Convergence acceleration of nonlinear iteration

Abstract

The solutions of nonlinear equations are generally derived by some iterative methods. However, due to the strong nonlinearities of some complicated nonlinear models, classical iterative methods may converge slowly or even fail to converge. In this study, an accelerating convergence scheme of iterative solution was introduced for nonlinear equations. The main concept involves fitting a polynomial based on the error of the derived approximate solution, and then extrapolating the error to zero to obtain a new approximation. The convergence rate of the proposed algorithm is rigorously proven which shows that the algorithm significantly accelerates the convergence rate. As an application of this acceleration technique, the performance of the algorithm in electronic structure calculations is also introduced. Numerical results for different types of nonlinear equations are presented to validate the efficiency of the proposed algorithm.

1 Introduction

Several problems in computational sciences and other disciplines can be stated in the form of nonlinear equations using mathematical modeling. In particular, numerous problems in applied mathematics and engineering have been resolved by finding solutions to these equations. With the rapid development of science and technology, the theory and method of nonlinear equation research have received increasing attention in practical applications, and more nonlinear problems have appeared in scientific fields in the process of development. For example, when investigating nonlinear mechanics, fluid mechanics, weather forecasting, petroleum geology and exploration, automatic control field, computational biology, computational quantum mechanics and other processes. Such practical problems often need to be built into mathematical models and transformed into nonlinear equations.

However, obtaining the exact solution in the practical process of solving a nonlinear equation is not easy; therefore, it is converted into a numerical solution. The iterative method is an important method for obtaining the numerical solutions of nonlinear equations. In other words, starting with an initial approximation of the predicted solution, a sequence of approximations is constructed using an iterative scheme to gradually approximate the true solution of the equation. Several representative iterative methods, such as the classical Newton iteration, secant iteration, and fixed-point iteration have been proposed. Detailed descriptions of these algorithms are provided in [7, 15, 16, 21, 23], etc. In particular, as a vital application of nonlinear iteration, there is a great demand in electronic structure calculations since it involves quite complex nonlinear models. The most common strategy for electronic structure calculations relies on approximate solutions of Schrödinger equations, and the so-called density functional theory (DFT) has been established as one of the most widely used first-principles methods in many fields. Modern electronic structure calculations in DFT settings require solving the well-known Kohn-Sham equation, which is adopted as a benchmark in this study. The Kohn-Sham equation is a complex nonlinear equation that must be solved using some efficient iteration schemes. In quantum mechanics, self-consistent field (SCF) iteration is the most general and widely-used method [2, 5, 6, 13, 20, 24]. However, these classical nonlinear iteration schemes may fail to

converge for complex models. This challenge can be partially overcome by implementing some mixing schemes which uses the combination of previous approximate solutions. By appropriately selecting the mixing coefficient, the mixing scheme causes the input and output functions to exhibit the smallest errors. Widely used mixing schemes include those in [1, 3, 4, 10, 12, 18, 19].

In this study, we construct a novel acceleration scheme for nonlinear iterations to improve the efficiency of classical nonlinear iteration schemes. The proposed method differs from the existing schemes in that it relies on the least squares method and an extrapolation scheme. More precisely, after deriving an initial approximate solution $\bar{u}_k$, we compute several approximate solutions $u_{k+1}, \cdots, u_{k+s-1}$ by performing s times the classical nonlinear iterations with the initial value $u_k := \bar{u}_k$. We then compute the error results for these approximate solutions, which use the differences between two consecutive solutions. In other words, for each approximate solution u_j, there is an error $u_{j+1} - u_j$, where $j = k, \cdots, k+s-1$. Subsequently, the corresponding errors are extrapolated to zero. The extrapolation process relies on the least squares method. Based on s two-dimensional points $(u_k, u_{k+1} - u_k), (u_{k+1}, u_{k+2} - u_{k+1}), \cdots, (u_{k+s-1}, u_{k+s} - u_{k+s-1})$, we fit a polynomial. Finally, we solve the zero point of the fitted polynomial and adopt it as the new approximate solution $\bar{u}_{k+1}$. For instance, based on these s points, we can fit a straight line denoted by $y = w_1 x + w_2$. After deriving the straight line $y = w_1 x + w_2$, we use its zero point $-w_2/w_1$ as the new approximate solution, which is denoted as $\bar{u}_{k+1}$. Because the fitted polynomial reflects the convergence tendency, the zero point will be a more precise solution. The convergence rate of the proposed algorithm is rigorously proved in this study and a higher convergence order is obtained compared with the classical iterations. This implies that the novel algorithm can accelerate the convergence rate of nonlinear iterations. Based on the theoretical results of this study, if the convergence order of the classical nonlinear iteration is p (> 1), then the proposed algorithm can improve the convergence order to $2p - 1$. If $p = 1$, the proposed algorithm can improve the convergence order to 2. Additionally, in some cases, even though the classical nonlinear iteration does not converge, the proposed algorithm can still derive the convergence results.

The remainder of this paper is organized as follows. In Section 2, we review basic knowledge of nonlinear iteration. In Section 3, we construct an accelerating iteration scheme to improve the convergence rate of nonlinear iterations. In Section 4, we introduce the way to perform the acceleration scheme for electronic structure calculations. In Section 5, the numerical experiments are presented to demonstrate the efficiency of the proposed method. Finally, concluding remarks are presented in Section 6.

2 Nonlinear iteration for nonlinear equations

In this section, we briefly introduce the basic concepts of nonlinear iterations. Let us consider a nonlinear equation as follows: Find $u \in \mathbb{R}$ such that

$$f(u) = 0. \tag{2.1}$$

To derive a iteration scheme, we change the equation (2.1) into

$$u = g(u). \tag{2.2}$$

Given an initial value u_0, the fixed point iteration scheme is designed as follows:

$$u_{k+1} = g(u_k), \qquad k = 0, 1, \cdots, \tag{2.3}$$

which is the basic form for the theoretical analysis of all the nonlinear iteration schemes.

Let u_* be the exact solution of (2.1), then we have

$$u_* = g(u_*). \tag{2.4}$$

The convergence order of the iteration scheme can be obtained through Taylor expansion. If $g^{(m)}(u_*) = 0$ for $m = 1, \cdots, p-1$, then we have

$$g(u_k) = g(u_*) + \frac{g^{(p)}(\xi_k)(u_k - u_*)^p}{p!}. \tag{2.5}$$

This means the iterative method is p-order convergent, that is

$$\frac{u_{k+1} - u_*}{(u_k - u_*)^p} = \frac{g^{(p)}(\xi_k)}{p!}, \tag{2.6}$$

or equivalently

$$u_{k+1} - u_* = C_k(u_k - u_*)^p, \tag{2.7}$$

where

$$\lim_{k\to\infty} C_k = C := \frac{g^{(p)}(u_*)}{p!}. \tag{2.8}$$

If one more item is used in the Taylor expansion, we have

$$g(u_k) = g(u_*) + \frac{g^{(p)}(u_*)(u_k - u_*)^p}{p!} + \frac{g^{(p+1)}(\xi_{k+1})(u_k - u_*)^{p+1}}{(p+1)!}. \tag{2.9}$$

The convergence rate can be expressed by:

$$\frac{u_{k+1} - u_*}{(u_k - u_*)^p} = \frac{g^{(p)}(u_*)}{p!} + \frac{g^{(p+1)}(\xi_{k+1})(u_k - u_*)}{(p+1)!}, \tag{2.10}$$

or equivalently

$$u_{k+1} - u_* = C(u_k - u_*)^p + \widetilde{C}_k(u_k - u_*)^{p+1}, \tag{2.11}$$

where

$$\lim_{k\to\infty} \widetilde{C}_k = \widetilde{C} := \frac{g^{(p+1)}(u_*)}{(p+1)!}. \tag{2.12}$$

3 Improved iteration scheme for nonlinear equations

For nonlinear equations, the approximate solutions should be derived using nonlinear iteration scheme. However, for some complicated nonlinear equations, classical nonlinear iteration schemes may converge slowly or even fail to converge.

In this study, we introduce an improved iteration scheme based on extrapolation and the least squares method to accelerate nonlinear iteration. Assuming that we have obtained an approximate solution $\bar{u}_k$, we introduce an iteration scheme to derive a new approximate solution $\bar{u}_{k+1}$ which has a better accuracy. Setting $u_k = \bar{u}_k$, we first derive s approximate solutions $u_{k+1}, \cdots, u_{k+s}$ by performing the classical nonlinear iterations s-times . Subsequently, for each approximate solution u_j, there exists an error $u_{j+1} - u_j$, $k \le j \le k+s-1$. Thus, we can construct

s two-dimensional point coordinates $(u_k,\ u_{k+1}-u_k), (u_{k+1},\ u_{k+2}-u_{k+1})\cdots, (u_{k+s-1},\ u_{k+s}-u_{k+s-1})$. Based on these s points, we can fit a straight line. Let us define the function for the straight line as $y = w_1x + w_2$. After deriving the straight line, we use its zero point $-w_2/w_1$ as the new approximate solution, which is denoted as $\bar{u}_{k+1}$.

The aforementioned fitting process for the straight line is performed using the least squares method. First, let us denote the coefficient matrix as follows:

$$A = \begin{pmatrix} u_k & 1 \\ \vdots & \vdots \\ u_{k+s-1} & 1 \end{pmatrix}_{s\times 2},$$

and the righthand vector

$$Y = \begin{pmatrix} u_{k+1}-u_k \\ \vdots \\ u_{k+s}-u_{k+s-1} \end{pmatrix}_{s\times 1},$$

and the unknown vector

$$W = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}_{2\times 1}.$$

Then the least squares method requires to solve the following minimization problem:

$$\min_{(w_1,w_2)} \sum_{j=k}^{k+s-1} \big((u_{j+1}-u_j) - w_1u_j - w_2\big)^2 = \min_{W}(AW-Y)^T(AW-Y). \tag{3.1}$$

The optimal solution of (3.1) can be derived by solving the following equation:

$$A^TAW = A^TY, \tag{3.2}$$

which yields

$$W = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = (A^TA)^{-1}A^TY. \tag{3.3}$$

Because A^TA is a 2×2 matrix:

$$A^TA = \begin{pmatrix} \sum_{j=k}^{k+s-1} u_j^2 & \sum_{j=k}^{k+s-1} u_j \\ \sum_{j=k}^{k+s-1} u_j & s \end{pmatrix}_{2\times 2}, \tag{3.4}$$

the corresponding inverse matrix can be derived easily as follows:

$$(A^TA)^{-1} = \frac{1}{|A^TA|}\begin{pmatrix} s & -\sum_{j=k}^{k+s-1} u_j \\ -\sum_{j=k}^{k+s-1} u_j & \sum_{j=k}^{k+s-1} u_j^2 \end{pmatrix}_{2\times 2}. \tag{3.5}$$

Since the final approximate solution is a quotient of w_1 and w_2, the value of $\frac{1}{|A^TA|}$ is not needed in actual calculation.

Thus, we only need the value of $|A^TA|W$ which is as follows:

$$|A^TA|W$$

$$
\begin{aligned}
&= \begin{pmatrix} s & -\sum_{j=k}^{k+s-1} u_j \\ -\sum_{j=k}^{k+s-1} u_j & \sum_{j=k}^{k+s-1} u_j^2 \end{pmatrix}_{2\times 2} \begin{pmatrix} u_k & 1 \\ \vdots & \vdots \\ u_{k+s-1} & 1 \end{pmatrix}^T_{s\times 2} \\
&\quad \cdot \begin{pmatrix} u_{k+1}-u_k \\ \vdots \\ u_{k+s}-u_{k+s-1} \end{pmatrix}_{s\times 1} \\
&= \begin{pmatrix} su_k - \sum_{j=k}^{k+s-1} u_j & \cdots & su_{k+s-1} - \sum_{j=k}^{k+s-1} u_j \\ \sum_{j=k}^{k+s-1} u_j^2 - u_k \sum_{j=k}^{k+s-1} u_j & \cdots & \sum_{j=k}^{k+s-1} u_j^2 - u_{k+s-1} \sum_{j=k}^{k+s-1} u_j \end{pmatrix}_{2\times s} \\
&\quad \cdot \begin{pmatrix} u_{k+1}-u_k \\ \vdots \\ u_{k+s}-u_{k+s-1} \end{pmatrix}_{s\times 1} .
\end{aligned}
$$

Moreover, the two components of the vector $|A^TA|W$ can be expressed as follows:

$$
\begin{aligned}
|A^TA|w_1 &= (u_{k+1}-u_k)(su_k - \sum_{j=k}^{k+s-1} u_j) \\
&\quad +(u_{k+2}-u_{k+1})(su_{k+1} - \sum_{j=k}^{k+s-1} u_j) \\
&\quad +\cdots \\
&\quad +(u_{k+s}-u_{k+s-1})(su_{k+s-1} - \sum_{j=k}^{k+s-1} u_j) \\
&= (u_{k+1}-u_k) \sum_{j=k}^{k+s-1} (u_k - u_j) \\
&\quad +(u_{k+2}-u_{k+1}) \sum_{j=k}^{k+s-1} (u_{k+1} - u_j) \\
&\quad +\cdots \\
&\quad +(u_{k+s}-u_{k+s-1}) \sum_{j=k}^{k+s-1} (u_{k+s-1} - u_j)
\end{aligned}
$$

and

$$
\begin{aligned}
|A^TA|w_2 &= (u_{k+1}-u_k)(\sum_{j=k}^{k+s-1} u_j^2 - u_k \sum_{j=k}^{k+s-1} u_j) \\
&\quad +(u_{k+2}-u_{k+1})(\sum_{j=k}^{k+s-1} u_j^2 - u_{k+1} \sum_{j=k}^{k+s-1} u_j) \\
&\quad +\cdots \\
&\quad +(u_{k+s}-u_{k+s-1})(\sum_{j=k}^{k+s-1} u_j^2 - u_{k+s-1} \sum_{j=k}^{k+s-1} u_j)
\end{aligned}
$$

$$
\begin{aligned}
= \quad & (u_{k+1}-u_k)\sum_{j=k}^{k+s-1}(u_j^2-u_k u_j) \\
& +(u_{k+2}-u_{k+1})\sum_{j=k}^{k+s-1}(u_j^2-u_{k+1}u_j) \\
& +\cdots \\
& +(u_{k+s}-u_{k+s-1})\sum_{j=k}^{k+s-1}(u_j^2-u_{k+s-1}u_j).
\end{aligned}
$$

Then, we use the zero point $\bar{u}_{k+1} := -(|A^TA|w_2)/(|A^TA|w_1)$ as the new approximate solution.

After performing the solving process, we then derive the new approximate solution $\bar{u}_{k+1}$ from $\bar{u}_k$ based on performing s-times nonlinear iterations and the extrapolation technique. For simplicity, we summarize this process into the following symbol

$$\bar{u}_{k+1} = ExtraLeast(\bar{u}_k, s). \tag{3.6}$$

The detailed process to accelerate the nonlinear iteration can be summarized in the following algorithm:

Algorithm 3.1. *Improved iteration scheme for nonlinear equations*

1. *Given an initial value $\bar{u}_1$, a tolerance TOL, and an extrapolation parameter s.*
2. *Set $k = 1$.*
3. *Derive a new approximate solution $\bar{u}_{k+1}$ from $\bar{u}_k$ by:*

$$\bar{u}_{k+1} = ExtraLeast(\bar{u}_k, s). \tag{3.7}$$

4. *if $|\bar{u}_{k+1} - \bar{u}_k| \le TOL$, stop. Else set $k = k+1$ and go to step 3.*

References

[1] D.G. Anderson, *Iterative procedures for nonlinear integral equations*, J. Assoc. Comput. Mach., 12(4) (1965), 547–560.

[2] Z. Bai, R.C. Li and D. Lu, *Optimal convergence rate of self-consistent field iteration for solving eigenvector-dependent nonlinear eigenvalue problems*, arxiv.org/abs/2009.09022v1.

[3] D.R. Bowler and M.J. Gillan, *An efiicient and robust technique for achieving self consistency in electronic structure calculations*, Chem. Phys. Lett., 325 (2000), 473–476.

[4] C. G. Broyden, *A class of methods for solving nonlinear simultaneous equations*, Math. Comp., 19 (1965), 577–593.

[5] X. Dai and A. Zhou, *Finiteelem entmethodsforelectronicstructurecalculations*, SCIENTIA SINICA Chimica, 45(8) (2015), 800–811.

[6] X. Dai and A. Zhou, *The design principle for the programming of real space parallel adaptive calculations for electronic structure*, SCIENTIA SINICA Informationis, 46(10) (2016), 1421–1441.

[7] P. Deuflhard, *Newton methods for nonlinear problems*, Springer, 2004.

[8] E. Fermi, *Un metodo statistics per la determinazione di alcune proprieta dell'atomoi*, Rend. Accad. Lincei, 6 (1927), 602–607.

[9] P. Hohenberg and W. Kohn, *Inhomogeneous electron gas*, Phys. Rev., 136 (1964), B864–B871.

[10] D. D. Johnson, *Modifled Broyden's method for accelerating convergence in self-consistent calculations*, Phys. Rev. B, 38 (1988), 12807–12813.

[11] W. Kohn and L. Sham, *Self-consistent equations including exchange and correlation effects*, Phys. Rev. A, 140 (1965), 1133–1138.

[12] L. Lin and C. Yang, *Elliptic preconditioner for accelerating the self-consistent field iteration in Kohn-Sham density functional theory*, SIAM J. Sci. Comput., 35(5) (2013), S277–S298.

[13] X. Liu, X. Wang, Z. Wen and Y. Yuan, *On the convergence of the self-consistent field iteration in Kohn-Sham density functional theory*, SIAM J. Matrix Anal. Appl., 2013, 35(2), 546–558.

[14] R. Martin, *Electronic Structure: Basic Theory and Practical Methods*, Cambridge: Cambridge University Press, 2020.

[15] A. M. Ostrowski, *Solutions of equations and system of equations*, New York: Academic Press, 1960

[16] J. M. Ortega and W. C. Rheinboldt, *Iterative solution of nonlinear equations in several variables*, Academic Press, 1972.

[17] J. P. Perdew and A. Zunger, *Self-interaction correction to density-functional approximations for many-electron systems*, Phys. Rev. B, 23 (1981), 5048–5079.

[18] P. Pulay, *Convergence acceleration of iterative sequences. the case of scf iteration*, Chem. Phys. Lett., 73 (1980), 393–398.

[19] P. Pulay, *Improved SCF convergence acceleration*, J. Comput. Chem., 3 (1982), 556–560.

[20] C.C.J. Roothaan, *New developments in molecular orbital theory*, Rev. Mod. Phys., 23(2):69, 1951

[21] A. Sergio and B. Sonia, *Advances in Iterative Methods for Nonlinear Equations*, Springer, Switzerland 2016

[22] L. Thomas, *The calculation of atomic fields*, Proc. Cambridge Phil. Soc., 23 (1927), 542–548.

[23] J. F. Traub, *Iterative methods for the solution of equations*, Englewood Cliffs New Jersey: Prentice-Hall, 1964

[24] C. Yang, W. Gao, J.C. Meza, *On the convergence of the self-consistent field iteration for a class of nonlinear eigenvalue problems*, SIAM J. Matrix Anal. Appl., 30(4) (2009), 1773–1788.