The W4 method: a new multi-dimensional root-finding scheme for nonlinear systems of equations

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Abstract

We propose a new class of method for solving nonlinear systems of equations, which, among other things, has four nice features: (i) it is inspired by the mathematical property of damped oscillators, (ii) it can be regarded as a simple extension to the Newton-Raphson (NR) method, (iii) it has the same local convergence as the NR method does, (iv) it has a significantly wider convergence region or the global convergence than that of the NR method. In this article, we present the evidence of these properties, applying our new method to some examples and comparing it with the NR method.

1. Introduction

One of the most important problems in computational science and engineering is a root-finding of functions. It is defined as a problem to solve the following equations numerically:

\[ F(x) = 0, \]  
(1)
where \( x \in \mathbb{R}^N, N \in \mathbb{Z} \) and \( F : \mathbb{R}^N \to \mathbb{R}^N \) is a generic system of nonlinear equations in \( x \).

Numerical root-finding methods are essentially categorized into two types. One is deterministic methods such as the Newton-Raphson (NR) method [1], which always give the same answer to the same initial condition. The other is stochastic methods such as the Monte-Carlo method [2], in which the answer may change in each trial even for identical initial conditions. The former method normally requires a larger computational cost but needs a very small number (mostly one) of trials, whereas the computational cost per trial is small but many trials are needed in the stochastic method.

Although the single-variable problem is rather simple, it becomes highly nontrivial when the dimension of variable space is higher than one. One may choose the NR method if the dimension is not prohibitively large in terms of numerical cost. The NR method can be regarded as an iterative solver based on the fixed point theorem and it is guaranteed to give a solution as long as the initial guess is sufficiently close to the solution [3]. In practice, there are two major drawbacks in the NR method: (i) very heavy computational cost in the inversion of a large Jacobian matrix (See Eq. (6)) and (ii) the strong dependence of convergence on the initial guess. The former is evaluated as \( O(N^3) \) for the direct inversion of an \( N \times N \) Jacobian matrix in the system of \( N \)-dimensions. So far, much attention has been paid to issue (i) and many efforts have been made to reduce the cost: for example, a number of quasi-Newton methods have been proposed, which successfully reduce the computational costs to \( O(N^2) \) [4, 5]. As for issue (ii), many studies have attempted to accelerate the normally quadratic convergence of the NR method. In fact, Halley’s and Householder’s methods proposed for single-variable problems are headed in this direction [6]. Also for multi-variable problems, a new approach emerged recently [6, 7].

It is the sensitivity of convergence to the initial guess that we focus most in this paper. It is well known that the NR method fails to find solutions when the initial guess is far from the solution, in particular, in multi-dimensional problems. We need to give a good consideration to the initial guess but there is no guarantee that it is always successful unless we know the solution. When the NR method fails to find solutions, we see either a divergence or a permanent oscillation of the successive solutions of the linearized equations as explicitly shown in Sec. 2.2. This is sometimes related to the existence of singularities in the Jacobian matrix and may be solved by modifying source terms in the linearized equations [8, 9, 10]. It should also be emphasized that the inversion of ill-conditioned matrices usually need high-precision calculations regardless of the iterative methods employed and a careless handling could easily produce an incorrect inverse matrix whose component is wrong from the leading figure. In such cases, we should pay proper attention to numerical errors accumulated during iterations. In this article, we focus especially on problems, for which the NR method fails to find solutions in spite of the fact that its Jacobian matrix is well-conditioned initially. The initial guess is likely to be a culprit then. We demonstrate that our new method can find a solution even when an initial guess is far from the solution.

This paper is organized as follows. Firstly, we define the problem we deal with in this paper. It will also make clear the motivation of this work, employing some concrete problems, in Sec. 2. Then, we present our new formulation to find roots of a system of nonlinear equations in Sec. 3 starting with the descriptions of other conventional methods in the literature on the same basis. In Sec. 4, we demonstrate the capabilities of our method for several sample problems, comparing them with those of other methods. Finally, we give a summary and comments on future prospects in Sec. 5.

2. Problem

As mentioned in the Introduction, our goal is to numerically solve generic systems of nonlinear equations, Eq. (1). In order to make clear the issues of our concern in this article, we consider some specific examples in the following. Although we are interested in multi-variable equations, we start with a single-variable problem for clarity.

2.1. single-variable problem

We first consider the root-finding of the following single-variable equation:

\[
f(x) = \arctan(x) + \sin(x) - 1 = 0,
\] (2)
where $x \in \mathbb{R}$. In the left panel of Fig. 1, we display the function, which has oscillatory behavior and has multiple solutions only on the positive $x$-axis ($x > 0$). In the NR method, one employs the following iteration map from the $n$-th step to $(n+1)$-th step,

$$x_{n+1} = x_n - \left( \frac{df}{dx}(x_n) \right)^{-1} f(x_n).$$  \hfill (3)

As demonstrated in Table 1, as long as it obtains a solution, the NR method requires only a small number of iteration steps to get to the solution within a prescribed accuracy, i.e., $|f(x)| < 10^{-6}$ in this example, thanks to its well known quadratic-convergence nature. The table also demonstrates that the NR method fails to find a solution if the initial guess is smaller than $x_i = -2.0$. We show typical trajectories of the NR map, Eq. (3), both for the successful and failed attempts in the right panel of Fig. 1. The iteration rapidly converges to one of the solutions ($x = 1$) when the initial guess is close to the solution whereas it shows an oscillation between two values and never reaches a solution if the initial guess is $x_i = -2.0$. Since the latter oscillation is a consequence of the oscillatory nature of the function $f(x)$, it is natural to soften its slope somewhat by hand in the evaluation of $x$ in the next step,

$$x_{n+1} = x_n - \Delta \tau \left( \frac{df}{dx}(x_n) \right)^{-1} f(x_n),$$  \hfill (4)

where we introduce a damping parameter $\Delta \tau$, which is a positive real number less than unity. The results for this so-called Damped Newton(DN) method are presented in Table 1 for the comparison with the original NR method. Although the number of iteration steps required to get a solution within the prescribed accuracy increases substantially in the DN method, the region of the initial guess where a solution is obtained becomes wider. This implies that the NR method, if appropriately modified, may find a solution even for initial guesses that are not very close to the solution at least for single-variable problems in principle.
2.2. multi-variable problem

The above situation is changed drastically when the dimension of variable space becomes higher than one. To observe what happens, we consider the following concrete problem:

\[ F_1(x, y) := x^2 + y^2 - 4 = 0, \]  
\[ F_2(x, y) := x^2 y - 1 = 0. \]  

The functions \( F_1 \) and \( F_2 \) represent a circle and a parabola, respectively, and the roots of this system correspond to the intersections of these two curves in the \( x - y \) plane. In the NR or DN method for multi-variable problems [3, 1], one can proceed just as in the single-variable case and employs the following iteration map from the \( n \)-th step to the \((n + 1)\)-th step,

\[ x_{n+1} = x_n - \Delta \tau J^{-1}F(x_n), \]  
where \( F := (F_1 \ F_2)^T \) and \( J^{-1} \) is the inverse of the Jacobian matrix associated with Eqs. (5), which is given as

\[ J = \begin{bmatrix} 2x & 2y \\ 2xy & x^2 \end{bmatrix}. \]  

Then, the iteration maps for \( \mathbf{x} = (x \ y)^T \) are expressed explicitly as

\[ x_{n+1} = x_n - \Delta \tau \left[ \frac{x_n}{2(x_n^2 - 2y_n^2)} F_1 - \frac{y_n}{x_n(x_n^2 - 2y_n^2)} F_2 \right], \]  
\[ y_{n+1} = y_n - \Delta \tau \left[ -\frac{y_n}{x_n^2 - 2y_n^2} F_1 + \frac{1}{x_n^2 - 2y_n^2} F_2 \right]. \]  

In Fig. 2 we display the Newton basin for the NR and DN maps in the left and right panels, respectively, as an indicator of the initial-guess dependence. Different colors (red, orange, green, blue) correspond to one of the four solutions,

\[ (x^*, y^*) \sim (\pm 1.9837924, 0.25410169), \quad (\pm 0.73307679, 1.8608059), \]  

Figure 2: Initial guess dependence by the NR method (Left) and the DN method (right) with \( \Delta \tau = 0.5 \) (Right). The red, orange, green and blue correspond to all solutions of Eqs. (5), while the black means the method cannot find any solution. In addition, four solutions are expressed by the black crosses.
to which each point converges. The black color implies that none of the solutions has been reached within 1000 iteration steps. For both methods, the local convergence is observed more or less as expected. It is evident, however, that the damping factor introduced in the DN method does not help as much in finding solutions in this two dimensional problem compared with the one-dimensional counterpart considered in the previous section.

3. The New Method

3.1. The NR method as a relaxation

The iteration map given in Eq. (6) can also be regarded as a discretized form of the continuous time-evolution equation:

$$\frac{dx}{d\tau} = -J^{-1}F(x).$$  \hspace{1cm} (10)

We will consider a bit more general time-evolution equation with a preconditioning matrix $M$ given as

$$\frac{dx}{d\tau} = -MF(x).$$  \hspace{1cm} (11)

The corresponding discretized form is obtained by the Euler forward discretization in time with the time interval $\Delta\tau$ as

$$x_{n+1} = x_n - \Delta\tau M F(x_n),$$  \hspace{1cm} (12)

where $x_n$ is the discretized solution at the $n$-th iteration step. If one employs the inverse of the Jacobian matrix as the preconditioner $M = J^{-1}$, then Eq. (10) is recovered.

**Theorem 1.** Suppose the solution of Eq. (1) exists and let $F: \mathbb{R}^n \to \mathbb{R}^n$ be Lipschitz continuous near the solution $x^*$, then the iteration map (12) for $M = J^{-1}$ with $0 < \Delta\tau < 1$ converges linearly to the solution $x^*$ starting from an arbitrary initial guess sufficiently close to the solution.

*Proof.* The Taylor expansion of the source function $F(x)$ around the solution $x^*$ up to the first order in the error defined as $e_n := x^* - x_n$ gives

$$F(x^*) = F(x_n) + J e_n + O(||e||^2).$$  \hspace{1cm} (13)

Since $x^*$ is the solution and $F(x^*) = 0$, one can express $F(x_n)$ in Eq. (12) in terms of the Jacobian matrix and the error to yield the error propagation equation as

$$e_{n+1} = (I - \Delta\tau M J) e_n,$$  \hspace{1cm} (14)

where $I$ is the $N \times N$ identity matrix. Under the present condition $M = J^{-1}$ and $0 < \Delta\tau < 1$ the error converges to zero in the $n \to \infty$ limit

$$\lim_{n \to \infty} \frac{||e_{n+1}||}{||e_0||} = \lim_{n \to \infty} (1 - \Delta\tau)^{n+1} = 0.$$  \hspace{1cm} (15)

As a result, we obtain the solution $x^*$ by the iteration map (12).

As a result, we obtain the solution $x^*$ by the iteration map (12).

1. In general, the necessary and sufficient conditions for the map (12) to converge to a solution are that the absolute values of all the eigenvalues for the matrix $E - \Delta\tau MJ$ should be less than unity.
3.2. A new approach for single-variable problems

Now we proceed to the new approach we propose in this article. For a nonlinear equation with a single variable

\[ F(x) = 0, \]  

we consider the following time-evolution equation with the second derivative in time

\[
\frac{d^2 x}{d\tau^2} + c \frac{dx}{d\tau} + \left\{ \frac{dF}{dx} \right\}^{-1} F(x) = 0, \tag{17}
\]

or equivalently two first-order equations,

\[
\frac{dx}{d\tau} := \dot{x} = p, \tag{18a}
\]

\[
\frac{dp}{d\tau} := \dot{p} = -cp - \left\{ \frac{dF}{dx} \right\}^{-1} F(x), \tag{18b}
\]

where the dot notation is introduced for the derivative with respect to \( \tau \) for later convenience and \( c \in \mathbb{R} \) is a constant parameter. These are nothing but damped oscillator’s equations of motion if \( F(x) = x \) and \( c > 0 \).

**Lemma 1.** Suppose there exists a solution of the nonlinear equation \[ (16) \] indicated with \( x^* \), if one sets the parameter \( c = 2 \), then a sufficiently small deviation from \( x^* \) always decays during its time evolution \[ (17). \]

**Proof.** The Taylor expansion around the solution yields

\[ F(x^* + \delta x) = F(x^*) + \frac{dF}{dx} \delta x + \mathcal{O}(\delta x^2). \tag{19} \]

One can then obtain the equation for the deviation \( \delta x \) valid up to the first order by the substitution \( x = x^* + \delta x \) into Eq. \[ (17) \] as

\[ \delta x + c\dot{\delta x} + \delta x = 0. \tag{20} \]

There exists a characteristic mode in the equation \[ (20) \], which is explicitly given by assuming \( \delta x = e^{i\omega \tau} \) as

\[ \omega = \frac{ic \pm \sqrt{-c^2 + 4}}{2}. \tag{21} \]

Thus, the deviation from the solution \( x^* \) with \( c = 2 \) decays exponentially as \( \delta x = e^{-\tau} \) during the time evolution.

**Theorem 2.** (Bendixson’s criterion) If on a simply connected region \( \mathcal{D} \subset \mathbb{R}^2 \) in the phase space \((x, p)\) the parameter \( c \) is nonzero, then there is no periodic orbits in \( \mathcal{D} \).

**Proof.** Any orbit of system \[ \text{(18)} \] in the two-dimensional real phase space \((x, p)\) is described by \( \frac{dp}{dx} = \dot{p}/\dot{x} \). A closed orbit \( \Gamma \) in the phase space satisfies

\[ \oint_{\Gamma} (\dot{x} dp - \dot{p} dx) = 0. \tag{22} \]

However, for a closed area \( \mathcal{D} \) bounded by \( \Gamma \), Green’s theorem gives

\[ \oint_{\Gamma} (\dot{x} dp - \dot{p} dx) = \iint_{\mathcal{D}} \left( \frac{\partial \dot{x}}{\partial x} + \frac{\partial \dot{p}}{\partial p} \right) dx dp = -c \mathcal{D}. \tag{23} \]

Consequently, no periodic orbit exists inside \( \mathcal{D} \) in the phase space with nonzero parameter \( c \).
Lemma 1 combined with Theorem 2 implies that the solution of our new time-evolution equation \((17)\) is all settled down asymptotically to one of the solutions of Eq. \((16)\).

We now show that the discretized version of equations \((18)\):

\[
x_{n+1} = x_n + \Delta \tau \quad (24a)
\]

\[
p_{n+1} = (1 - c \Delta \tau) p_n - \Delta \tau \left\{ \frac{dF}{dx} \right\}^{-1} F(x_n), \quad (24b)
\]

also converges to the same solution under a certain condition. In deriving these equations, we employ the explicit Euler difference in time with an interval \(\Delta \tau\).

**Proposition 1.** Suppose there exists a solution of Eq. \((16)\) and let \(F : \mathbb{R} \rightarrow \mathbb{R}\) be Lipschitz continuous near the solution \(x^*\), then the iteration map \((24)\) with \(c = 2\) and \(0 < \Delta \tau < 1\) yields a series of \(x^*\) starting from \(p_0 = 0\) and an arbitrary initial guess \(x_0\) that is sufficiently close to the solution \(x = x^*\).

**Proof.** Just as in the proof of Theorem 1 we evaluate the error propagation for the map \((24)\) up to the first order in \(e^{(x)}_n := x^* - x_n\) and \(e^{(p)}_n := 0 - p_n\), using \(F(x_n) = \frac{dF}{dx} e^{(x)}_n\), as follows:

\[
e^{(x)}_{n+1} = e^{(x)}_n - \Delta \tau e^{(p)}_n, \quad (25a)
\]

\[
e^{(p)}_{n+1} = (1 - 2 \Delta \tau) e^{(p)}_n + \Delta \tau e^{(x)}_n. \quad (25b)
\]

We then obtain the following solution to these equations

\[
e^{(x)}_n = e^{(x)}_0 (1 - \Delta \tau)^{n-1} [1 + (n - 1) \Delta \tau], \quad (26a)
\]

\[
e^{(p)}_n = n e^{(x)}_0 \Delta \tau (1 - \Delta \tau)^{n-1}, \quad (26b)
\]

which can be easily confirmed by substitution. The convergence is now evident for \(0 < \Delta \tau < 1\).

\[
\lim_{n \rightarrow \infty} e^{(x)}_n = \lim_{n \rightarrow \infty} e^{(p)}_n = 0. \quad (27)
\]

### 3.3. The new formulation for multi-variable problems

Now we move on to the multi-variable case, the main part of this paper. Unlike the NR method discussed in Sec. 3.1 the following second-order time-evolution equations instead of the first-order ones, Eq. \((11)\):

\[
\frac{d^2 x}{d\tau^2} + M_1 \frac{dx}{d\tau} + M_2 F(x) = 0, \quad (28)
\]

where we introduce two preconditioning matrices, \(M_1, M_2 : \mathbb{R}^N \rightarrow \mathbb{R}^N\). These equations are then divided into two sets of first-order differential equations as follows:

\[
\frac{dx}{d\tau} = X p, \quad (29a)
\]

\[
\frac{dp}{d\tau} = -2p - Y F, \quad (29b)
\]

which \(x \in \mathbb{R}^N\) and \(p \in \mathbb{R}^N\) are generalized coordinates and associated momenta, respectively; another pair of preconditioners \(X\) and \(Y\) are introduced, which will be determined later. We also adopt the damping

\[\text{footnote}{^2}\]This analysis will not hold for higher dimensional problems since chaos may kick in and trajectories will not be closed.
factor $c = 2$ for the multi-variable case. The explicit Euler discretization in time with the time interval $\Delta \tau$ then yields the following iteration map:

$$
\begin{align*}
x_{n+1} &= x_n + \Delta \tau X p_n, \\
p_{n+1} &= (1 - 2\Delta \tau) p_n - \Delta \tau Y F(x_n).
\end{align*}
$$

(30a) (30b)

Again linearizing the above nonlinear map around the solution ($x = x^*$ and $p = 0$), we obtain the following error propagation equations:

$$
\begin{align*}
e_{n+1}^{(x)} &= e_n^{(x)} - X\Delta \tau e_n^{(p)}, \\
e_{n+1}^{(p)} &= (1 - 2\Delta \tau) e_n^{(p)} + Y J \Delta \tau e_n^{(x)},
\end{align*}
$$

(31a) (31b)

which can be cast into a more compact form as

$$
e_{n+1}^{(z)} = W e_n^{(z)}, \quad e_n^{(z)} := \begin{pmatrix} e_n^{(x)} \\ e_n^{(p)} \end{pmatrix}, \quad W := \begin{pmatrix} I & -\Delta \tau X \\ \Delta \tau Y J & (1 - 2\Delta \tau) I \end{pmatrix},$$

(32)

where $I$ denotes the $N \times N$ identity matrix. We name this map the W4 map.

**Lemma 2.** Suppose there exists a complete set of eigenvectors $v_i \in \mathbb{R}^N$ of the matrix $W$ and let $P$ be an $N \times N$ matrix composed of $v_i$ and $\lambda_i$ be the eigenvalues corresponding to $v_i$, then the error $e_n^{(z)}$ converges to the zero vector if the maximum eigenvalue satisfies $|\lambda_{\text{max}}| < 1$.

**Proof.** The matrix $W$ can be decomposed as $W = P^{-1} \Lambda P$ in terms of the matrix $P := [v_1 \ v_2 \ \cdots \ v_N]$ and the diagonal matrix $\Lambda := \text{diag} [\lambda_1, \lambda_2, \cdots, \lambda_N]$. Then the error propagates as

$$
e_{n+1} = P^{-1} \Lambda P e_n = (P^{-1} \Lambda P)^n e_0 = P^{-1} \Lambda^n P e_0$$

(33)

and converges to the zero vector if the maximum eigenvalue $|\lambda_{\text{max}}|$ is less than unity.

Our problem is then reduced to finding the eigenvalues of the matrix $W$ in Eq. (32).

**Lemma 3.** Suppose $A, B, C, D$ are $N \times N$ matrices and $M := \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ is a $2N \times 2N$ matrix. If $A$ and $B$ commute with each other and $A$ is invertible, then the determinant of the matrix $M$ is given as

$$
\det [M] = \det [AD - CB].
$$

(34)

**Proof.** Following Ref. [11], we consider the identity

$$
\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} I & -B \\ O & A \end{pmatrix} = \begin{pmatrix} A & BA - AB \\ C & DA - CB \end{pmatrix},
$$

(35)

where $O$ denotes the $N \times N$ zero matrix. Since $A$ and $B$ commute with each other, the upper-right block vanishes. The determinant of the identity (35) yields

$$
\det [M] \det [A] = \det [A] \det [DA - CB].
$$

(36)

Since $\det [A] \neq 0$, we have

$$
\det [M] = \det [DA - CB].
$$

(37)

**Proposition 2.** Suppose there exists a solution of Eq. (1) and let $F : \mathbb{R}^N \rightarrow \mathbb{R}^N$ be Lipschitz continuous near the solution $x^*$ and $X$ and $Y$ be $N \times N$ real nonsingular matrices, then the iteration map (30) with $Y = X^{-1} J^{-1}$ and $0 < \Delta \tau < 1$ yields a series of vectors $x_n$ that converges to the solution $x^*$ from an arbitrary initial guess $x_0$ sufficiently close to the solution.
Proof. Let $\lambda_W$ be an eigenvalue of the matrix $W$. Then the following equation is satisfied:

$$\det [W - \lambda_W I] = \det [(1 - \lambda_W)(1 - 2\Delta\tau - \lambda_W)I + \Delta\tau^2 YJX] = 0, \quad (38)$$

where we use Lemma 3. Under the given condition $Y = X^{-1}J^{-1}$, Eq. (38) is reduced to

$$\det [W - \lambda_W I] = \det [(1 - \Delta\tau - \lambda_W)^2 I] = 0, \quad (39)$$

leading to $\lambda_W = 1 - \Delta\tau$. The iteration (30) hence converges to the solution $x = x^*$ and $p = 0$ as long as $0 < \Delta\tau < 1$, according to Lemma 2.

The proposition implies the local convergence of our formulation. Note that Eqs. (29) are combined into the following second-order differential equations:

$$\ddot{x} + 2\dot{x} + \dot{XX}^{-1}\dot{x} + XYF(x) = 0. \quad (40)$$

It is apparent then that the third term, which may be regarded as a part of the friction term, does not vanish unless the matrix $X$ is constant. It means that the “damping factor” is in general time-dependent, a key property for the local convergence in our formulation and completely different from the NR or DN method.

### 3.4. UDL decomposition

Next we discuss the choice of the preconditioners $X$ and $Y$. Although we have several options of the matrices $X$ and $Y$, we propose here one of the most useful decompositions.

**Definition 1.** Suppose the $N \times N$ Jacobian matrix is decomposed into $J := UDL$ where $U$, $D$ and $L$ are $N \times N$ upper triangular, diagonal and lower triangular matrices, respectively. In our formulation they are employed to give $X = L^{-1}$ and $Y = D^{-1}U^{-1}$.

Eqs. (29) then become the following:

$$x_{n+1} = x_n + \Delta\tau L_n^{-1}p_n, \quad (41a)$$

$$p_{n+1} = (1 - 2\Delta\tau)p_n - \Delta\tau D_n^{-1}U_n^{-1}F(x_n), \quad (41b)$$

where $L_n^{-1}$, $D_n^{-1}$ and $U_n^{-1}$ are the inverted matrices evaluated at $x_n$: e.g., $L_n^{-1} := L^{-1}(x_n)$. As mentioned in Sec. 3.3 the eigenvalue in the close vicinity of the solution is $1 - \Delta\tau$ to the first order.

### 4. Results

We show here the results of some applications of our new method, referred to as the W4 method, to some sample problems and comparisons of its performance with those of the NR and DN methods.

#### 4.1. Example 1

We will return to the very first problem for a single variable given in Eq. (2):

$$f(x) = \arctan(x) + \sin(x) - 1 = 0.$$ 

The iteration map for this problem in our W4 method is given as

$$x_{n+1} = x_n + \Delta\tau p_n, \quad (42a)$$

$$p_{n+1} = (1 - 2\Delta\tau)p_n - \Delta\tau \frac{\arctan(x_n) + \sin(x_n) - 1}{1 + x_n^2 + \cos(x_n)}, \quad (42b)$$

where $0 < \Delta\tau < 1$. In Table 2 we summarize the performance of the W4 method together with those for the NR and DN methods. Although the numbers of iteration steps are larger than those of the DN method, the W4 method successfully finds the solution where the other two methods fail. The inertia term or the second derivative term, which is absent in the NR or DN method, is supposed to be responsible for the “slower” convergence in our method. The case with $x_i = -2.5$ is an exceptional case, in which this effect is particularly remarkable. It is somewhat expected because Theorem 2 guarantees that there does not exist any permanent oscillation in the continuous time-evolution equation.
Table 2: The same as Table 1, but the performance of the W4 method is included. The convergence criterion is the same: \(|f(x)| < 10^{-6}\). The time interval is set as \(\Delta \tau = 0.5\) for the W4 method. The symbol \(\infty\) implies again that no solution is obtained within \(10^4\) iteration steps.

| Method | \(x_i\) | -3.0 | -2.5 | -2.0 | -1.5 | -1.0 | -0.5 | 0 | 0.5 | 1.0 | 1.5 | 2.0 | 2.5 | 3.0 |
|--------|--------|------|------|------|------|------|------|---|-----|-----|-----|-----|-----|-----|
| NR     | \(\infty\) | \(\infty\) | \(\infty\) | 4    | 5    | 4    | 3    | 2  | 4   | 8   | 4   | 3   |     |     |
| DN     | 25    | \(\infty\) | 41   | 20   | 20   | 19   | 15   | 18 | 19  | 17  | 19  | 18  |     |     |
| W4     | 1434  | 33   | 70   | 22   | 25   | 26   | 25   | 20 | 22  | 28  | 30  | 25  | 24  |     |

4.2. Example 2

Next, we consider the multi-variable problem given in Eqs. (5)

\[ F_1(x, y) = x^2 + y^2 - 4 = 0, \]
\[ F_2(x, y) = x^2y - 1 = 0. \]

The W4 method with the UDL decomposition discussed in Sec. 3.4 gives the following iteration map for this problem:

\[ x_{n+1} = x_n + \Delta \tau p_n, \quad \text{(44a)} \]
\[ y_{n+1} = y_n + \Delta \tau \left[ -\frac{2y_n}{x_n} p_n + q_n \right], \quad \text{(44b)} \]
\[ p_{n+1} = (1 - 2\Delta \tau) p_n - \Delta \tau \left[ \frac{x_n}{2(x_n^2 - 2y_n^2)} F_1 - \frac{y_n}{x_n(x_n^2 - 2y_n^2)} F_2 \right], \quad \text{(44c)} \]
\[ q_{n+1} = (1 - 2\Delta \tau) q_n - \frac{\Delta \tau}{x_n^2} F_2, \quad \text{(44d)} \]

in which \(\mathbf{x} = (x \ y)^T\) and \(\mathbf{p} = (p \ q)^T\).

In the left panel of Fig. 3 we display the initial-guess dependence of the W4 method with \(X = L^{-1}, Y = D^{-1}U^{-1}\) and \(\Delta \tau = 0.5\). Four colors (red, orange, green, blue) correspond to the four different solutions just as in Fig. 2. We first note that the local convergence is observed also for the W4 method, more or less in a similar way to the NR method as expected. What is most remarkable, however, is the fact that the
black region in Fig. 2, where the NR method fails to find a solution within 1000 iteration steps, disappears completely in our new method within the initial value space that we have explored. In the right panel of Fig. 3, we compare the sequences that the iteration maps of the two methods produce for the same initial conditions, \((x, y) = (1, 4)\) or \((2, -4)\). It is apparent that the NR method immediately finds the solution for the former whereas it fails to obtain a solution for the latter. In fact the sequence is oscillatory for the latter case and there is no hint of convergence at least up to 1000 iterations. The W4 method, on the other hand, always manages to find a solution although it takes more iterations to reach it, compared with the NR method when it does find a solution.

4.3. Example 3

The last problem is new and given by the following equations:

\[
F_1(x, y) = x^2 - y^2 - 4x + 6 = 0, \tag{45a}
\]

\[
F_2(x, y) = 2xy + 4y - 2 = 0, \tag{45b}
\]

which have actually two solutions at

\[
(x^*, y^*) \sim (-1.7505169, 4.0082886), \quad (-2.2244718, -4.4549031). \tag{46}
\]

The Jacobian for this problem is given as

\[
J = \begin{bmatrix}
2(x - 2) & -2y \\
2y & 2(x + 2)
\end{bmatrix}. \tag{47}
\]

(i) The iteration maps for the NR or DN method are written as

\[
x_{n+1} = x_n - \frac{\Delta \tau}{2(x_n^2 + y_n^2 - 4)} \left[ (x_n + 2) F_1 + y_n F_2 \right], \tag{48a}
\]

\[
y_{n+1} = y_n - \frac{\Delta \tau}{2(x_n^2 + y_n^2 - 4)} \left[ -y_n F_1 + (x_n - 2) F_2 \right], \tag{48b}
\]

where \(x\) and \(y\) are defined as \(\mathbf{x} = (x\ y)^T\).
(ii) In the W4 method with the UDL decomposition, we solve the following iteration maps for \( x = (x, y)^T \) and \( p = (p, q)^T \):

\[
\begin{align*}
x_{n+1} &= x_n + \Delta \tau p_n, & (49a) \\
y_{n+1} &= y_n + \Delta \tau \left[ \frac{y_n}{x_n + 2} p_n + q_n \right], & (49b) \\
p_{n+1} &= (1 - 2\Delta \tau) p_n - \frac{\Delta \tau (x_n + 2)}{2(x_n^2 + y_n^2 - 4)} \left[ F_1 + \frac{y_n}{x_n + 2} F_2 \right], & (49c) \\
q_{n+1} &= (1 - 2\Delta \tau) q_n - \frac{\Delta \tau}{2(x_n + 2)} F_2. & (49d)
\end{align*}
\]

In Fig. 4, we show the Newton basins for the iteration map (i) of the NR method (left) and for the iteration map (ii) of the W4 method with \( X = L^{-1}, Y = D^{-1}U^{-1} \) and \( \Delta \tau = 0.5 \) (right). The red and blue colors correspond to the initial conditions that converge to one of the solutions indicated with the black crosses while the black dots again imply that no solution is reached within 1000 iteration steps. It is found that for the NR method the blue or red region is clustered near the solution, to which it converges and whereas two colors appear rather randomly in the region between the two solutions. It is also evident that the NR method sometimes fails to find a solution whereas the W4 method always reaches one of the solutions. Which one is obtained is unpredictable.

4.4. Global convergence

In this section, we elucidate the difference between the NR method and the W4 method, using the following two-variable problem, which is somewhat similar to Example 2 in Sec. 4.2,

\[
F_1(x, y) = x^2 + xy^2 - 4 = 0, \tag{50a}
\]

\[
F_2(x, y) = x^2y - 1 = 0, \tag{50b}
\]

which has three solutions at

\[
(x^*, y^*) \sim (-2.0296789, 0.24274223), (1.9668697, 0.25849302), (0.65417501, 2.3367492). \tag{51}
\]

The Jacobian matrix for this system is given as

\[
J = \begin{bmatrix} 2x + y^2 & 2xy \\ 2xy & x^2 \end{bmatrix}. \tag{52}
\]

Note that this is a \( 2 \times 2 \) symmetric matrix and has two real eigenvalues \( \lambda_{\pm} \):

\[
\lambda_{\pm} = \frac{1}{2} \left( A \pm \sqrt{A^2 - 4B} \right), \tag{53}
\]

where we define \( A := \text{tr}J \) and \( B := \det J \). Then the corresponding eigenvectors are given as

\[
v_{\pm} = \begin{bmatrix} 2xy \\ a_{\pm} \end{bmatrix}, \quad a_{\pm} := \sqrt{4x^2y^2 + (\lambda_{\pm} - 2x - y^2)^2}. \tag{54}
\]

The iteration map for the DN method can be expressed in terms of these eigenvalues and eigenvectors as

\[
x_{n+1} = x_n - P_n \Lambda_n^{-1} P_n^{-1} F(x_n) \Delta \tau, \tag{55}
\]

where we introduce \( P_n = Q_n / \det(Q_n) \), \( Q_n := [v_n^+, v_n^-] \), and \( \Lambda_n^{-1} = \text{diag} \left[ \frac{1}{\lambda_n^+}, \frac{1}{\lambda_n^-} \right] \) for nonzero \( \lambda_n^- \) and \( \Lambda_n^{-1} = \text{diag} \left[ \frac{1}{\lambda_n^+}, 0 \right] \) for \( \lambda_n^- = 0 \). Note that the determinant of \( P_n \) is unity. On the other hand, the iteration map for the W4 method is given as

\[
\begin{align*}
x_{n+1} &= x_n + P_n p_n \Delta \tau, \tag{56a} \\
p_{n+1} &= (1 - 2\Delta \tau) p_n - \Lambda_n^{-1} P_n^{-1} F(x_n) \Delta \tau. \tag{56b}
\end{align*}
\]
Figure 5: Initial guess dependence by NR method (Upper-Left) and W4 method with $X = P, Y = \Lambda^{-1} P^{-1}$ and $\Delta \tau = 0.5$ (Upper-Right). The red, green, and blue correspond to all solutions of Eq. (50), while the black means the method cannot find any solution before 1000 iterations. Each solution is described by the black crosses. The white circles are initial guesses for the lower figures showing its evolutions by NR method (Lower-Left) and our new method (Lower-Right).

Note in particular that the eigenvalues and eigenvectors are defined pointwise and change for each iteration in general.

In the upper panels of Fig. 5 we exhibit the Newton basins for the NR (left) and the W4 (right) methods. The red, blue, and green colors correspond to the initial conditions that produce one of the three solutions indicated with the black crosses whereas the black points indicate that no solution is reached within 1000 iterations. It is clear that the W4 method always finds some solution in sharp contrast to the NR method, which sometimes fails to reach any of the solutions. In the lower panels of Fig. 5 we show the specific sequences starting from the white circles displayed in the upper panels. The NR method reaches a solution very quickly within 10 iterations normally whenever it is successful. This happens usually when the initial guess is close to the solution. On the other hand, the W4 method needs more iterations but always manages to find some solution. In the following, we investigate the possible cause of this difference more in detail, picking up the case for the initial guess $(x_i, y_i) = (0.1, -1.0)$.

We display in the upper panels of Fig. 6 three evolutions of $x$ (left) and $y$ (right) by the NR method, the DN method with $\Delta \tau = 0.5$, and the W4 method with $\Delta \tau = 0.5$. One can see that $(x_n, y_n)$ go to $(0, -\infty)$.
Figure 6: The evolutionary sequences of $x$ (upper left), $y$ (upper right), $|\lambda_+|$ (lower left) and $|\lambda_-|$ (lower right) generated by the iteration maps of the NR, DN and W4 methods. $\lambda_{\pm}$ are the maximum and minimum eigenvalues of the Jacobian matrix, respectively.

as $n \to \infty$ both for the NR method and DN methods. In the lower panels of Fig. 6, we draw the evolutions of absolute values of the maximum ($\lambda^+$, left) and minimum ($\lambda^-$, right) eigenvalues. It is evident that the ratio of $|\lambda^-/\lambda^+|$ tends to zero again both in the NR and the DN method. In what follows, we pay particular attention to this behavior of $\lambda^-/\lambda^+$ and analyze the situation when $|\lambda^-/\lambda^+|$ becomes quite small at $x \sim 0$.

**Lemma 4.** Suppose there exists a complete set of eigenvectors $v_n^{\pm} \in \mathbb{R}^2$ of the symmetric Jacobian matrix $J_n$ at the $n$-th iteration step and let $P_n$ be an $N \times N$ orthogonal matrix composed of $v_n^{\pm}$ and $\lambda_n^{\pm}$ be the corresponding eigenvalues, then the increment $x_{n+1} - x_n$ at this particular step tends to be aligned with $v_n^-$ if $|\lambda_n^-/\lambda_n^+| \to 0$ as $n \to \infty$.

**Proof.** The iteration map (55) with $\Delta \tau = 1$ gives the increment in $x$ at the $n$-th step in terms of the eigenvectors as

$$x_{n+1} - x_n = -P_n \Lambda_n^{-1} P_n^{-1} F(x_n) = -\frac{c_n^+}{\lambda_n} v_n^+ - \frac{c_n^-}{\lambda_n} v_n^- = \frac{\lambda_n^-}{\lambda_n} \frac{c_n^+}{\lambda_n} v_n^+ - \frac{c_n^-}{\lambda_n} v_n^- \to -\frac{c_n^-}{\lambda_n} v_n^-,$$

where we introduce the inner product $c_n^\pm := (v_n^\pm)^T F(x_n)$ and take the limit $|\lambda_n^-/\lambda_n^+| \to 0$. $\square$

This lemma explains the behavior of the sequences produced by the iteration map of the DN method. In fact, Taylor-expanding the eigenvalues and eigenvectors as well as the coefficients $c_n^\pm$ in the neighborhood of
Lemma 5. Suppose there exists a complete set of eigenvectors $\mathbf{v}_n^\pm \in \mathbb{R}^2$ of the symmetric Jacobian matrix $J_n$ also at the $(n-1)$-th step and let $P_n$ be an $N \times N$ orthogonal matrix composed of $\mathbf{v}_n^\pm$ and $\lambda_n^\pm$ be the corresponding eigenvalues, then in the iteration map of the W4 method with $\Delta \tau = 0.5$ the increment in $x$ is not aligned completely with $\mathbf{v}_n^-$ but depends also on $\mathbf{v}_n^+$ as $|\lambda_n^-/\lambda_n^*| \to 0$ if $\mathbf{v}_n^+ \neq \mathbf{v}_n^-$. 

Proof. From the iteration map (55) of the W4 method with $\Delta \tau = 0.5$, we can obtain 

$$x_{n+1} - x_n = \frac{1}{4} P_n \Lambda_{n-1}^{-1} P_n^{-1} \mathbf{F}(x_{n-1}) = \frac{1}{4} \lambda_{n-1}^{-1} c_n^+ \mathbf{v}_n^+ - \frac{1}{4} \lambda_{n-1}^{-1} c_n^- \mathbf{v}_n^- \to \frac{1}{4} \lambda_{n-1}^{-1} c_n^- \mathbf{v}_n^-.$$  

where $a^\pm$ are certain constants, the increment in $x_n$ can be rewritten as 

$$x_{n+1} - x_n = \frac{a^+ c_n^-}{4 \lambda_{n-1}} \mathbf{v}_n^+ - \frac{a^- c_n^-}{4 \lambda_{n-1}} \mathbf{v}_n^-,$$  

and hence includes the contribution from $\mathbf{v}_n^+$ unless $a^+$ is exactly zero, $a^+ = 0$.  

The important thing in the above lemma is that the degeneracy of the Jacobian matrix at a certain iteration step affects the direction of the sequence at the next step but $\mathbf{v}_n^+$ is the direction of crucial importance so that the sequence could get out of the vicinity of $x = 0$, in which the sequence of the DN method is trapped. 

Fig. 7 shows the specific evolutions of $x$ (left) and $y$ (right) for the iteration maps of the DN method with $\Delta \tau = 0.25$ and of the W4 method with $\Delta \tau = 0.5$, both starting from the same initial condition $(x,y) = (0.5, -1.0)$ and $(p,q) = (0,0)$. Note that $(x_1,y_1)$ at the first step in the DN method is identical to $(x_2,y_2)$ in the W4 method but the following evolutions are different from each other. In fact, $x_2$ in the DN method gets closer to $x = 0$ whereas $x_3$ in the W4 method is farther away, since the momentum gained in the previous steps prevents it from changing the direction of motion in the latter method.  

5. Conclusion

We have proposed a new iterative method, which we named the W4 method, to solve nonlinear systems of equations. In this paper, we have considered a couple of representative problems, for which the Newton-Raphson method, or the NR method, fails to find any one of the solutions and have applied the new method to them to see if any improvement is made. The results are summarized in Table 2 for the single-variable problems and in Fig. 2 and 3 for the multi-variable problems. 

Our findings are listed as follows:

$x = 0,$

$$\lambda^+ = y^2 + 2x + 4x^2 + \mathcal{O}(x^3), \quad \lambda^- = -3x^2 + \mathcal{O}(x^3),$$  

(58)

$$\mathbf{v}^+ = \left( -1 + \frac{2x^2}{y^2} + \mathcal{O}(x^3) \right) \left( -\frac{2x}{y} + \frac{4x^2}{y^2} + \mathcal{O}(x^3) \right)^T,$$  

(59)

$$\mathbf{v}^- = \left( \frac{2x}{y} - \frac{4x^2}{y^2} + \mathcal{O}(x^3) \right) \left( 1 + \frac{2x^2}{y^2} + \mathcal{O}(x^3) \right)^T,$$  

(60)

$$c^+ = 4 + \left(-y^2 + \frac{2}{y}\right) x + \mathcal{O}(x^2), \quad c^- = 1 - \frac{8x}{y} + \mathcal{O}(x^2),$$  

(61)

one realizes that once the sequence enters the region with $y < 0$, it heads to $x = 0$ and $y = -\infty$. This is also understood from the fact that $\mathbf{v}^+$ is the only way out of this region.
1. When the NR method or its modified version, the DN method, fails in these problems, their iteration maps produce sequences, which either diverge or oscillate as shown in Fig. 3.
2. The W4 method, which introduces the second time derivative term, can be hence regarded as an extension of the NR method as argued in Sec. 3.2 and Sec. 3.3.
3. The W4 method has the same local convergence as the NR method is well-known to possess, as demonstrated in Sec. 3.3.
4. In the W4 method the Newton basins that lead to no solution in the NR method are eliminated as exhibited in Figs. 2, 3 and 4. This strongly suggests that the W4 method has a global-convergence property in multi-variable problems.
5. In the W4 method, the convergence occurs only linearly just as in the DN method. The NR method, in contrast, has a quadratic convergence nature. This was discussed in Sec. 3.1 and Sec. 3.3.
6. The computational cost of the current version of the W4 method, which employs the UDL decomposition of the Jacobian matrix, is no higher than that of the NR method because of the decomposition into \( U, D \) and \( L \).

We believe that our new method, having the better global-convergence nature, should be very useful in many fields of science, particularly when the NR method fails to work more often than not.

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