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Performance of cubic convergent methods for implementing nonlinear constitutive models

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ABSTRACT

Suitability of nonlinear root-solvers whose convergence rates are better than the quadratic Newton–Raphson method and that do not require higher derivatives is examined for solving nonlinear equations encountered in the implementation of constitutive models. First, the performance of six cubic convergent methods is demonstrated by means of examples. These cubic methods are used in place of the Newton–Raphson method to solve the nonlinear equations in the J_2 plasticity and Gurson plasticity constitutive models. Few cubic methods are found to be computationally efficient and relatively insensitive to the initial guess when compared to the Newton–Raphson method for the considered models.

1. Introduction

A number of physical processes in nature are modeled as nonlinear systems and are mathematically represented by a system of nonlinear algebraic equations. The solutions of these nonlinear equations – which is equivalent to finding roots or zeros of the equations – then are of interest as they embody the behavior of the system under consideration. This process of determining roots of a set of nonlinear equations is a very commonly encountered problem in engineering applications. Till date, there are no analytical solutions for finding the roots of a general set of nonlinear equations. Numerical procedures based on iterative schemes are the methods of choice for solving such systems [1,2]. Among these iterative schemes, the Newton–Raphson method is perhaps one of the most popular method used to solve a set of nonlinear equations. The Newton–Raphson method exhibits an asymptotic rate of quadratic convergence in a neighborhood of the roots, and can be used for both scalar and multivariate cases. Moreover, the performance of Newton–Raphson method is sensitive to the initial guess, and its performance can be improved by using line search techniques [3,4]. Advantages and disadvantages of the Newton–Raphson method together with its variants can be found in Ref. [5].

The computational cost for evaluating roots of a system of nonlinear equations using iterative methods can be reduced by either improving the order of convergence or by reducing the amount of time required per iteration. Although both these techniques have been explored in the past [6–15], the former idea is the point of discussion in this study. For increasing the order of convergence, a number of iterative methods have been proposed in literature for scalar cases with order of convergence greater than two. Usually these higher order methods require higher order derivatives of the functions and multiple function evaluations at each iteration. These methods are usually classified as multipoint methods; see Ref. [5] for a comprehensive overview of multipoint methods. In fact this topic was extensively investigated before 1970s by several researchers [14–17]. However, this topic regained a lot of attention in the recent past due to advances in computational mathematics. In the past decade, many higher order multipoint methods were developed to solve a system of nonlinear equations, see for example [11,13,17]. Although the order of convergence of multipoint methods are extensively reported [17], the computational efficiency of these methods in practical engineering applications is rarely investigated.

In applications that are of interest in this study, the derivatives of order greater than one are usually very expensive to evaluate. Specially, in multivariate cases the first order derivative represents the Jacobian that can be evaluated, whereas the second order derivative will be a multilinear higher order tensor that is expensive to evaluate. Thus, the focus of this study is the multipoint iterative methods with asymptotic rate of cubic convergence that requires only first order derivative information. These multipoint methods with cubic convergence require additional evaluation of function and first order derivatives when compared to the Newton–Raphson method. In general, these additional computations will increase the computational cost per iteration. However,

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due to the higher order of convergence the number of iterations required to converge to accurate roots are reduced when compared to the Newton–Raphson method. For this reason, the methods with cubic convergence can be computationally efficient when compared to the Newton–Raphson method. Such methods can then replace the Newton–Raphson method in numerous engineering applications where roots of nonlinear algebraic system of equations are required. In addition, as the Newton–Raphson and the higher order methods are sensitive to the initial guess, it will be elucidating to compare the sensitivity of these methods to the initial guess. In practice, a method that is relatively insensitive to the initial guess will be considered as robust. Finally, as most of the cubic methods are proposed to solve a single nonlinear equation, for practical purposes, these methods should be extended to multivariate cases and their corresponding convergence rates should be investigated to establish if the cubic rates are preserved.

Nonlinear equations are frequently encountered in the constitutive modeling of materials. The class of constitutive models that employs rate equations to describe the materials behavior is of interest in this study. The integration of these rate equations ultimately result in a set of nonlinear equations that have to be simultaneously solved. The number of nonlinear equations that are needed to be solved depends on the constitutive model under consideration. For example a rate independent J_2 plasticity problem has a single nonlinear equation [18], a Lemaitre type plastic damage model has two nonlinear equations [19], and a porous plasticity model like Gurson model [20] requires solution of four nonlinear equations. Solving these systems of nonlinear equations is generally accomplished through the Newton–Raphson method. However, it might be advantageous to use higher order methods to solve these nonlinear equations. The higher order methods may result in one or more of the following advantages: (a) may be computationally efficient; and/or (b) may be less sensitive to initial guess when compared to the Newton–Raphson method. At present, there are no studies that have investigated the performance of higher order methods for solving such material nonlinearity. This issue is investigated in the current work.

In this exploratory study, the performance of a special class of root-solvers, which converge cubically in a neighborhood of the roots, is investigated for their suitability in constitutive modeling of the J_2 and the Gurson plasticity. This paper is organized as follows: Section 2 provides a summary of six cubic methods used in this study. The performance of these cubic methods by means of examples is demonstrated in Section 3. Section 4 provides the details related to the constitutive models that are used in this study. Detailed discussion about the suitability of cubic methods for solving material nonlinearity is presented in Section 5. Finally, Section 6 contains the summary and conclusions of this study.

2. Newton–Raphson method and cubic root-solvers

This section provides a brief summary of six cubic convergent methods along with the Newton–Raphson method for single and multivariate problems. No attempt is made to review all the existing cubic methods; see Ref. [5] for an elaborate discussion on these methods. Instead, the methods whose computational efficiency is comparable to the Newton–Raphson method are chosen. Furthermore, none of the presented cubic method requires the evaluation of higher order derivatives.

2.1. NR – Newton Raphson method

The Newton Raphson (NR) scheme for finding a root of a nonlinear equation, $f(x) = 0$, is given as

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{1}$$

where $f'(\boldsymbol{x}_n) \neq 0$ is the first derivative of $f(x)$ at $x = x_n$. The corresponding scheme for a multivariate case with a system of m-nonlinear equations, $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$, where $\boldsymbol{x} \in \mathbb{R}^m$ and $\boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^m$ can be expressed as

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n - \boldsymbol{F}(\boldsymbol{x}_n)^{-1}\boldsymbol{f}(\boldsymbol{x}_n) \tag{2}$$

where $\boldsymbol{F}(\boldsymbol{x}_n) \in \mathbb{R}^{m\times m}$ is a nonsingular matrix also referred to as the Jacobian which is given as

$$\boldsymbol{F}(\boldsymbol{x}_n) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_m} \end{bmatrix}_{\boldsymbol{x}=\boldsymbol{x}_n} \tag{3}$$

Informational efficiency index (Θ) is typically used (Ref. [16]) to compare different iterative procedures based on the convergence rates and the amount of information (function evaluations) required at each iteration and is defined as

$$\Theta = r^{\frac{1}{d}} \tag{4}$$

where r is the rate of convergence and d is the number of function evaluations required in the procedure. The NR method exhibits quadratic convergence in a neighborhood of roots and requires one derivative value and one function value at every iteration. Hence, the informational efficiency index of the NR method is 1.414. However, it is important to note that the informational efficiency index is not a measure of computational efficiency, as it does not account for the relative complexity of different function evaluations. For example, the informational efficiency index does not account for the difference in the evaluation of a function and it's Jacobian. Although this difference is nominal for small system of equations, it can be considerable in a relatively large system of equations. In the rest of this section, a brief review of cubic methods with efficiency index close to Newton–Raphson method is provided. All these methods can find single non-repetitive root in the vicinity of the trial root value.

2.2. M1 – Weerakoon and Fernando (2000) [21]

Weerakoon and Fernando [21] proposed a multipoint method with cubic convergence. As noted in Ref. [17], this method was earlier proposed by Traub [15], whereas Weerakoon and Fernando [21] derived this method using numerical integration. The iterative scheme for this two point nonlinear solver is given as

$$x_{n+1} = x_n - \frac{2f(x_n)}{\left[f'(x_n) + f'\left(x_n - \frac{f(x_n)}{f'(x_n)}\right)\right]} \tag{5}$$

The multivariate counterpart can be expressed as

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n - 2\left[\boldsymbol{F}(\boldsymbol{x}_n) + \boldsymbol{F}(\boldsymbol{x}_n - \boldsymbol{F}(\boldsymbol{x}_n)^{-1}\boldsymbol{f}(\boldsymbol{x}_n))\right]^{-1}\boldsymbol{f}(\boldsymbol{x}_n) \tag{6}$$

The method M1 requires one function value and the value of first derivative at two different points to update the roots at every iteration. It should be noted that the multivariate case requires two matrix inversions and this method has an efficiency index of $\Theta = 1.442$.

2.3. M2 – Frontini and Sormani (2003) [22], Özban (2004) [23]

Frontini and Sormani [22] rediscovered one of the multipoint methods proposed by Traub [15] following the procedure adopted