called secant stiffness matrix, which depends on both \mathbf{U} and the structure's initial configuration. Another important quantity is the tangent stiffness matrix \mathbf{K}_T , which is also nonlinearly dependent on \mathbf{U} and structure's configuration. In a nonlinear analysis, the secant stiffness matrix serves to calculate the residual force vector, while the tangent stiffness matrix is mainly utilized to calculate the incremental quantities. A descriptive figure of \mathbf{K}_S and \mathbf{K}_T is depicted in Fig.(1).

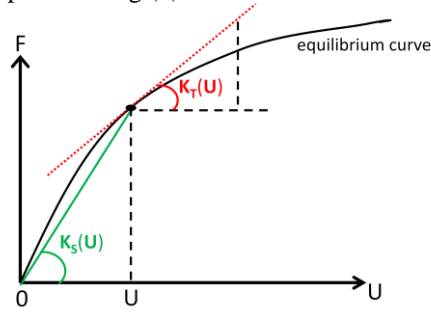


Figure 1: Secant and tangent stiffness matrix at the equilibrium point \mathbf{U}

Detailed discussions about the secant stiffness matrix are found in [20-26]. It is especially worth mentioning that, explicit analytical expressions of both secant and tangent stiffness matrices for linear triangular and tetrahedral elements are presented [25-27]. It provides the possibilities of analytical evaluation of stiffness matrices and their derivatives, and is thus a powerful tool for in-depth investigation on nonlinear sensitivity analysis.

4.2. Geometric nonlinear analysis with non-zero prescribed displacement loads

Geometric nonlinear problem with non-zero prescribed displacements analyze the large deformation behavior of a structure under both external mechanical force loads and non-zero prescribed displacement loads. The governing equation is:

$$\mathbf{K}_S(\mathbf{U}) \cdot \begin{bmatrix} \mathbf{U}^f \\ \mathbf{U}^p \end{bmatrix} = \begin{bmatrix} \mathbf{F}^f \\ \mathbf{F}^p \end{bmatrix} \quad (3)$$

, where \mathbf{U}^p is part of \mathbf{U} that corresponds to the given prescribed displacements, \mathbf{F}^f is the given external forces, \mathbf{U}^f is the unknown displacements, and \mathbf{F}^p is the unknown reaction force vector corresponds to \mathbf{U}^p . The nonlinear residual force vector \mathbf{R} is defined as:

$$\begin{bmatrix} \mathbf{R}^f \\ \mathbf{R}^p \end{bmatrix} = \mathbf{K}_S(\mathbf{U}) \cdot \begin{bmatrix} \mathbf{U}^f \\ \mathbf{U}^p \end{bmatrix} - \begin{bmatrix} \mathbf{F}^f \\ \mathbf{F}^p \end{bmatrix} \quad (4)$$

Newton-Raphson method is often employed to solve this nonlinear problem iteratively [28]. In the initial step, the unknown displacement $\mathbf{U}^{f,0}$ and reaction force $\mathbf{F}^{p,0}$ are obtained by solving the linear system of equations:

$$\mathbf{K}_T(\mathbf{0}, \mathbf{U}^p) \cdot \begin{bmatrix} \mathbf{U}^{f,0} \\ \mathbf{U}^p \end{bmatrix} = \begin{bmatrix} \mathbf{F}^f \\ \mathbf{F}^{p,0} \end{bmatrix} \quad (5)$$

Then the residual force vector is calculated by Eq.(4), and the incremental reaction forces and displacements of the iteration are obtained by solving the following linear problem:

$$\mathbf{K}_T(\mathbf{U}^{f,i}, \mathbf{U}^p) \cdot \begin{bmatrix} \Delta \mathbf{U}^{f,i+1} \\ \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{R}^{f,i} \\ \Delta \mathbf{F}^{p,i+1} \end{bmatrix} \quad (6)$$

Both displacements and reaction forces are then updated before the start of the next iteration:

$$\mathbf{U}^{f,i+1} = \mathbf{U}^{f,i} + \Delta \mathbf{U}^{f,i+1} \quad (7)$$

$$\mathbf{F}^{p,i+1} = \mathbf{F}^{p,i} + \Delta \mathbf{F}^{p,i+1} \quad (8)$$

The procedure terminates until the residual force vector is small enough.

4.3. Discrete analytical sensitivity analysis with adjoint approach

In this research, the sensitivity is derived with discrete method, which will provide the straightforward implementation with general finite element codes. Since the number of design variables is usually much larger than that of system responses in nonparametric shape optimization, the adjoint method is preferable for efficiency. For a system response g , it is a function of the design variable s , displacement vector \mathbf{U} and force vector \mathbf{F} . Therefore the sensitivity of $g(\mathbf{U}(s), \mathbf{F}(s), s)$ with respect to s is:

$$\frac{Dg}{Ds} = \frac{\partial g}{\partial s} + (\nabla_{\mathbf{U}}g)^T \cdot \frac{D\mathbf{U}}{Ds} + (\nabla_{\mathbf{F}}g)^T \cdot \frac{D\mathbf{F}}{Ds} \quad (9)$$

Rewrite the governing equation as:

$$\mathbf{R}(\mathbf{U}(s), \mathbf{F}(s), s) = \mathbf{K}_S(\mathbf{U}(s), s) \cdot \mathbf{U}(s) - \mathbf{F}(s) \equiv 0 \quad (10)$$

Total derivative of \mathbf{R} with respect to s is:

$$0 = \frac{D\mathbf{R}}{Ds} = \frac{\partial \mathbf{R}}{\partial s} + (\nabla_{\mathbf{U}}\mathbf{R})^T \cdot \frac{D\mathbf{U}}{Ds} + (\nabla_{\mathbf{F}}\mathbf{R})^T \cdot \frac{D\mathbf{F}}{Ds} = \frac{\partial \mathbf{K}_S}{\partial s} \cdot \mathbf{U} + \mathbf{K}_T \cdot \frac{D\mathbf{U}}{Ds} - \frac{D\mathbf{F}}{Ds} \quad (11)$$

Introducing the adjoint variable $\boldsymbol{\lambda} = [\boldsymbol{\lambda}^f \quad \boldsymbol{\lambda}^p]^T$ by multiplying to Eq.(11) and subtracting from Eq.(9),

$$\begin{aligned} \frac{Dg}{Ds} &= \frac{\partial g}{\partial s} + (\nabla_{\mathbf{U}}g)^T \cdot \frac{D\mathbf{U}}{Ds} + (\nabla_{\mathbf{F}}g)^T \cdot \frac{D\mathbf{F}}{Ds} - \boldsymbol{\lambda}^T \cdot \left(\frac{\partial \mathbf{K}_S}{\partial s} \cdot \mathbf{U} + \mathbf{K}_T \cdot \frac{D\mathbf{U}}{Ds} - \frac{D\mathbf{F}}{Ds} \right) \\ &= \frac{\partial g}{\partial s} - \boldsymbol{\lambda}^T \cdot \frac{\partial \mathbf{K}_S}{\partial s} \cdot \mathbf{U} + (\mathbf{K}_T \cdot \boldsymbol{\lambda} - \nabla_{\mathbf{U}}g)^T \cdot \frac{D\mathbf{U}}{Ds} + (\nabla_{\mathbf{F}}g + \boldsymbol{\lambda})^T \cdot \frac{D\mathbf{F}}{Ds} \end{aligned} \quad (12)$$

It is always assume that the external forces and prescribed displacements are independent of design variables. Therefore,

$$\frac{D\mathbf{U}}{Ds} = \begin{bmatrix} D\mathbf{U}^f/Ds \\ \mathbf{0} \end{bmatrix} \quad (13)$$

$$\frac{D\mathbf{F}}{Ds} = \begin{bmatrix} \mathbf{0} \\ D\mathbf{F}^p/Ds \end{bmatrix} \quad (14)$$

Therefore the third term in Eq.(12) is:

$$(\mathbf{K}_T \cdot \boldsymbol{\lambda} - \nabla_{\mathbf{U}}g)^T \cdot \frac{D\mathbf{U}}{Ds} = \left(\begin{bmatrix} \mathbf{K}_T^{ff} & \mathbf{K}_T^{fp} \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{\lambda}^f \\ \boldsymbol{\lambda}^p \end{bmatrix} - \nabla_{\mathbf{U}}g \right)^T \cdot \frac{D\mathbf{U}^f}{Ds} \quad (15)$$

Also, the fourth term in Eq.(12) is:

$$(\nabla_{\mathbf{F}}g + \boldsymbol{\lambda})^T \cdot \frac{D\mathbf{F}}{Ds} = (\nabla_{\mathbf{F}^p}g + \boldsymbol{\lambda})^T \cdot \frac{D\mathbf{F}^p}{Ds} \quad (16)$$

Force both terms in the parenthesis of Eq.(15) and Eq.(16) to zero. It leads to:

$$\boldsymbol{\lambda}^p = -\nabla_{\mathbf{F}^p}g \quad (17)$$

And $\boldsymbol{\lambda}^f$ is obtained by solving the linear problem:

$$\mathbf{K}_T \cdot \begin{bmatrix} \boldsymbol{\lambda}^f \\ -\nabla_{\mathbf{F}^p}g \end{bmatrix} = \begin{bmatrix} \mathbf{K}_T^{ff} & \mathbf{K}_T^{fp} \\ \mathbf{K}_T^{pf} & \mathbf{K}_T^{pp} \end{bmatrix} \cdot \begin{bmatrix} \boldsymbol{\lambda}^f \\ -\nabla_{\mathbf{F}^p}g \end{bmatrix} = \begin{bmatrix} \nabla_{\mathbf{U}^f}g \\ \mathbf{Y} \end{bmatrix} \quad (18)$$

, where \mathbf{Y} is the force vector corresponds to prescribed displacement $-\nabla_{\mathbf{F}^p}g$.

And finally, the sensitivity of response g is expressed as:

$$\frac{Dg}{Ds} = \frac{\partial g}{\partial s} - \begin{bmatrix} \boldsymbol{\lambda}^f \\ -\nabla_{\mathbf{F}^p}g \end{bmatrix} \cdot \frac{\partial \mathbf{K}_S}{\partial s} \cdot \mathbf{U} \quad (19)$$

4.4. Semi-analytical sensitivity analysis procedure

The semi-analytical method is used to approximate the partial derivatives of the secant stiffness matrix:

$$\frac{\partial \mathbf{K}_S(\mathbf{U}, s)}{\partial s} \approx \frac{\mathbf{K}_S(\mathbf{U}, s+\Delta s) - \mathbf{K}_S(\mathbf{U}, s)}{\Delta s} \quad (20)$$

When secant stiffness matrix is not available, which is the case so far in common commercial finite element codes, the approximation could be replaced by finite differencing on reaction force results. According to Eq.(2), the multiplication of secant stiffness matrix and corresponding displacement vector equals to the reaction force vector, therefore the semi-analytical approximation could be modified as:

$$\frac{\partial \mathbf{K}_S(\mathbf{U},s)}{\partial s} \cdot \mathbf{U} \approx \frac{\mathbf{K}_S(\mathbf{U},s+\Delta s) \cdot \mathbf{U} - \mathbf{K}_S(\mathbf{U},s) \cdot \mathbf{U}}{\Delta s} = \frac{\mathbf{F}(\mathbf{U},s+\Delta s) - \mathbf{F}(\mathbf{U},s)}{\Delta s} \quad (21)$$

This approximation avoids the direct evaluation of the secant stiffness matrix, and the reaction force results could be obtained directly by nonlinear finite element analysis. Due to the design variables in nonparametric shape optimization are usually the coordinates of design variables, the semi-analytical approximation and thus the nonlinear analysis only needs to be carried out on element level, which ensures the computational efficiency. The following procedure for the sensitivity analysis is developed, which is a straightforward realization of Eq.(18), Eq.(19) and Eq.(21).

Step 1: Full model geometric nonlinear analysis to find the equilibrium point \mathbf{U}^* .

Step 2: Linear perturbation analysis at \mathbf{U}^* with external force loads $\nabla_{\mathbf{U}} f \mathbf{g}$ and prescribed displacements $-\nabla_{\mathbf{F}} p \mathbf{g}$ as boundary conditions. Denote the displacement result of the analysis by λ .

And then the following steps are carried out for each design variable separately:

Step 3: Extract neighbor elements around the design node, and denote their nodal force results in Step 1 by $\mathbf{F}(\mathbf{U}^*,s)$.

Step 4: Run a nonlinear analysis on the extracted small model with perturbed design node and with \mathbf{U}^* as its boundary conditions. The nodal force results of this analysis is $\mathbf{F}(\mathbf{U}^*,s+\Delta s)$.

Step 5: Evaluate explicit expression of $\partial \mathbf{g} / \partial s$.

Step 6: Calculate the sensitivity of response \mathbf{g} with respect to design variable according to Eq.(19).

For a system with M responses and N design variables, the total computational effort of the procedure is 1 time full nonlinear analysis of the structure, M times linear perturbation analysis at the equilibrium point plus N times nonlinear analysis on element level models around each design node.

Obviously, this procedure is consistent with sensitivities analysis for geometric nonlinear structure under only mechanical force loads, where the term $-\nabla_{\mathbf{F}} p \mathbf{g}$ in Step 2 vanishes. And it degenerates to linear sensitivity analysis by replacing the nonlinear analysis in Step 1 and Step 4 with linear analysis.

5. Example and numerical results

The procedure is implemented in an in-house finite element code. In this solver, the analytical secant and tangent stiffness matrices for four-node linear tetrahedral element in [26, 27] is adopted. The numerical result of a benchmark cantilever beam example is presented. And the accuracy problem is discussed thereafter.

5.1. Introduction to the cantilever beam example

As shown in Fig.(2a), a 3D cantilever beam is taken as an example. The beam is of size 300mm×15mm×15mm and are loaded with two prescribed displacements on the end that is not fixed, $u_{1y} = u_{2y} = -100\text{mm}$. It is meshed with 3D four-node linear tetrahedral solid element with a total number of 286. Linear isotropic material is assumed with Young's modulus 209GPa, Poisson's ratio 0.3. The sum of the downward reaction forces at the two points is chosen to be the system response, i.e. $\mathbf{g} = \mathbf{F}_{1y} + \mathbf{F}_{2y}$. The design variables are y -coordinates of middle nodes of the bottom surface (red points shown in Fig.(2b)).

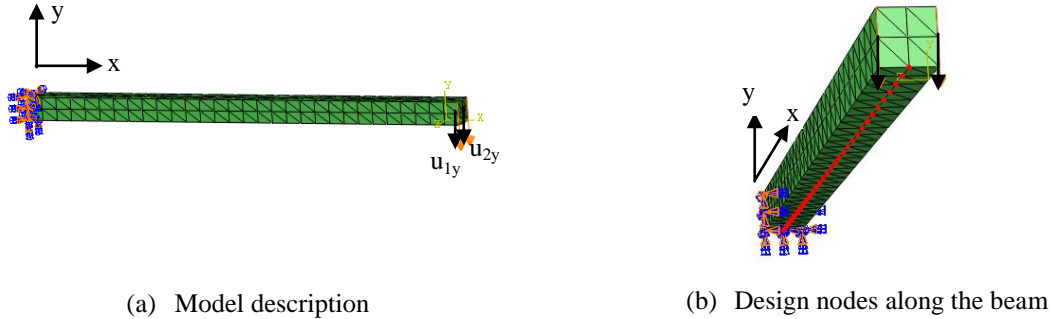


Figure 2: Cantilever beam model

5.2. Sensitivity results

With the definition of the system response,

$$\nabla_{\mathbf{U}} f \mathbf{g} = \mathbf{0} \quad (22)$$

$$\nabla_{\mathbf{F}^D} \mathbf{g} = \begin{bmatrix} \frac{\partial \mathbf{g}}{\partial F_{1y}} \\ \frac{\partial \mathbf{g}}{\partial F_{2y}} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad (23)$$

$$\frac{\partial \mathbf{g}}{\partial s} = 0 \quad (24)$$

The sensitivity results are depicted in Fig.(3), where the results of the semi-analytical approach is compared with the result of global finite difference method which is taken as the reference result here. The perturbation size in the semi-analytical method is 10^{-5} mm and in global finite difference is 5×10^{-4} mm, both of which are properly for their own method. The figure shows that the semi-analytical results match well with the reference results.

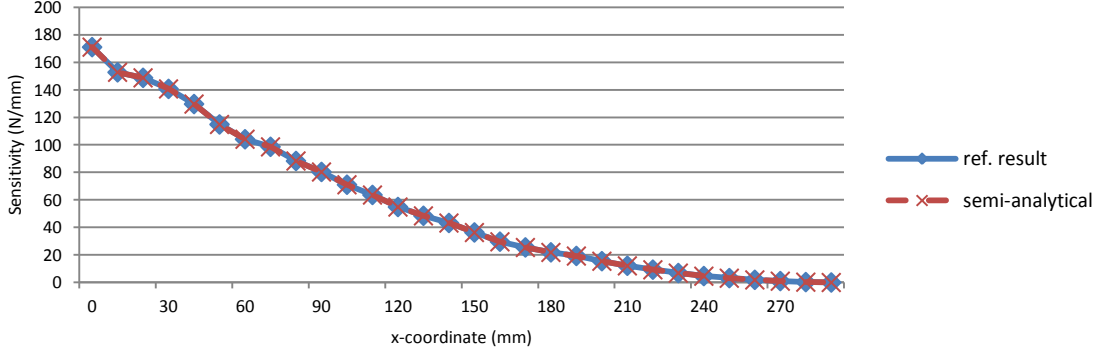


Figure 3: Sensitivity results

However, the scaled sensitivities in Fig.(4) shows that, the relative error increases as the position of design nodes getting close to the loading end (as x-coordinate increasing). This phenomenon is consistent with that in linear case [10], which is caused by the rigid “rotation” of elements.

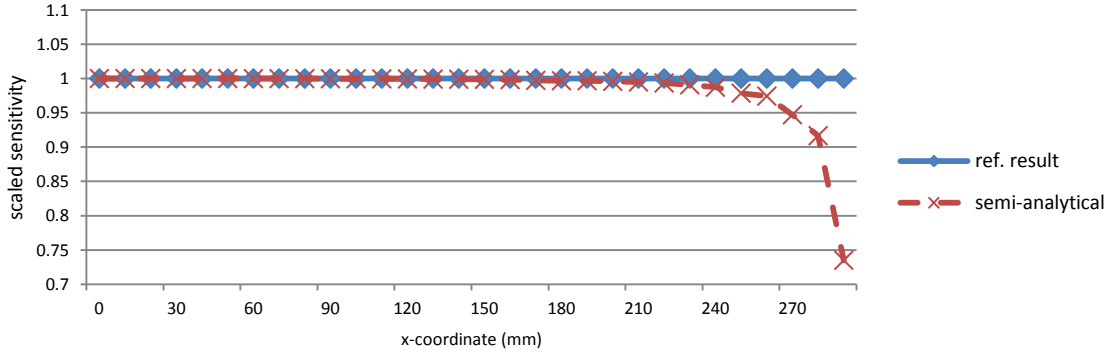


Figure 4: Scaled sensitivity results

5.3. Influence of perturbation size and higher-order finite difference scheme

It should be noted that, the accuracy of sensitivity results relies highly on the selection of perturbation size, and a higher-order finite difference scheme helps to reduce the error. A central finite difference scheme is implemented to take the place of forward scheme in Eq.(21):

$$\frac{\partial \mathbf{K}_S(\mathbf{U}^*, s)}{\partial s} \cdot \mathbf{U}^* \approx \frac{\mathbf{F}(\mathbf{U}^*, s + \Delta s) - \mathbf{F}(\mathbf{U}^*, s - \Delta s)}{2 \cdot \Delta s} \quad (25)$$

The sensitivity result of the forward and central scheme with different perturbation size are compared in Fig.(4). Clearly, the central scheme well improves the stability of the sensitivity results.

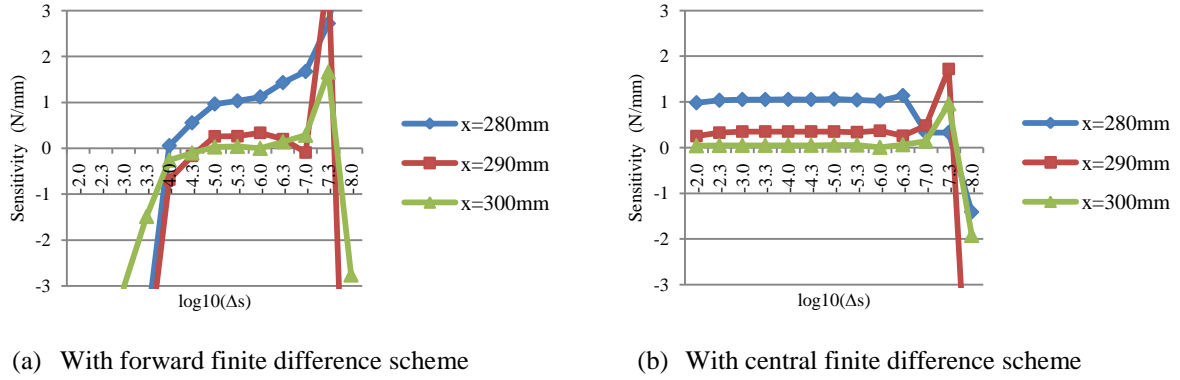


Figure 5: Sensitivity results with different perturbation size

The value of sensitivity at a design node near the loading end is listed in Table.(1). The relative errors are calculated with respect to the reference result.

Table 1: Sensitivity results at a point near loading end ($x=290\text{mm}$, ref. value= 0.354N/mm)

Perturbation size (mm)	forward semi-analytical		central semi-analytical	
	Sensitivity(N/mm)	Error	Sensitivity (N/mm)	Error
10^{-2}	-103	-29200%	0.252	-29%
10^{-3}	-9.98	-2917%	0.351	-0.8%
10^{-4}	-0.681	-292%	0.352	-0.6%
10^{-5}	0.260	-27%	0.352	-0.6%
10^{-6}	0.338	-4.6%	0.37	4.0%
10^{-7}	-0.0929	-126%	0.482	36%
10^{-8}	-10.90	-3179%	-7.24	-2145%

It could be seen that by using the central finite difference scheme, the accuracy of the results is significantly improved. The results well match the reference in a much larger range of perturbation size. But it also shows that this type of error can't be fully corrected solely with higher order finite difference schemes.

5.4. Discussion on correction of the error

In linear sensitivity analysis, this type of error could be corrected by “exact” semi-analytical approach or “refined” semi-analytical approach. The idea is to add a correction term, which is constructed with rigid body motion vectors of elements, to partial derivatives of their stiffness matrix or pseudo load vector so that the approximation still satisfies so-called rigid body conditions.

Both of these methods could also be extended to the nonlinear case. The key point lies in finding the rigid body movement vectors correspond to the secant stiffness matrix at equilibrium point instead of initial tangent stiffness matrix. Given the analytical expression of secant stiffness matrix in [26], investigation on the rigid body motion vectors and the extension of exact and refined semi-analytical methods is possible. This topic is postponed for a future study.

6. Conclusions

In this paper, the formula for discrete analytical sensitivity analysis of geometric nonlinear problem with prescribed displacements is derived. A corresponding semi-analytical approach is presented for the calculation. The procedure is implemented in an in-house finite element code and demonstrated with a cantilever beam example. With higher-order finite difference scheme, the accuracy could be greatly improved. And the existence of the error caused by rigid rotation of elements going along with the semi-analytical approach is also discussed.

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