Continuation Newton Method with the Trust-region Time-stepping Scheme

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Abstract For the problem of nonlinear equations, the homotopy methods (continuation methods) are popular in engineering fields since their convergence regions are large and they are fairly reliable to find a solution. The disadvantage of the classical homotopy methods is that their consumed time is heavy since they need to solve many auxiliary systems of nonlinear equations during the intermediate continuation processes. In order to overcome this shortcoming, we consider the special continuation method based on the Newton flow and follow its trajectory with the new time-stepping scheme based on the trust-region technique. Furthermore, we analyze the global convergence and local superlinear convergence of the new method. Finally, the promising numerical results of the new method for some real-world problems are also reported, with comparison to the traditional trust-region method (the built-in subroutine fsolve.m of the MATLAB environment [30,33] and the classical homotopy continuation methods (HOMPACK90 [47] and the built-in subroutines psolve.m for polynomial systems, GaussNewton.m for non-polynomial systems of the NAClab environment [49]).

Keywords Continuation Newton method · trust-region technique · nonlinear equations · homotopy continuation method · equilibrium problem

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1 Introduction

In engineering fields, we often need to solve the equilibrium state of the differential equation \[25,32,39,45,46\]
\[
\frac{dx}{dt} = F(x), \quad x(t_0) = x_0,
\]
which introduces the problem of nonlinear equations as follows:
\[
F(x) = 0,
\]
where \(F: \mathbb{R}^n \to \mathbb{R}^n\) is a vector function. For problem (2), there are some popular traditional optimization methods such as the trust-region methods \([6,10,24,31,35]\) and the classical homotopy continuation methods \([1,12,36,47]\).

For the traditional optimization methods, they obtain the numerical solution of nonlinear equations (2) via solving the following equivalent nonlinear least-square problem

\[
\min_{x \in \mathbb{R}^n} f(x) = \|F(x)\|^2,
\]
where \(\|\cdot\|\) denotes the Euclidean vector norm or its induced matrix norm. Generally speaking, the traditional optimization methods such as the trust-region methods and the line search methods are efficient for the large-scale problems since they have the local superlinear convergence near the optimal solution \(x^*\) \([6,35]\).

However, the line search methods and the trust-region methods are apt to stagnate at a local minimum point \(x^*\) of problem (3), when the Jacobian matrix \(J(x^*)\) of function \(F(x^*)\) is singular or nearly singular (see p. 304 in \([35]\)). Furthermore, the termination condition of line search methods and trust-region methods is given by
\[
\|\nabla f(x_k)\| = ||J(x_k)^T F(x_k)|| < \epsilon,
\]
which causes the algorithm to early stop far away from the local minimum \(x^*\) in some cases. For example, consider
\[
F(x) = Ax = 0, \quad A = \begin{bmatrix} 1 & 0 \\ 0 & 10^{-6} \end{bmatrix},
\]
which has a unique solution \(x^* = 0\). If we select the termination condition of problem (5) as equation (4) and set \(\epsilon = 10^{-6}\), they will cause the algorithm to early stop far away from \(x^*\) when \(x_k = (0, c), \ c < 10^6\).

For the classical homotopy methods, they obtain the solution of nonlinear equations (2) via constructing the following homotopy function
\[
H(x, t) = (1 - t)G(x) + tF(x),
\]
where the zero points of the auxiliary smooth function \(G(x)\) are known, and attempting to trace an implicitly defined curve \(\lambda(t) \in H^{-1}(0)\) from the starting point \((x_0, 0)\)
to a solution \((x^*, 1)\) by the predictor-corrector methods \([1, 12]\). Generally speaking, the homotopy continuation methods are fairly reliable to find a solution of nonlinear equations and they are very popular in engineering fields \([25]\). The disadvantage of the classical homotopy methods is that their consumed time is heavy since they need to solve many auxiliary systems of nonlinear equations during the intermediate continuation processes.

In order to overcome this shortcoming, in this article, we consider the special continuation method based on the following Newton flow \([3, 4, 7, 44]\)

\[
\frac{dx(t)}{dt} = -J(x)^{-1}F(x), \quad x(t_0) = x_0,
\]

where \(J(\cdot)\) is the Jacobian matrix of the function \(F(\cdot)\), i.e. \(J(x) = F'(x)\). Then, we construct a special ODE method based on the implicit Euler method to trace the trajectory of the Newton flow \([7]\). Finally, in order to improve its computational efficiency and ensure its global convergence, we devise a new time-stepping scheme based on the trust-region technique \([6, 19, 35]\).

The rest of this article is organized as follows. In the next section, we give a continuation Newton method with the new time-stepping scheme based on the trust-region technique for nonlinear equations \([4]\). In section 3, under the standard assumptions, we analyze the global convergence and the local superlinear convergence of the new method. In section 4, some promising numerical results of the new method are also reported, with comparison to the traditional optimization method (the built-in subroutine fsolve.m of the MATLAB environment \([30, 33]\)) and the classical homotopy continuation methods (HOMPACK90 \([47]\), and the built-in subroutines psolve.m and GaussNewton.m of Numerical Algebraic Computing Toolbox for MATLAB (NAClab) \([23, 49, 50]\)). Finally, some conclusions and the further work are discussed in section 5.

## 2 Continuation Newton method

In this section, based on the trust-region technique, we construct a new time-stepping scheme for the continuation Newton method to trace the trajectory of the Newton flow and obtain its equilibrium point \(x^*\).

### 2.1 The continuous Newton flow

If we consider the Newton method with the line search strategy for nonlinear equations \([22, 35]\), we have

\[
x_{k+1} = x_k - \Delta t_k J(x_k)^{-1} F(x_k).
\]

In equation (8), if we regard \(x_{k+1} = x(t_k + \Delta t_k), x_k = x(t_k)\) and let \(\Delta t_k \to 0\), we obtain the continuous Newton flow \([7]\). Actually, if we apply an iteration with the explicit
Euler method [15, 42] for the continuous Newton flow (7), we can also obtain the damped Newton method (8). Since the Jacobian matrix $J(x)$ may be singular, we reformulate the continuous Newton flow (7) as the following more general formula:

$$-J(x)\frac{dx(t)}{dt} = F(x), \quad x(t_0) = x_0. \quad (9)$$

The continuous Newton flow (9) is an old method and can be traced back to Davidenko's work [7] in 1953, after that it is investigated by Branin [4], Deuflhard et al. [9], Tanabe [44] and Kalaba et al. [20] in 1970s, and Axelsson and Sysala [3]. The reason of the sustained research interest for this method is that it has some nice properties. We describe them as the following property 1.

**Property 1** (Branin [4] and Tanabe [44]) Assume that $x(t)$ is the solution of the continuous Newton flow (9), then the energy function $f(x(t)) = \|F(x)\|^2$ converges to zero as $t$ tends to infinity. Namely, for every limit point $x^*$ of $x(t)$, it is also the solution of nonlinear equations (2). Furthermore, $F(x)$ has the linear convergence rate $e^{-t}$. If its Jacobian matrix $J(x)$ is nonsingular, $x(t)$ can not converge to its equilibrium $x^*$ on finite interval.

**Proof.** Assume that $x(t)$ is the solution of the continuous Newton flow (9), then we have

$$\frac{d}{dt} (e^t F(x)) = e^t J(x) \frac{dx(t)}{dt} + e^t F(x) = 0,$$

which gives

$$F(x) = F(x_0) e^{-t}. \quad (10)$$

From equation (10), it is not difficult to know that $F(x(t))$ converges to zero with linear convergence rate $e^{-t}$ when $t$ tends to infinity. Thus, if the solution $x(t)$ of the continuous Newton flow (9) falls in a compact set, it converges to a limit point $x^*$ when $t$ tends to infinity, and this limit point $x^*$ is also a solution of nonlinear equations (2).

Furthermore, if the Jacobian matrix $J(x)$ is nonsingular, the ordinary differential equation (ODE) (9) is equivalent to the continuous Newton flow (7). Thus, from the dynamical property of the ODE, it is not difficult to know that the ODE (7) has a unique solution $x(t)$ and it can not converge to its equilibrium $x^*$ on finite interval (pp. 79-82, [38]).

The inverse matrix $J(x)^{-1}$ can be regarded as the preconditioner of $F(x)$ such that the solution elements $x_i(t) (i = 1, 2, \ldots, n)$ of the Newton flow (7) have the roughly same convergence rates and it mitigates the stiff property of the ODE (7) (on the definition of the stiff problem, one can refer to the ODE textbooks [16, 48]). This property is very useful since it makes us adopt the explicit ODE method to follow the trajectory of the Newton flow. We show it as follows.
Actually, if we consider the linear case $F(x) = Ax$ of the ODE (9), we have
\[
\frac{dx}{dt} = -Ax, \quad x(0) = x_0.
\] (11)

Integrating the linear ODE (11), we obtain
\[
x(t) = e^{-t}x_0.
\] (12)
From equation (12), we know that the solution $x(t)$ of the ODE (11) linearly converges to zero with the same rate $e^{-t}$ when $t$ tends to infinity.

2.2 The continuation Newton method

From subsection 2.1, we know that the continuous Newton flow (9) has the nice global convergence property. On the other hand, when the Jacobian matrix $J(x)$ is singular or nearly singular, the ODE (9) is the system of differential-algebraic equations and its trajectory is not efficiently followed by the general ODE method such as the backward differentiation formulas (the built-in subroutine bdf15s.m of the MATLAB environment [2,16,30,42]). Thus, we need to construct the special method to handle this problem and we expect that the new method has the same global convergence as the homotopy continuation methods and the fast convergence near the solution $x^*$ as the traditional optimization methods. In order to attain these two aims, we consider the continuation Newton method and construct a new time-stepping scheme based on the trust-region technique for problem (9).

Firstly, we apply the implicit Euler method to the continuous Newton flow (9) [2,5], then we obtain
\[
J(x_{k+1}) \frac{x_{k+1} - x_k}{\Delta t_k} = -F(x_{k+1}).
\] (13)
The scheme (13) is an implicit method and it needs to solve a system of nonlinear equations at every iteration. To avoid solving the system of nonlinear equations, we replace $J(x_{k+1})$ with $J(x_k)$ and $F(x_{k+1})$ with $F(x_k) + J(x_k)s_k$ in equation (13). Thus, we obtain its explicit continuation Newton method as follows:
\[
J(x_k)s_k = -\frac{\Delta t_k}{1 + \Delta t_k}F(x_k),
\] (14)
\[
x_{k+1} = x_k + s_k.
\] (15)
The continuation Newton method (14)-(15) is similar to the damped Newton method (8) if we regard $\Delta t_k/(1 + \Delta t_k)$ in equation (14) as $\Delta t_k$ in equation (8). However, from the view of the ODE method, they are very different. The damped Newton method (8) is obtained by the explicit Euler scheme applied to the continuous Newton flow (9), and its time-stepping size $\Delta t_k$ is restricted by the numerical stability [16,42,48]. Namely, the large time-stepping size $\Delta t_k$ can not be adopted in the steady-state phase. The continuation Newton method (14)-(15) is obtained by the semi-implicit
Euler method applied to the continuous Newton flow (9), and its time-stepping size $\Delta t_k$ is not restricted by the numerical stability. Therefore, the large time-stepping size can be adopted in the steady-state phase, the continuation Newton method (14)-(15) of which mimics the Newton method and is expected to have the fast convergence rate. The most of all, the continuation Newton method (14)-(15) is favourable to adopt the trust-region technique to accurately follow the trajectory of the continuous Newton flow in the transient-state phase and to maintain its fast convergence rate near the the equilibrium point $x^\ast$.

For some practical problems, the Jacobian matrix $J(x)$ may be singular, which arises from the physical property of the problem. For example, for the chemical kinetic reaction problem (1), the elements of $x(t)$ represent the reaction concentrations and they must satisfy the linear conservation law (26). A system is called to satisfy the linear conservation law (40, or p. 35, 42), if there is a constant vector $c \neq 0$ such that

$$c^T x(t) = c^T x(0) \text{ for all } t \geq 0$$

(16)

is satisfied. If there exists a constant vector $c$ such that

$$c^T F(x) = 0, \text{ for all } x \in \mathbb{R}^n$$

(17)

is satisfied, we have

$$c^T J(x) = 0, \text{ for all } x \in \mathbb{R}^n.$$  

(18)

From equation (18), we know that the Jacobian matrix $J(x)$ is singular. For this case, the solution $x(t)$ of the ODE (1) satisfies the linear conservation law (16).

For the singularity of the Jacobian matrix $J(x)$, there are some efficient approaches [14] to handle this problem. Here, we only simply adopt the regularization technique [17,21] to modify the continuation Newton method (14)-(15) as follows:

$$\langle \mu_k I - J(x_k) \rangle s_k = F(x_k),$$

(19)

$$s_k = \frac{\Delta t_k}{1 + \Delta t_k} s_k,$$

(20)

$$x_{k+1} = x_k + s_k,$$

(21)

where $\mu_k$ is a small positive number. In order to achieve the fast convergence rate near the solution $x^\ast$, the regularization continuation Newton method (19)-(21) is required to approximate the Newton method $x_{k+1} = x_k - J(x_k)^{-1} F(x_k)$ near the solution $x^\ast$ [11]. Thus, we select the regularization parameter $\mu_k$ as follows:

$$\mu_k = \begin{cases} c_\varepsilon, & \text{if } \Delta t_k \leq 1/c_\varepsilon, \\ 1/\Delta t_k, & \text{others}, \end{cases}$$

(22)

where $c_\varepsilon$ is a small positive constant such as $c_\varepsilon = 10^{-6}$ in practice.

It is not difficult to verify that the regularization continuation Newton method (19)-(21) satisfies the linear conservation law (16) when it exists a constant $c$ to satisfy
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\[ c^T F(x) = 0 \] for all \( x \in \mathbb{R}^n \). Actually, from \( c^T F(x) = 0 \), we have \( c^T J(x) = 0 \). Therefore, from equations (19)-(21), we obtain

\[
\begin{align*}
    c^T x_{k+1} &= c^T x_k + c^T s_k = c^T x_k + \frac{1}{\mu_k} c^T (\mu s_k) \\
    &= c^T x_k + \frac{1}{\mu_k} c^T \left( \frac{\Delta t_k}{1 + \Delta t_k} F(x_k) + J(x_k) s_k \right) \\
    &= c^T x_k = \cdots = c^T x_0.
\end{align*}
\] (23)

Namely, the regularization continuation Newton method (19)-(21) preserves the linear conservation law (16).

### 2.3 The trust-region time-stepping scheme

Another issue is how to adaptively adjust the time-stepping size \( \Delta t_k \) at every iteration. A popular way to control the time-stepping size is based on trust-region technique [6,8,19,29]. For the trust-region time-stepping scheme, it needs to construct an approximation model of the merit function. Here, we adopt the residual \( \|F(x_k)\| \) as the merit function and use \( \|F(x_k) + J(x_k)(x_{k+1} - x_k)\| \) as the approximation model of \( \|F(x_{k+1})\| \). Thus, according to the following ratio:

\[
\rho_k = \frac{\|F(x_k)\| - \|F(x_{k+1})\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)(x_{k+1} - x_k)\|},
\] (24)

we enlarge or reduce the time-stepping size \( \Delta t_k \) at every iteration. A particular adjustment strategy is given as follows:

\[
\Delta t_{k+1} = \begin{cases} 
    \gamma_1 \Delta t_k, & \text{if } |1 - \rho_k| \leq \eta_1, \\
    \Delta t_k, & \text{if } \eta_1 < |1 - \rho_k| < \eta_2, \\
    \gamma_2 \Delta t_k, & \text{if } |1 - \rho_k| \geq \eta_2,
\end{cases}
\] (25)

where the constants are selected as \( \gamma_1 = 2, \gamma_2 = 0.5, \eta_1 = 0.25, \eta_2 = 0.75 \) according to the numerical experiments.

According to the above discussions, we give the detailed implementation of the continuation Newton method with the trust-region time-stepping scheme for nonlinear equations in Algorithm [1]

### 3 Convergence analysis

In this section, we discuss some theoretical properties of Algorithm [1]. Firstly, we estimate the lower bound of the predicted reduction \( \|F(x_k)\| - \|F(x_k) + J(x_k)(x_{k+1} - x_k)\| \), which is similar to the estimation result of the trust-region method for the unconstrained optimization problem [37].
Algorithm 1 Continuation Newton Method with the Trust-region Time-stepping Scheme (The CNMTr method)

Input:
the nonlinear function: $F(x)$;
the initial point: $x_0$ (optional);
the terminated parameter: $\varepsilon$ (optional).

Output:
the approximation solution $x^*$ of nonlinear equations.

1: If the called function does not provide $x_0$ and $\varepsilon$, we set $x_0 = [1, 1, \ldots, 1]^T$ and $\varepsilon = 10^{-6}$, respectively.
2: Initialize the parameters: $\eta = 10^{-6}, \eta_1 = 0.25, \gamma_1 = 2, \eta_2 = 0.75, \gamma_2 = 0.5$.
3: Compute $F(x_0)$ and the Jacobian matrix $J(x_0)$. Select the initial time-stepping size as

$$\Delta t_0 = \min \left\{ 0.01, \frac{1}{\|F(x_0)\|} \right\}$$

Compute the residual $Res_0 = \|F(x_0)\|$.
4: while $Res_k \geq \varepsilon$ do
5: Solve the linear system of equations (19)-(20) to obtain the trial step $s_k$.
6: Set $x_{k+1} = x_k + s_k$.
7: Evaluate $F(x_{k+1})$.
8: Compute the residual $Res_{k+1} = \|F(x_{k+1})\|$.
9: if $\|F(x_k)\| < \|F(x_k) + J(x_k)s_k\|$ then
10: $\rho_k = -1$;
11: else
12: Compute the ratio $\rho_k$ from equation (23).
13: end if
14: Adjust the time-stepping size $\Delta t_{k+1}$ based on the trust-region scheme (25).
15: if $\rho_k \geq \eta$ then
16: Accept the trial step $s_k$. Set $x_k = x_{k+1}, \Delta t_k = \Delta t_{k+1}$ and $Res_k = Res_{k+1}$. Evaluate the Jacobian matrix $J(x_k)$.
17: else
18: Set $\Delta t_k = \Delta t_{k+1}$.
19: end if
20: Set $k \leftarrow k + 1$.
21: end while

Lemma 1 Assume that the Jacobian matrix $J(x_k)$ of the function $F(x_k)$ is nonsingular. Namely, it exists a positive constant $m$ such that

$$\|J(x_k)y\| \geq m\|y\|, \forall y \in \mathbb{R}^n, k = 0, 1, 2, \ldots,$$  (26)

are satisfied. If $s_k$ is the solution of the regularization continuation Newton method (19)-(21), when the regularization parameter $\mu_k$ defined by equation (22) and the constant $c_\varepsilon$ satisfy $\mu_k \leq c_\varepsilon < 0.5m$, we have

$$\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\| \geq c_r \frac{\Delta t_k}{1 + \Delta t_k} \|F(x_k)\|,$$  (27)

where the constant $c_r$ satisfies $0 < c_r < 1$. 
Proof. From equations (19)-(20), we have

\[-J(x_k)s_k + \mu_k s_k = F(x_k) \frac{\Delta t_k}{1 + \Delta t_k},\]

which gives

\[\|J(x_k)s_k + F(x_k)\| = \left\| \mu_k s_k + \frac{1}{1 + \Delta t_k} F(x_k) \right\| \]
\[= \left\| \mu_k \frac{\Delta t_k}{1 + \Delta t_k} (-J(x_k) + \mu_k I)^{-1} F(x_k) + \frac{1}{1 + \Delta t_k} F(x_k) \right\| \]
\[\leq \frac{1}{1 + \Delta t_k} \left( \Delta t_k \left\| (-\frac{1}{\mu_k} J(x_k) + I)^{-1} \right\| + 1 \right\| F(x_k)\|. \quad (28)\]

According to the definition of the induced matrix norm [13], we have

\[\left\| (-\frac{1}{\mu_k} J(x_k) + I)^{-1} \right\| = \max_{\|y\| = 1} \left\| (-\frac{1}{\mu_k} J(x_k) + I)^{-1} y \right\| \]
\[= \max_{\|y\| = 1} \left\| (-\frac{1}{\mu_k} J(x_k) + I)^{-1} y \right\| \]
\[= \frac{1}{\min_{\|y\| = 1} \left\| (-\frac{1}{\mu_k} J(x_k) + I)^{-1} y \right\|} \quad (29)\]

On the other hand, when \(\|y\| = 1\), from the nonsingular assumption [20] of the Jacobian matrix \(J(x_k)\), we have

\[\left\| (-\frac{1}{\mu_k} J(x_k) + I) y \right\| = \left\| -\frac{1}{\mu_k} J(x_k) y + y \right\| \]
\[\geq \frac{1}{\mu_k} \|J(x_k)y\| - \|y\| \geq \frac{1}{\mu_k} (m - 1). \quad (30)\]

Thus, from the definition [22] of the parameter \(\mu_k\) and equations [29]-[30], if we select the parameter \(c_e < 0.5m\), we have

\[\left\| (-\frac{1}{\mu_k} J(x_k) + I)^{-1} \right\| \leq \frac{\mu_k}{m - \mu_k} \leq \frac{c_e}{m - c_e}. \quad (31)\]

Therefore, if we replace equation [31] into equation [28], we have

\[\|J(x_k)s_k + F(x_k)\| \leq \frac{1}{1 + \Delta t_k} \left( 1 + \frac{c_e}{m - c_e} \Delta t_k \right) \|F(x_k)\|, \]

which gives

\[\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\| \geq \left( \frac{m - 2c_e}{m - c_e} \right) \frac{\Delta t_k}{1 + \Delta t_k} \|F(x_k)\|. \quad (32)\]

Thus, if we select the constant \(c_e = (m - 2c_e)/(m - c_e)\), from equation [32], we obtain equation [27]. \(\Box\)

In order to prove that the sequence \(\{\|F(x_k)\|\}\) converges to zero when \(k\) tends to infinity, we also use the following result about the lower bound estimation of the time-stepping size \(\Delta t_k\).
Lemma 2 Assume that the function $F : \mathbb{R}^n \to \mathbb{R}^m$ is continuously differentiable and its Jacobian matrix $J(x)$ satisfies the Lipschitz continuity. Namely, it exists a positive number $L$ such that

$$
\|J(x) - J(y)\| \leq L \|x - y\|, \ \forall x, y \in \mathbb{R}^n,
$$

are satisfied. Furthermore, we assume that the nonsingular condition (26) of the Jacobian matrix $J(x_k)$ is satisfied. If the sequence $\{x_k\}$ is generated by Algorithm 1 when the regularization parameter $\mu_k$ defined by equation (22) and the constant $c_\mu \leq c_\epsilon < 0.5m$, it exists a positive number $\delta_{\Delta t}$ such that

$$
\Delta t_k \geq \delta_{\Delta t} > 0, \ k = 1, 2, \ldots
$$

are satisfied, where $\Delta t_k$ is adaptively adjusted by formulas (24)-(25).

Proof. According to the Lipschitz continuity assumption (33) of the Jacobian matrix $J(x)$, we have

$$
\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\| = \left\| \int_0^1 J(x_k + ts_k)s_k dt - J(x_k)s_k \right\|
$$

$$
= \left\| \int_0^1 (J(x_k + ts_k) - J(x_k))s_k dt \right\| \leq \int_0^1 \| (J(x_k + ts_k) - J(x_k))s_k \| dt
$$

$$
\leq \int_0^1 \| J(x_k + ts_k) - J(x_k) \| \| s_k \| dt \leq \int_0^1 L \| s_k \|^2 dt = \frac{1}{2} L \| s_k \|^2. \tag{35}
$$

On the other hand, from equations (19)-(20), we have

$$
\| s_k \| = \frac{\Delta t_k}{1 + \Delta t_k} \left\| (-J(x_k) + \mu_k I)^{-1} F(x_k) \right\|
$$

$$
\leq \frac{\Delta t_k}{1 + \Delta t_k} \left\| (-J(x_k) + \mu_k I)^{-1} \right\| \| F(x_k) \|. \tag{36}
$$

Similar to the estimation of inequality (31), from the definition (22) of the parameter $\mu_k$ and the nonsingular assumption (26) of the Jacobian matrix $J(x_k)$, we have

$$
\left\| (-J(x_k) + \mu_k I)^{-1} \right\| \leq \frac{1}{m - \mu_k} \leq \frac{1}{m - c_\mu}. \tag{37}
$$

Thus, from equations (35)-(37), we obtain

$$
\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\| \leq \frac{1}{2} \frac{L}{(m - c_\mu)^2} \left( \frac{\Delta t_k}{1 + \Delta t_k} \right)^2 \| F(x_k) \|^2. \tag{38}
$$

Therefore, from the definition (24) the ratio $\rho_k$, equation (32) of Lemma 1 and equation (38), we have

$$
|\rho_k - 1| = \frac{\|F(x_k)\| - \|F(x_{k+1})\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} - 1 = \frac{\|F(x_{k+1})\| - \|F(x_k) + J(x_k)s_k\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} - 1
$$

$$
\leq \frac{\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} \leq \frac{1}{2} \frac{L}{(m - 2c_\mu)^2} \left( \frac{\Delta t_k}{1 + \Delta t_k} \right) \| F(x_k) \|. \tag{39}
$$
Furthermore, according to Algorithm 1, we know that \( \| F(x_k) \| \) is monotonically decreasing, which gives \( \| F(x_k) \| \leq \| F(x_0) \|, \quad k = 1, 2, \ldots \). We select the constant \( \delta_{\Delta t} \) as

\[
\delta_{\Delta t} = \frac{2(m - 2c_\epsilon)^2}{\| F(x_0) \| L} \eta_1. \tag{40}
\]

If we assume that \( K \) is the first index such that \( \Delta t_k \leq \delta_{\Delta t} \), from equations (39)-(40), we know that \( | \rho_{k} - 1 | < \eta_1 \). Consequently, \( \Delta t_{k+1} \) will be enlarged according to the time-stepping scheme (25). Therefore, if we select \( \delta_{\Delta t} = \min \{ \Delta t_k, \delta_{\Delta t} \} \), we know that \( \Delta t_k \geq \delta_{\Delta t} \) for all \( k = 0, 1, 2, \ldots \). \( \square \)

Now, using the analysis results of Lemma 1 and Lemma 2, we know that the sequence \( \{ \| F(x_k) \| \} \) converges to zero when \( k \) tends to infinity. We state it as the following theorem.

**Theorem 1** Assume that the function \( F : \mathbb{R}^n \rightarrow \mathbb{R}^n \) is continuously differentiable and its Jacobian matrix \( J(x) \) satisfies the Lipschitz continuity (33) and the nonsingular assumption (26). If the sequence \( \{ x_k \} \) is generated by Algorithm 1 when the regularization parameter \( \mu_k \) defined by equation (22) and the constant \( c_\epsilon \) satisfy \( \mu_k \leq c_\epsilon < 0.5m \), we have

\[
\lim_{k \to \infty} \inf \| F(x_k) \| = 0. \tag{41}
\]

**Proof.** According to Algorithm 1, we know that it exists an infinite subsequence \( \{ x_{k_l} \} \) to satisfy

\[
\frac{\| F(x_{k_l}) \| - \| F(x_{k_l+1}) \|}{\| F(x_{k_l}) \| - \| F(x_{k_l}) + J(x_{k_l})s_{k_l} \|} \geq \eta_{\alpha}. \tag{42}
\]

Using the result of Lemma 1, i.e. equation (27), from equation (42), we have

\[
\| F(x_{k_l}) \| - \| F(x_{k_l+1}) \| \geq \eta_{\alpha} c_r \frac{\Delta t_{k_l}}{1 + \Delta t_{k_l}} \| F(x_{k_l}) \|,
\]

which gives

\[
\| F(x_{k_l+1}) \| \leq \left( 1 - \eta_{\alpha} c_r \frac{\Delta t_{k_l}}{1 + \Delta t_{k_l}} \right) \| F(x_{k_l}) \| \leq \left( 1 - \eta_{\alpha} c_r \frac{\delta_{\Delta t}}{1 + \delta_{\Delta t}} \right) \| F(x_{k_l}) \|. \tag{43}
\]

In the second inequality of the above estimation (43), we use the result of Lemma 2, i.e. \( \Delta t_k \geq \delta_{\Delta t} \) for all \( k = 0, 1, 2, \ldots \). From equation (43), we obtain

\[
\lim_{k_l \to \infty} \| F(x_{k_l}) \| = 0,
\]

which proves the result of equation (41). \( \square \)

Under the nonsingular assumption (26) of the Jacobian matrix \( J(x^*) \), where \( x^* \) is the solution of nonlinear equations (2), we analyze the local superlinear convergence of Algorithm 1 as follows.
Theorem 2 Assume that the function $F : \mathbb{R}^n \to \mathbb{R}^n$ is continuously differentiable and it has a zero point $x^*$. Furthermore, we assume that the Jacobian matrix $J(x)$ satisfies the Lipschitz continuity (33) and the Jacobian matrix $J(x^*)$ is nonsingular. If the sequence $\{x_k\}$ is generated by Algorithm [7] when the regularization parameter $\mu_k$ defined by equation (22) and the constant $c_k$ satisfy $\mu_k \leq c_k < 0.5m$, it exists a neighborhood of $x^*$ with a radius $r > 0$ such that the sequence $\{x_k\}$ converges superlinearly to $x^*$ when the initial point belongs to the set $B_r(x^*)$, where the closed ball $B_r(x^*)$ is defined by

$$B_r(x^*) = \{x : \|x - x^*\| \leq r\}.$$  \hfill (44)

Proof. Firstly, we prove that the sequence $\{x_k\}$ linearly converges to $x^*$ when the initial point $x_0$ sufficiently nears $x^*$. Then, we prove that the time-stepping size $\Delta t_k$ tends to infinity. Finally, we prove that the search step $s_k$ approximates the Newton step $s_k^N$ and the sequence $\{x_k\}$ superlinearly converges to $x^*$.

According to the nonsingular and continuous assumption of the Jacobian matrix $J(x^*)$, it exists a constant $m$ and a neighborhood of $x^*$ with a radius $r_1$ such that

$$\|J(x)y\| \geq m\|y\|, \forall y \in \mathbb{R}^n,$$  \hfill (45)

is satisfied when $x \in B_{r_1}(x^*)$, where $B_{r_1}(x^*)$ is defined by equation (44). Similar to the proof of inequality (31), from the definition (22) of the parameter $\mu_k$, we have

$$\|\mu_k I - J(x_k)\|^{-1} \leq \frac{1}{m - c_k}, \forall x_k \in B_{r_1}(x^*), k = 0, 1, 2, \ldots.$$  \hfill (46)

Thus, if we denote $e_k = x_k - x^*$, from equations (19)-(20), we have

$$e_{k+1} = e_k + s_k = e_k + \frac{\Delta t_k}{1 + \Delta t_k} (\mu_k I - J(x_k))^{-1} F(x_k)$$

$$= e_k + \frac{\Delta t_k}{1 + \Delta t_k} (\mu_k I - J(x_k))^{-1} \int_0^1 J(x^* + t e_k) e_k dt$$

$$= \frac{1}{1 + \Delta t_k} e_k + \frac{\Delta t_k}{1 + \Delta t_k} (\mu_k I - J(x_k))^{-1} \int_0^1 (J(x^* + t e_k) - J(x_k)) e_k dt.$$  \hfill (47)

From the Lipschitz continuous assumption (33) of the Jacobian matrix $J(x)$, inequalities (46)-(47) and the definition (22) of the parameter $\mu_k$, we have

$$\|e_{k+1}\| \leq \frac{1}{1 + \Delta t_k} \|e_k\|$$

$$+ \frac{\Delta t_k}{1 + \Delta t_k} \|\mu_k I - J(x_k)\|^{-1} \left\| \int_0^1 (\|J(x^* + t e_k) - J(x_k)\| + \mu_k) e_k dt \right\|$$

$$\leq \frac{1}{1 + \Delta t_k} \|e_k\| + \frac{\Delta t_k}{1 + \Delta t_k} \left( \mu_k + \frac{1}{2} L \|e_k\| \right) \frac{1}{m - c_k} \|e_k\|$$

$$= \frac{1 + \frac{1}{m - c_k} \left( \mu_k + \frac{1}{2} L \|e_k\| \right) \Delta t_k}{1 + \Delta t_k} \|e_k\| \leq \frac{1 + \frac{1}{m - c_k} \left( c_k + \frac{1}{2} L \|e_k\| \right) \Delta t_k}{1 + \Delta t_k} \|e_k\|.$$  \hfill (48)
We denote
\[ q_k = \frac{1 + \frac{1}{m-\epsilon} \left( \epsilon + \frac{1}{2} L \| e_k \| \right) \Delta t_k}{1 + \Delta t_k}, \] (49)
and select \( x_0 \in B_{r_1}(x^*) \) to satisfy
\[ \| e_0 \| < \frac{m - 2c_\epsilon}{L}. \] (50)
Thus, if we select \( r = \min \{ r_1, (m - 2c_\epsilon)/L \} \), when \( x_0 \in B_r(x^*) \), from equations (48)-(50) and the assumption \( c_\epsilon < 0.5m \), by the mathematical induction, we have
\[ \| e_{k+1} \| \leq q_k \| e_k \|, \quad q_k < \frac{1 + \frac{m}{2(m-\epsilon)} \delta_M}{1 + \delta_M} < 1. \] (51)

It is not difficult to know that the function \( f(t) = \frac{(1 + \alpha t)}{(1 + t)} \) is monotonically decreasing when \( 0 \leq \alpha < 1 \). Thus, from the result (34) of Lemma 2 and equation (51), we obtain
\[ \| e_{k+1} \| \leq \left( q_{\delta_M} \right)^{k} \| e_0 \| \rightarrow 0, \text{ when } k \rightarrow \infty. \] (52)
Namely, we have \( \lim_{k \rightarrow \infty} x_k = x^* \).

On the other hand, from equations (19)-(20) and equation (46), we have
\[ \| s_k \| = \frac{\Delta t_k}{1 + \Delta t_k} \left\| \left( -J(x) + \mu_k I \right)^{-1} F(x_k) \right\| \]
\[ \leq \frac{\Delta t_k}{1 + \Delta t_k} \left\| \left( -J(x) + \mu_k I \right)^{-1} \right\| \| F(x_k) \| \leq \frac{1}{m-\epsilon} \frac{\Delta t_k}{1 + \Delta t_k} \| F(x_k) \|. \] (53)

Similar to the proof of equation (39), from the definition (24) of the ratio \( \rho_k \), equations (32) and (53), we have
\[ |\rho_k - 1| = \left| \frac{\| F(x_k) \| - \| F(x_{k+1}) \|}{\| F(x_k) \| - \| F(x_k) + J(x_k) s_k \|} - 1 \right| \]
\[ \leq \frac{1}{2} \left( \frac{L}{m-2c_\epsilon} \right)^2 \left( \frac{\Delta t_k}{1 + \Delta t_k} \right) \| F(x_k) \| \leq \frac{1}{2} \left( \frac{L}{m-2c_\epsilon} \right)^2 \| F(x_k) \|. \] (54)

Since \( \lim_{k \rightarrow \infty} x_k = x^* \) and \( F(x^*) = 0 \), we can select a sufficiently large number \( K_F \) such that
\[ \| F(x_k) \| \leq \frac{2\eta_1 (m - 2c_\epsilon)^2}{L}, \forall k \geq K_F, \] (55)
is satisfied. From equations (54)-(55), we have
\[ |\rho_k - 1| \leq \eta_1, \] for all \( k \geq K_F, \)
which means \( \Delta t_k \) will be enlarged every iteration after \( k \geq K_F \) according to the time-stepping scheme (25). Namely, we have
\[ \lim_{k \to \infty} \Delta t_k = \infty. \] (56)

From the definition (22) of the regularization parameter \( \mu_k \) and \( \lim_{k \to \infty} \Delta t_k = \infty \), we know that \( \mu_k = 1/\Delta t_k \) when \( k \geq K_\mu \), where we select the sufficient index \( K_\mu \) such that \( 1/\Delta t_k < \epsilon \epsilon \) when \( k \geq K_\mu \). Thus, from equation (48), when \( k \geq K_\mu \), we have
\[ \|e_{k+1}\| \leq \frac{1 + \frac{1}{m-1} (\mu_k + \frac{1}{2}L\|e_k\|) \Delta t_k}{1 + \Delta t_k} \]
\[ = \frac{1}{1 + \Delta t_k} + \frac{1}{m-1/\Delta t_k} \left( \frac{1}{\Delta t_k} + \frac{1}{2}L\|e_k\| \right) \frac{\Delta t_k}{1 + \Delta t_k} \to 0, \]
where we use the properties \( \lim_{k \to \infty} \|e_k\| = 0 \) and \( \lim_{k \to \infty} \Delta t_k = \infty \). Namely, the sequence \( \{x_k\} \) superlinearly converges to \( x^* \).

For some practical problems, the singularity of the Jacobian matrix \( J(x) \) is introduced by the linear conservation law such as the conservation of mass or the conservation of charge [28,40,41,42]. In the rest of this section, we analyze convergence properties of Algorithm 1 for the singular case of the Jacobian matrix \( J(x) \). Similar to the standard assumption of the nonlinear dynamical system, we assume that the Jacobian matrix \( J(x) \) satisfies the one-sided Lipschitz condition (see p. 303, [8] or p. 180, [16]) as follows:
\[ y^T J(x)y \leq -v\|y\|^2, \] for \( y \in S_c = \{y|c^Ty = 0\} \), \( v > 0 \), (57)
where the constant vector \( c \) satisfies \( c^TF(x) = 0 \) for all \( x \in \mathbb{R}^n \), which leads to \( c^TJ(x) = 0 \) for all \( x \in \mathbb{R}^n \). The positive number \( v \) is called the one-sided Lipschitz constant. Under the assumption of the one-sided Lipschitz condition (57), we know that the matrix \( (\mu I - J(x)) \) is nonsingular when \( \mu > 0 \). We restate it as the following property.

**Property 2** Assume that the Jacobian matrix \( J(x) \) satisfies the one-sided Lipschitz condition (57) in the vertical space of vector \( c \). Then, the matrix \( (\mu I - J(x)) \) is nonsingular when \( \mu > 0 \) and the solution \( s_k \) of equations (19)-(20) belongs to the vertical space of vector \( c \).

**Proof.** If the matrix \( (\mu I - J(x)) \) is singular, it exists a nonzero vector \( y \) such that
\[ (\mu I - J(x))y = 0 \] (58)
is satisfied. Thus, from (58), we have
\[ \mu c^Ty = \frac{1}{\mu} c^T J(x)y = \frac{1}{\mu} (c^T J(x))y = 0. \]


Namely, the vector \( y \) belongs to the vertical space of vector \( c \). Therefore, from the one-sided Lipschitz condition (57) and equation (58), we have

\[
y^T (\mu I - J(x)) y = \mu ||y||^2 - y^T J(x) y \geq (\mu + \nu) ||y||^2 > 0,
\]

which contradicts equation (58). It means that the matrix \((\mu I - J(x))\) is nonsingular. From equations (19)-(20) and the assumption \( c^T F(x_k) = 0 \), we have

\[
(\mu_k I - J(x_k)) s_k = \frac{\Delta t_k}{1 + \Delta t_k} F(x_k),
\]

which gives

\[
c^T (\mu_k I - J(x_k)) s_k = \frac{\Delta t_k}{1 + \Delta t_k} c^T F(x_k) = 0.
\]

Thus, using the property \( c^T J(x_k) = 0 \), from equation (60), we have

\[
c^T s_k = \frac{1}{\mu_k} c^T J(x_k) s_k = (c^T J(x_k)) s_k = 0.
\]

Namely, \( s_k \) belongs to the vertical space of vector \( c \).

Similar to the nonsingular case of the Jacobian matrix \( J(x) \), we have the lower-bounded estimation of the predicted reduction \(|F(x_k)| - |F(x_k) + J(x_k) s_k|\).

**Lemma 3** Assume that the Jacobian matrix \( J(x) \) of the function \( F(x) \) satisfies the one-sided Lipschitz condition (57) in the vertical space of vector \( c \), where the vector \( c \) satisfies \( c^T F(x) = 0 \) for all \( x \in \mathbb{R}^n \). Let \( s_k \) be the solution of the regularization continuation Newton method (19)-(21), then we have

\[
|F(x_k)| - |F(x_k) + J(x_k) s_k| \geq c_s \frac{\Delta t_k}{1 + \Delta t_k} ||F(x_k)||,
\]

where the constant \( c_s \) satisfies \( 0 < c_s < 1 \).

**Proof.** From the result of Property 2, we know that the matrix \((\mu I - J(x_k))\) is nonsingular and \( s_k \) belongs to the vertical space of vector \( c \). From equations (19)-(20) and the Cauchy-Schwartz inequality \( ||x^T y|| \leq ||x|| ||y|| \), we have

\[
\mu_k ||s_k||^2 - s_k^T J(x_k) s_k = \frac{\Delta t_k}{1 + \Delta t_k} s_k^2 F(x_k) \leq \frac{\Delta t_k}{1 + \Delta t_k} ||s_k|| ||F(x_k)||.
\]

Using the assumption of the one-sided Lipschitz condition (57), from equation (63), we have

\[
(\mu_k + \nu) s_k^2 \leq \mu_k ||s_k||^2 - s_k^T J(x_k) s_k \leq \frac{\Delta t_k}{1 + \Delta t_k} ||s_k|| ||F(x_k)||,
\]

which gives

\[
||s_k|| \leq \frac{1}{\mu_k + \nu} \frac{\Delta t_k}{1 + \Delta t_k} ||F(x_k)||.
\]
Thus, from equations (19)-(20) and (64), we have
\[
\|F(x_k) + J(x_k)s_k\| = \left\| \mu_k s_k + \frac{1}{1 + \Delta t_k} F(x_k) \right\| \leq \mu_k \|s_k\| + \frac{1}{1 + \Delta t_k} \|F(x_k)\|
\]
which gives
\[
\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\| \geq \frac{\Delta t_k}{\mu_k + \nu} \frac{\nu}{1 + \Delta t_k} \|F(x_k)\|
\]
where we use the definition (22) of the parameter \(\mu_k\). If we select \(c_s = \frac{\nu}{\epsilon + \nu}\), from inequality (65), we obtain inequality (62). \(\square\)

Similar to the nonsingular case of Jacobian matrix \(J(x)\), for the singular case of Jacobian matrix \(J(x)\), we also has the lower-bounded estimation of time-stepping sizes \(\Delta t_k\) for all \(k = 0, 1, \ldots\), where \(\Delta t_k\) is updated by the trust-region time-stepping scheme (24)-(25).

**Lemma 4** Assume that the function \(F : \mathbb{R}^n \rightarrow \mathbb{R}^n\) is continuously differentiable and its Jacobian matrix \(J(x)\) satisfies the Lipschitz continuity (33) and the one-sided Lipschitz condition (57). If the sequence \(\{x_k\}\) is generated by Algorithm 1, it exists a positive \(\delta_{\Delta t}\) such that
\[
\Delta t_k \geq \delta_{\Delta t} > 0, \quad k = 1, 2, \ldots
\]
are satisfied, where \(\Delta t_k\) is adaptively updated by the trust-region scheme (24)-(25).

**Proof.** According to the Lipschitz continuity (33) of the Jacobian matrix \(J(x)\), we have
\[
\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\| = \left\| \int_0^1 J(x_k + ts_k)s_k dt - J(x_k)s_k \right\|
\]
\[
= \left\| \int_0^1 (J(x_k + ts_k) - J(x_k))s_k dt \right\| \leq \int_0^1 \|J(x_k + ts_k) - J(x_k))s_k\| dt
\]
\[
\leq \int_0^1 \|J(x_k + ts_k) - J(x_k))\|\|s_k\| dt \leq \int_0^1 L\|s_k\|^2 dt = \frac{1}{2} L\|s_k|^2.
\]
On the other hand, using the result of property 2 and the one-sided Lipschitz condition (57), from equations (19)-(20), we obtain the upper-bounded estimation (64) of the trial step \(s_k\). Therefore, from equations (64) and (67), we have
\[
\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\| \leq \frac{1}{2} \frac{L}{(\mu_k + \nu)^2} \left( \frac{\Delta t_k}{1 + \Delta t_k} \right)^2 \|F(x_k)\|^2.
\]
From the result (65) of Lemma 3 and equation (68), we have

$$|p_k - 1| = \left| \frac{\|F(x_k)\| - \|F(x_{k+1})\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} - 1 \right| \leq \frac{\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} \leq \frac{L}{2v^2} \left( \frac{\Delta t_k}{1 + \Delta t_k} \right) \|F(x_k)\|.$$  \hspace{1cm} (69)

Furthermore, according to Algorithm 1, we know that the sequence \{\|F(x_k)\|\} is monotonically decreasing. Namely, we have \|F(x_k)\| \leq \|F(x_0)\| for all k = 1, 2, \ldots. Let

$$\delta_{M} = \frac{2v^2}{\|F(x_0)\|L} \eta_1.$$  \hspace{1cm} (70)

If we assume that K is the first index such that \(\Delta t_K \leq \delta_{M}\), from inequalities (69)–(70), we know that \(|p_k - 1| < \eta_1\). Consequently, \(\Delta t_{K+1}\) will be enlarged according to the time-stepping scheme (25). Therefore, if we select \(\delta_{M} = \min\{\Delta t_K, \delta_{M}\}\), we know that \(\Delta t_k \geq \delta_{M}\) for all \(k = 0, 1, 2, \ldots\). \hfill \Box

Now, using the results of Lemma 3 and Lemma 4, we know that the sequence \{\|F(x_k)\|\} converges to zero when \(k\) tends to infinity and its proof is similar to Theorem 1. We state it as the following theorem and omit its proof.

**Theorem 3** Assume that the function \(F : \mathbb{R}^n \to \mathbb{R}^n\) is continuously differentiable and its Jacobian matrix \(J(x)\) satisfies the Lipschitz continuity (57) and the one-sided Lipschitz condition (57). If the sequence \(\{x_k\}\) is generated by Algorithm 1, we have

$$\liminf_{k \to \infty} \|F(x_k)\| = 0.$$  \hspace{1cm} (71)

When the Jacobian matrix \(J(x)\) satisfies the one-sided Lipschitz condition (57), the sequence \(\{x_k\}\) generated by Algorithm 1 also has the local superlinear convergence property.

**Theorem 4** Assume that the function \(F : \mathbb{R}^n \to \mathbb{R}^n\) is continuously differentiable and its Jacobian matrix \(J(x)\) satisfies Lipschitz continuity (57) and one-sided Lipschitz condition (57). Furthermore, assume that \(x^*\) is a solution of nonlinear equations (1). If the sequence \(\{x_k\}\) is generated by Algorithm 1 and there is a subsequence \(\{x_{k_i}\}\) such that it converges to \(x^*\), the sequence \(\{x_{k_i}\}\) superlinearly converges to \(x^*\).

**Proof.** From Property 2, we know that the matrix \((\mu I - J(x_k))\) is nonsingular and \(s_k\) belongs to the vertical space of vector \(c\), where \(x_k\) is the solution of equations (19)–(20) and the vector \(c\) satisfies \(c^T F(x) = 0\) for all \(x \in \mathbb{R}^n\).

Firstly, we prove that it exists an index \(K_F\) such that \(\Delta t_k\) will be enlarged at every iteration when \(k \geq K_F\). Consequently, \(\Delta t_k\) tends to infinity. From equation (65) of
Lemma 3 and equation (69) of Lemma 4, we have

$$|p_k - 1| = \left| \frac{\|F(x_k)\| - \|F(x_{k+1})\|}{\|F(x_k)\| - \|F(x_k) + J(x_k) e_k\|} - 1 \right| \leq\frac{1}{2} \frac{L}{\nu(\mu + \nu)} \left( \frac{\Delta t_k}{1 + \Delta t_k} \right) \|F(x_k)\| \leq\frac{1}{2} \frac{L}{\nu^2} \|F(x_k)\|. \quad (72)$$

Since there is a subsequence \( \{x_k\} \) such that it converges to \( x^* \), it exists an index \( K_F \) such that

$$\|F(x_{K_F})\| \leq \frac{2\eta_1 \nu^2}{L} \quad (73)$$

is monotonically decreasing. Consequently, we have \( \|F(x_k)\| \leq \|F(x_{K_F})\| \) when \( k \geq K_F \). From equations (72)-(73), we have

$$|p_k - 1| \leq \eta_1, \quad \text{when } k \geq K_F. \quad (74)$$

Thus, from equation (74) and the time-stepping scheme (25), we know that \( \Delta t_k \) will be enlarged at every iteration when \( k \geq K_F \). Consequently, we have \( \lim_{k \to \infty} \Delta t_k = \infty \).

We denote

$$e_k = x_k - x^*. \quad (75)$$

From equations (19)-(20) and (75), we have

$$e_{k+1} = e_k + s_k = e_k + (\mu_k I - J(x_k))^{-1} \frac{\Delta t_k}{1 + \Delta t_k} F(x_k). \quad (76)$$

Reformulating equation (76), we obtain

$$\begin{align*}
(\mu_k I - J(x_k)) e_{k+1} &= (\mu_k I - J(x_k)) e_k + \frac{\Delta t_k}{1 + \Delta t_k} (F(x_k) - F(x^*)) \\
&= -\frac{1}{\Delta t_k} J(x_k) e_k + \frac{\Delta t_k}{1 + \Delta t_k} \int_0^1 (J(x^* + t e_k) - J(x_k)) e_k dt. \quad (77)
\end{align*}$$

Since \( c^T s_k = 0 \) and the subsequence \( \{x_k\} \) converges to \( x^* \), from equation (76), we have

$$c^T e_{k+1} = c^T e_k + c^T s_k = c^T e_k = \cdots = c^T e_k \to 0. \quad (78)$$

Namely, the error vectors \( e_k (k = 0, 1, \ldots) \) belong to the vertical space of vector \( c \). Thus, from the one-sided Lipschitz condition (57) and the Cauchy-Schwarz inequality \( |x^T y| \leq \|x\| \|y\| \), we have

$$\|e_{k+1}\| \|\mu_k I - J(x_k)\| e_{k+1} \| \geq e_{k+1}^T (\mu_k I - J(x_k)) e_{k+1} \geq (\mu_k + \nu) \|e_{k+1}\|^2. \quad (79)$$
Reformulating equation (78), we have

$$\|e_{k+1}\| \leq \frac{1}{\mu_k + \nu} \|(\mu_k I - J(x_k))e_{k+1}\|.$$  \hspace{1cm} (79)

From the continuity of the Jacobian matrix $J(x)$ at $x^*$, it exists the positive constants $M$ and $\varepsilon_1$ such that

$$\|J(x)\| \leq M \text{ when } \|x - x^*\| < \varepsilon_1.$$

Since the subsequence $\{x_k\}$ converges to $x^*$, it exists the index $K_1$ such that $\|x_{K_1} - x^*\| < \varepsilon_1$. Furthermore, we have proved that $\lim_{k \to \infty} \Delta t_k = \infty$. Thus, we can select a sufficiently large index $K_2$ such that $\Delta t_{K_2} \geq (4M)/\nu$ and $\|e_{K_2}\| \leq \nu/(2\mu)$. We select $K = \max\{K_1, K_2\}$.

From equation (77) and the Lipschitz continuity (33), we have

$$\|(\mu_k I - J(x_k))e_{k+1}\| \leq \mu_k \|e_k\| + \frac{1}{\Delta t_k} \|J(x_k)\| \|e_k\|$$

$$\leq \left(\mu_k + \frac{1}{\Delta t_k} M\right) \|e_k\| + \int_0^1 L \|e_k\|^2 dt$$

$$\leq \left(\mu_k + \frac{1}{\Delta t_k} M + \frac{1}{2} L \|e_k\|^2\right) \|e_k\|.$$  \hspace{1cm} (80)

Replacing equation (80) into equation (79), we obtain

$$\|e_{k+1}\| \leq \frac{\mu_k + \frac{1}{\Delta t_k} M + \frac{1}{2} L \|e_k\|}{\mu_k + \nu} \|e_k\| \leq \frac{\mu_k + 1/2 \mu}{\mu_k + \nu} \|e_k\| = \|e_k\|.$$  \hspace{1cm} (81)

In the second inequality of equation (81), we use the assumptions $\Delta t_k \geq (4M)/\nu$ and $\|e_{K_2}\| \leq \nu/(2\mu)$. Thus, by the mathematical induction and the definition (22) of the regularization parameter $\mu$, we have

$$\|e_{k+1}\| \leq \frac{\mu_k + \frac{1}{\Delta t_k} M + \frac{1}{2} L \|e_k\|}{\mu_k + \nu} \|e_k\|$$

$$\leq \frac{\mu_k + 1/2 \nu}{\mu_k + \nu} \|e_k\| \leq \frac{c_k + 1/2 \nu}{c_k + \nu} \|e_k\|, \quad k = K, K + 1, \ldots.$$  \hspace{1cm} (82)

Consequently, we obtain $\lim_{k \to \infty} \|e_k\| = 0$.

From the definition (22) of the regularization parameter $\mu_k$ and $\lim_{k \to \infty} \Delta t_k = \infty$, we know that $\mu_k = 1/\Delta t_k$ when $k \geq K_\mu$, where we select the sufficient index $K_\mu$ such that $1/\Delta t_k < \varepsilon_\nu$ when $k \geq K_\mu$. Thus, from equation (82), when $k \geq K_\mu$, we have

$$\|e_{k+1}\| \leq \frac{\mu_k + \frac{1}{\Delta t_k} M + \frac{1}{2} L \|e_k\|}{\mu_k + \nu} = \frac{\mu_k + \frac{1}{\Delta t_k} M + \frac{1}{2} L \|e_k\|}{\mu_k + \nu} \to 0,$$

where we use the properties $\lim_{k \to \infty} \Delta t_k = \infty$ and $\lim_{k \to \infty} \|e_k\| = 0$. Namely, the sequence $\{x_k\}$ superlinearly converges to $x^*$. \hfill \Box
4 Numerical Experiments

In this section, for some practical equilibrium problems and the classical test problems of nonlinear equations, we test the performance of Algorithm 1 (CNMTr) and compare it with the trust-region method (the built-in subroutine fsolve.m of the MATLAB environment [30,33]) and the homotopy continuation methods (HOMPACK90 [47] and NAClab [23,49,50]).

The trust-region method is a popular optimization method for nonlinear equations and its efficient implementation is given by Jorge Moré [33]. At every iteration, its trial step $s_k$ is obtained via solving the following linear system:

$$
(J(x_k)^T J(x_k) + \lambda_k I) s_k = -J(x_k)^T F(x_k),
$$

where the parameter $\lambda_k$ is updated according to the following ratio

$$
r_k = \frac{\|F(x_k)\|^2 - \|F(x_k + s_k)\|^2}{\|F(x_k)\|^2 - \|F(x_k) + J(x_k)s_k\|^2}.
$$

If $r_k$ is close to one, the parameter $\lambda_{k+1}$ of the next iteration is reduced such as $\lambda_{k+1} = 0.5\lambda_k$. If $r_k$ is close to zero, the parameter $\lambda_{k+1}$ of the next iteration is enlarged such as $\lambda_{k+1} = 2\lambda_k$. From equations (24) and (84), we know that the trust-region technique of Algorithm 1 is slightly different from the classical trust-region technique. $p_k$ in equation (24) more accurately reflects the approximation $F(x_k) + J(x_k)s_k$ of $F(x_k + s_k)$ than $r_k$ in equation (84).

HOMPACK90 [47] is a classical homotopy method implemented by Fortran 90 for nonlinear equations and it is very popular in engineering fields. Another state-of-the-art homotopy method is the built-in subroutine psolve.m of the NAClab environment [23,49]. Since psolve.m only solves the polynomial systems, we replace psolve.m with its subroutine GaussNewton.m (the Gauss-Newton method) for non-polynomial systems. Therefore, we compare these two homotopy methods with Algorithm 1 too.

We collect 26 test problems of nonlinear equations, some of which come from the equilibrium problems of chemical reactions [16,18,39,46], and some of which come from the classical test problems [8,10,27,34,35]. We put them in Appendix A. The dimensions of test problems vary from 1 to 3000. Some problems have the singular Jacobian matrix $J(x)$ of function $F(x)$. The codes are executed by a HP Pavilion notebook with Intel quad-core CPU, and the termination condition is

$$
\|F(x^k)\|_{\infty} \leq 10^{-12}.
$$

The numerical results are put in Table [1] and Table [2]. The number of iterations of CNMTr and fsolve is illustrated by Figure [1]. The consumed time of these four methods (CNMTr, HOMPACK90, fsolve and NAClab) is illustrated by Figure [2]. From Table [1] and Table [2], we find that CNMTr (Algorithm 1) performs well for nonlinear equations. However, the trust-region method (fsolve) and the classical homotopy methods (HOMPACK90 and NAClab) can not correctly work out for some problems,
which especially comes from the practical problems with the non-isolated singular Jacobian matrices such as examples 1, 2, 3, 4, 6, 21, 23. Furthermore, from Figures 1 and 2, we also find that CNMTr retains the fast convergence property of the traditional optimization methods such as the trust-region method (fsolve). The following parts of this section are the detailed descriptions of numerical examples.

For example 1, the solutions computed by CNMTr and fsolve are $x_{\text{CNMTr}} = (4.41\times10^{-5}, 1.76\times10^{-10}, 1.00)$ and $x_{\text{fsolve}} = (6.29\times10^{-5}, 2.44\times10^{-10}, 1.032691)$ respectively, which are close to the steady-state solution of the original chemical reaction problem and satisfies the linear conservation law $c^T x = 1$ and the nonnegative constraints, where $c^T = [1, 1, 1]$. The solutions computed by HOMPACK90 and NAClab are $x_{\text{HOMPACK90}} = (47.24, -4.09\times10^{-6}, -46.24)$ and $x_{\text{NAClab}} = (0, 0, 0)$, respectively. Since the third element of $x_{\text{HOMPACK90}}$ violates the nonnegative constraint of the chemical reaction concentration, and the $x_{\text{NAClab}}$ can not satisfy the linear conservation law $c^T x = c^T x_0 = 1$, we regard that HOMPACK90 and NAClab both fail to solve this problem.

For example 2, the solution computed by CNMTr is $x_{\text{CNMTr}} = (1.20\times10^{-9}, 4.72\times10^{-15}, -8.96\times10^{-21}, 3.76\times10^{-21})$, which is close to the steady-state solution $x^* = (0, 0, 0, 0)$. However, since the solution computed by HOMPACK90 is $x_{\text{HOMPACK90}} = (-1.15\times10^4, 3.01\times10^{-4}, -2.67\times10^{-11}, 3.01\times10^{-4})$ and its residual is 3.06 which is far away from the termination condition $\epsilon_5$, we regard that HOMPACK90 fails to solve this problem. Since the solutions computed by fsolve and NAClab are $x_{\text{fsolve}} = (1.76\times10^{-3}, 0, -1.26\times10^{-19}, -1.30\times10^{-23})$ and $x_{\text{NAClab}} = (1.18\times10^{-1}, -9.73\times10^{-3}, -7.37\times10^{-17}, -7.36\times10^{-17})$ respectively, which are far away from its steady-state solution $x^* = (0, 0, 0, 0)$, we regard that they both fail to solve this problem, too.

For example 3, the solution computed by CNMTr is close to a steady-state solution and it satisfies the linear conservation law. Since the residuals of the solutions computed by HOMPACK90 and fsolve are 3.12 and 2.77E-03 respectively, which are far away from the termination condition $\epsilon_5$, we regard that HOMPACK90 and fsolve both fail to solve this problem. Since the solution computed by NAClab is zero,
Table 1: Numerical results.

| Problem | CNMTr | HOMPACK90 | fsolve | NAClab (psolve) |
|---------|-------|-----------|--------|----------------|
|         | CPU (s) | $||F(x^*)||_\infty$ | CPU (s) | $||F(x^*)||_\infty$ | CPU (s) | $||F(x^*)||_\infty$ |
| Exam 1 (n=3) | 7.46E-02 | 4.87E-13 | 6.31E-01 | 5.01E-04 (failed) | 2.52E-01 | 1.64E-07 | 6.84E-01 | 0 (failed) |
| Exam 2 (n=4) | 2.55E-02 | 9.86E-14 | 1.09 | 3.06 (failed) | 3.57E-02 | 1.39E-12 (far sol.) | 7.55E-01 | 4.27E-20 (failed) |
| Exam 3 (n=20) | 1.39E-02 | 9.61E-14 | 1.02 | 3.12 (failed) | 3.32E-02 | 9.24E-05 (far sol.) | 1.42 | 0 (failed) |
| Exam 4 (n=5) | 1.71E-02 | 1.17E-15 | 7.94E-01 | 0.74 (failed) | 1.34E-03 | 1.93 (failed) | 1.35 | 1.40E+01 (failed) |
| Exam 5 (n=1) | 2.98E-02 | 4.66E-15 | 5.87E-01 | 2.60E-12 | 4.67E-02 | 5.51E-01 (failed) | 1.36 | 1.96 (failed) |
| Exam 6 (n=2) | 3.01E-02 | 1.11E-16 | 5.49E-01 | 1.34E-02 (failed) | 2.87E-02 | 3.44E-15 | 3.43E+01 | 4.39 (failed) |
| Exam 7 (n=2) | 1.18E-02 | 3.05E-13 | 7.52E-01 | 0 | 1.36E-02 | 2.34E-09 | 2.85E-01 | 0 |
| Exam 8 (n=3000) | 1.24E+01 | 4.21E-02 | 5.12E-13 | 8.64E+02 | 3.20E-13 | 3.65E+04 | 7.12E-12 |
| Exam 9 (n=3000) | 2.07E+01 | 4.01E-13 | 6.84E-12 | 3.55E+02 | 7.50E-13 | 3.97E+04 | 5.21E-13 |
| Exam 10 (n=3000) | 1.94E+01 | 4.05E-13 | 6.31E-15 | 3.85E+03 | 6.75 | 4.02E+03 | 1.20E+04 (failed) |
| Exam 11 (n=3) | 4.37E-02 | 2.58E-13 | 8.37E-01 | 2.15E-14 | 1.69E-02 | 1.39E-17 | 4.39E-01 | 9.90E+02 (failed) |
| Exam 12 (n=4) | 1.24E-01 | 6.77E-13 | 7.53E-01 | 8.94E-13 | 2.07E-01 | 5.25E-01 (failed) | 8.62E-01 | 6.02E-12 |
| Exam 13 (n=4) | 4.30E+01 | 9.58E-13 | 6.03E-02 | 9.68E-13 | 6.91E+02 | 4.57E-01 (failed) | 4.13E+03 | 4.84E+08 (failed) |
| Exam 14 (n=2) | 1.87E+01 | 6.31E-13 | 5.91E-02 | 8.41E-13 | 4.12E+02 | 1.48E-06 | 4.10E+04 | 8.13E-12 |
| Exam 15 (n=10) | 3.80E-02 | 1.42E-14 | 8.06 | 6.013.84E-14 | 1.99E-02 | 5.72E-13 | 4.71E+02 | 5.18E-13 |
| Exam 16 (n=10) | 4.67E-02 | 2.44E-14 | 2.94 | 6.57E-14 | 1.16E-02 | 6.76E-13 | 9.20E-01 | 4.15E-13 |
| Exam 17 (n=100) | 1.30 | 6.07E-13 | 3.54E+01 | 5.71E-13 | 2.51E-02 | 8.88E-16 | 9.13E+01 | 3.16E-12 |
| Exam 18 (n=5) | 1.40E-02 | 3.81E-16 | 2.09 | 6.14E-16 | 8.02E-03 | 7.19E-12 | 7.74E-01 | 1 (failed) |
| Exam 19 (n=3) | 2.07E-02 | 5.47E-15 | 2.54 | 6.58E-12 | 8.13E-03 | 4.96E-13 | 5.45E-01 | 0 |
| Exam 20 (n=2) | 6.57E-03 | 2.66E-15 | 5.28 | 5.14E-13 | 1.09E-02 | 2.22E-16 | 3.51E-01 | 8.53 |
| Exam 21 (n=2) | 1.23E-03 | 8.77E-15 | 7.53E-01 | 1.22E-02 (failed) | 5.29E-02 | 3.55E-05 | 4.17E-01 | 1 (failed) |
| Exam 22 (n=2) | 5.58E-03 | 0 | 7.79E-01 | 0 | 6.73E-02 | 2.73 (failed) | 5.41E-01 | 0 |
| Exam 23 (n=6) | 1.62E-02 | 4.48E-13 | 4.92 | 1.09E+02 (failed) | 4.84E-02 | 1.05E+02 (failed) | 8.31E-01 | 5.47E+14 (failed) |
| Exam 24 (n=10) | 5.30E-02 | 1.24E-14 | 7.63E-01 | 6.26E-13 | 9.83E-03 | 4.23E-12 | 9.00E-01 | 2.22E-16 |
| Exam 25 (n=3000) | 7.94E-02 | 6.09E-13 | 4.87E-02 | 4.13E-13 | 3.91E+03 | 3.55E-15 | 4.07E+04 | 1.45E-12 |
| Exam 26 (n=3000) | 1.31E+03 | 2.30E-13 | 9.12E+02 | 6.14E-12 | 7.77E+03 | 5.55E-16 | 7.09E+04 | 6.14E-12 |
Table 2: Statistical results.

|                | CNMTr | HOMPACK90 | fsolve | NAClab |
|----------------|-------|-----------|--------|--------|
| the ratio of failed problems | 0/26  | 7/26      | 9/26   | 13/26  |
| the ratio of the minimum consumed time | 19/26 | 0/26      | 7/26   | 0/26   |

which can not satisfy the linear conservation law $c^T x_{NAClab} = c^T x_0 = 0.657$ where $c = \text{ones}(20, 1)$, we regard that NAClab fails to solve this problem, too.

For example 4, since the residual of the solution computed by CNMTr is 1.17E-15, we regard that CNMTr successfully solves this problem. However, since the residuals of the solutions computed by HOMPACK90, fsolve and NAClab are 0.74, 1.93 and 14 respectively, which are far away from the termination condition (85), we regard that these three methods fail to solve this problem.

For example 5, since the residuals of the solutions computed by CNMTr and HOMPACK90 are 4.66E-15 and 2.60E-12 respectively, we regard that they both successfully solve this problem. However, since the residuals of the solutions computed by fsolve and NAClab are 0.551 and 1.96 respectively, which are far away from the termination condition (85), we regard that these two methods fail to solve this problem.

For example 6, since the residuals of the solutions computed by CNMTr and fsolve are 1.11E-16 and 3.44E-15 respectively, we regard that they both successfully solve this problem. However, the residuals of the solutions computed by HOMPACK90 and NAClab are 1.34E-02 and 4.39 respectively, which are far away from the termination condition (85), we regard that these two methods fail to solve this problems.

For examples 7, 8, 9, since the residuals of the solutions computed by these four methods are small, we regard that these four methods successfully solve these three problems.

For example 10, since the residuals of the solutions computed by CNMTr and HOMPACK90 are 4.05E-13 and 6.31E-15 respectively, we regard that they both successfully solve this problem. However, since the residuals of the solutions computed by fsolve and NAClab are 6.75 and 1.20E+04 respectively, which are far away from the termination condition (85), we regard that these two methods fail to solve this problem.

For example 11, since the residuals of the solutions computed by CNMTr, HOMPACK90 and fsolve are 2.58E-13, 2.15E-14 and 1.39E-17 respectively, we regard that these three methods successfully solve this problem. However, since the residual of the solution computed by NAClab is 9.90E + 02, which is far away from the termination condition (85), we regard that NAClab fails to solve this problem.

For example 12, since the residuals of the solutions computed by CNMTr, HOMPACK90 and NAClab are 6.77E-13, 8.94E-13 and 6.02E-12, we regard that these
three methods successfully solve this problem. However, since the residual of the solution computed by fsolve is 5.25E-01, which is far away from the termination condition (85), we regard that fsolve fails to solve this problem.

For example 13, since the residuals of the solutions computed by CNMTr and HOMPACK90 are 9.58E-13 and 9.68E-13 respectively, we regard that they both successfully solve this problem. However, since the residuals of the solutions computed by fsolve and NAClab are 4.57E-01 and 4.84E+08 respectively, which are far away from the termination condition (85), we regard that these two methods fail to solve this problem.

For examples 14, 15, 16, 17, these four methods (CNMTr, HOMPACK90, fsolve and NAClab) successfully solve these four problems.

For example 18, since the residuals of the solutions computed by CNMTr, HOMPACK90 and fsolve are 3.81E-16, 6.14E-16 and 7.19E-12 respectively, we regard that these three methods successfully solve this problem. However, since the residual of the solution computed by NAClab is 1, which is far away from the termination condition (85), we regard that NAClab fails to solve this problem.

For example 19, since the residuals of the solutions computed by CNMTr, HOMPACK90, fsolve and NAClab are 5.84E-15, 6.58E-12, 4.96E-13 and 0 respectively, we regard that these four methods successfully solve this problem.

For example 20, since the residuals of the solutions computed by CNMTr, HOMPACK90 and fsolve are 2.66E-15, 5.14E-13 and 2.22E-16 respectively, we regard that these three methods successfully solve this problem. However, the residual of the solution computed by NAClab is 8.53, which is far away from the termination condition (85), we regard that NAClab fails to solve this problem.

For example 21, since the residuals of the solutions computed by CNMTr and fsolve are 2.91E-12 and 3.55E-05 respectively, we regard that they both successfully solve this problem. However, since the residuals of the solutions computed by HOMPACK90 and NAClab are 1.22E-02 and 1 respectively, which are far away from the termination condition (85), we regard that these two methods fail to solve this problem.

For example 22, since the residuals of the solutions computed by CNMTr, HOMPACK90 and NAClab are very close to zeroes, we regard that these three methods successfully solve this problems. However, since the residual of the solution computed by fsolve is 2.73, which is far away from the termination condition (85), we regard that fsolve fails to solve this problem.

For example 23, since the residual of the solution computed by CNMTr is 4.48E−13, we regard that it successfully solves this problem. However, since the residuals of the solutions computed by HOMPACK90, fsolve and NAClab are 1.09E+02, 1.05E+02 and 5.47E+14 respectively, which are far away from the termination condition (85), we regard that these three methods fail to solve this problem.
For examples 24, 25, and 26, these four methods (CNMTr, HOMPACK90, fsolve and NACLab) successfully solve these three problems.

5 Conclusion and future work

In this article, we consider the special continuation method based on the continuous Newton flow and construct a new time-stepping scheme based on the trust-region technique (CNMTr) for nonlinear equations. We also analyze the local and global convergence of the new method under the standard assumptions. Finally, for some classical test problems, we compare it with the classical homotopy methods (HOMPACK90 and psolve) and the traditional optimization method (the trust-region method, fsolve). Numerical results show that the new method maintains the robust convergence of the classical homotopy method and the fast convergence of the trust-region method. Therefore, the CNMtr method (Algorithm 1) is worth investigating further as a special continuation method. We will also apply it to the global optimization problems and report it promising numerical results soon.

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A Test Problems

Example 1. ROBER- An autocatalytic reaction problem with the singular Jacobian matrix [16,39]

This problem is proposed by H. H. Robertson in 1966 and it describes the kinetics of an autocatalytic reaction. Under some idealized conditions, an ODE model can be set up as follows:

\[
\begin{align*}
\dot{x}_1 &= -k_1 x_1 + k_3 x_2 x_3, \\
\dot{x}_2 &= k_1 x_1 - k_2 x_2^2 - k_3 x_2 x_3, \\
\dot{x}_3 &= k_2 x_2^2,
\end{align*}
\]

where \(x_1, x_2, x_3\) represent the concentrations and \(k_1, k_2, k_3\) are the reaction rate constants. It is not difficult to verify that it exists a constant vector \(c = [1, 1, 1]\) to satisfy

\[
\begin{align*}
c^T F(x) &= -k_1 x_1 + k_3 x_2 x_3 + k_1 x_1 - k_2 x_2^2 - k_3 x_2 x_3 + k_2 x_2^2 = 0.
\end{align*}
\]

Consequently, this problem satisfies the linear conservation law \(c^T x(t) = c^T x(0)\).

We assume that the reaction rate constants are \(k_1 = 0.04, k_2 = 3E + 7, k_3 = 1.0E + 4\), and the initial concentrations are \(x_1(0) = 1, x_2(0) = 0, x_3(0) = 0\). This problem is a stiff system because the reaction rate constants \(k_i (i = 1, 2, 3)\) vary in a large range. Generally speaking, it is difficult to find its equilibrium point for many solvers.

Example 2. The E5 problem with the singular Jacobian matrix [16]

This test problem is a model for the chemical pyrolysis and describes a reaction involving six reactants. According to conservation of mass and other some idealized assumptions, the corresponding math-
where $x_i$ ($i = 1, 2, \ldots, 6$) are the concentrations of the reactants $A_i$ ($i = 1, 2, \ldots, 6$). Generally, we use the first four equations as a stiff integration comparison \cite{16}. It is easy to verify that there exists a constant vector $c = [0, 1, -1, -1, 0, 0]$ to satisfy

$$c^T F(x) = (k_1 x_1 - k_2 x_2 x_3) - (k_1 x_1 - k_2 x_2 x_3 - k_3 x_1 x_3 + k_4 x_4) - (k_3 x_1 x_3 - k_4 x_4) = 0.$$  

Consequently, it satisfies the linear conservation law $c^T x(t) = c^T x(0)$. The reaction rate constants are given by $k_1 = 7.89E - 10$, $k_2 = 1.1E + 9$, $k_3 = 1.1E + 7$, $k_4 = 1.13E + 3$, and initial concentrations are set to zeroes except for $x_1(0) = 1.76E - 3$.

**Example 3. The pollution problem with the singular Jacobian matrix \cite{45, 46}**

This test problem arises from the chemical reaction part of the air pollution model. The original system has 25 reactions and 20 reacting compounds. The function has the following form:

$$F(x) = \begin{pmatrix}
-(x_1 + x_{10} + x_{14} + x_{23} + x_{24}) + (x_2 + x_3 + x_9 + x_{11} + x_{12} + x_{22} + x_{23}) \\
-(x_2 + x_3 + x_9 + x_{12}) + (x_1 + x_{21}) \\
x_1 + (x_1 + x_{17} + x_{19} + x_{22}) \\
-(x_2 + x_{16} + x_{17} + x_{21}) + x_{15} \\
x_3 + (2 x_4 + x_6 + x_7 + x_{13} + x_{20}) \\
-(x_6 + x_8 + x_{14} + x_{20}) + (x_3 + 2 x_{18}) \\
-(x_4 + x_5 + x_6) + x_{13} \\
x_4 + x_5 + x_6 + x_7 \\
-(x_7 + x_8) \\
-x_{12} + x_7 + x_9 \\
-(x_9 + x_{10}) + (x_8 + x_{11}) \\
x_9 \\
-x_{11} + x_{10} \\
-x_{13} + x_{12} \\
x_{14} \\
-(x_{18} + x_{19}) + x_{16} \\
-x_{20} \\
x_{20} \\
-(x_{21} + x_{22} + x_{24}) + (x_{23} + x_{25}) \\
-x_{25} + x_{24}
\end{pmatrix}.$$  

It is not difficult to verify that it exists a constant vector $c = [1, 1, \ldots, 1]^T$ to satisfy $c^T F(x) = 0$. Consequently, it satisfies the linear conservation law $c^T x(t) = c^T x(0)$. The initial point is $x_0 = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0.007, 0, 0, 0)$.
Example 4. The stability problem of an aircraft (p. 279, [35])

This test problem in control is to analyze the stability of an aircraft in response to the commands of the pilot. The equilibrium equations for a particular aircraft are given by a system of 5 equations in 8 unknowns of the form

\[ F(x) = Ax + \varphi(x) = 0, \]

where \( F : \mathbb{R}^8 \to \mathbb{R}^5 \), the matrix \( A \) is given by

\[
A = \begin{bmatrix}
-3.933 & 0.107 & 0.126 & 0 & -9.99 & 0 & -45.83 & -7.64 \\
0 & -0.987 & 0 & -22.95 & 0 & -28.37 & 0 & 0 \\
0.002 & 0 & -0.235 & 0 & 5.67 & 0 & -0.921 & -6.51 \\
0 & 1.0 & 0 & -1.0 & 0 & -0.168 & 0 & 0 \\
0 & 0 & -1.0 & 0 & -0.196 & 0 & -0.0071 & 0
\end{bmatrix},
\]

and the nonlinear part is defined by

\[
\varphi(x) = \begin{bmatrix}
-0.727x_2x_3 + 8.39x_1x_4 - 684.4x_2x_5 + 63.5x_4x_2 \\
0.949x_1x_3 + 0.173x_1x_5 \\
-0.716x_1x_2 - 1.578x_1x_4 + 1.132x_4x_2 \\
-x_1x_5 \\
x_1x_4
\end{bmatrix}.
\]

The first three variables \( x_1, x_2, x_3 \), represent the rates of roll, pitch and yaw, respectively, while \( x_4 \) is the incremental angle of attack and \( x_5 \) is the sideslip angle. The last three variables \( x_6, x_7, x_8 \) are the controls; they represent the deflections of the elevator, aileron and rudder, respectively. The initial point is \((0.5, 0.5, 0.5, 2, 0)\) and let the other three variables \( x_6 = 0.5, x_7 = 0.5, x_8 = 0.5 \).

Example 5. \( F(x) = \sin(5x) - x \) (p. 279, [35])

This test function has three zeroes located at zero and approximately \( \pm 0.519148 \). The initial value is set by \( x_0 = -1 \).

Example 6. Problem with the singular Jacobian matrix (p. 149, [8])

This test problem has the following form:

\[
\exp(x^2 + y^2) - 3 = 0,
\]

\[
x + y - \sin(3(x + y)) = 0.
\]

Its singular Jacobian matrix can be calculated by the straight line

\[ y = x, \]

and the family of parallels

\[ y = -x \pm \frac{1}{3} \arccos \left( \frac{1}{7} \right) \pm \frac{2}{3} \pi j, \ j = 0, 1, 2 \ldots. \]

We choose the initial point \((-1, -1)\) for this test problem.

Example 7. The Jacobian matrix of the function with positive and negative eigenvalues

We construct a simple test function whose Jacobian matrix includes the positive and negative eigenvalues. It has the following form:

\[
F(x) = \begin{bmatrix} 1 & 0 \\ 0 & -2 \end{bmatrix} x.
\]
Obviously, its Jacobian matrix has two eigenvalues, i.e. 1 and -2. We choose the initial point $(1, 2)$ for this test problem.

**Example 8. The extended Rosenbrock function (p. 362, [10] or [34])**

The Rosenbrock function is proposed by H. H. Rosenbrock in 1960. Here is its extended form as follows:

\[
\begin{align*}
    n &= \text{any positive multiple of 2,} \\
    \text{for } i &= 1, \ldots, n/2 \\
    f_{2i-1}(x) &= 10(x_{2i} - x_{2i-1}^2); \\
    f_{2i}(x) &= 1 - x_{2i-1}; \\
\end{align*}
\]

We set \( n = 3000 \) and the initial point \( x_0 = (-1.2, 1, \ldots, -1.2, 1) \) for this test problem. Its zero point is located at \( x^* = (1, 1, \ldots, 1, 1, 1) \).

**Example 9. The extended Powell singular function (p. 362, [10] or [34])**

The Powell singular function is proposed by M. J. D. Powell as an unconstrained optimization software. Here, we regard it as the test problem of nonlinear equations. The function is convex and its Hessian matrix is singular at the solution. It has the following form:

\[
\begin{align*}
    n &= \text{any positive multiple of 4,} \\
    \text{for } i &= 1, \ldots, n/4 \\
    f_{4i-3}(x) &= x_{4i-3} + 10x_{4i-2}; \\
    f_{4i-2}(x) &= \sqrt{5} (x_{4i-1} - x_4); \\
    f_{4i-1}(x) &= (x_{4i-2} - 2x_{4i-1})^2; \\
    f_{4i}(x) &= \sqrt{10} (x_{4i-3} - x_{4i})^2; \\
\end{align*}
\]

We set \( n = 3000 \). Its zero point is located at \( x^* = (0, 0, 0, \ldots, 0, 0, 0, 0) \). The initial point is \( (3, -1, 0, 1, \ldots, 3, -1, 0, 1) \).

**Example 10. The trigonometric function (p. 362, [10] or [34])**

This classical test function has the following form:

\[
\begin{align*}
    n &= \text{any positive integer,} \\
    \text{for } i &= 1, \ldots, n \\
    f_i(x) &= n - \sum_{j=1}^{n} \left( \cos x_j + i(1 - \cos x_j) - \sin x_j \right); \\
\end{align*}
\]

We set \( n = 3000 \) and choose \((100/n, 100/n, \ldots, 100/n)\) as the initial point for this problem.

**Example 11. The helical valley function (p. 362, [10])**

This test function has the following form:

\[
\begin{align*}
    n &= 3, \\
    f_1(x) &= 10(x_3 - 10\theta(x_1, x_2)), \\
    f_2(x) &= 10\left( x_1^2 + x_2^2 \right)^{1/2} - 1, \\
    f_3(x) &= x_3, \\
\end{align*}
\]
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where

\[ \theta(x_1, x_2) = \begin{cases} \frac{1}{\pi} \arctan(x_2/x_1), & \text{if } x_1 > 0, \\ \frac{1}{\pi} \arctan(x_2/x_1) + 0.5, & \text{if } x_1 < 0. \end{cases} \]

Example 12. The Wood function (p. 363, [10])

The Wood function has the following form:

\[
f(x) = 100(x_1^2 - x_2)^2 + (1 - x_1)^2 + 90(x_3^2 - x_4)^2 + (1 - x_3)^2 \\
+ 10.1 \left( (1 - x_2)^2 + (1 - x_4)^2 \right) + 19.8(1 - x_2)(1 - x_4).\]

This function has a global minimum point at \( x^* = (1, 1, 1, 1) \). We use its gradient \( F(x) = \nabla f(x) \) as the test problem of nonlinear equations. The initial point is \((-30, -10, -30, -10)\).

Example 13. The extended Cragg and Levy function [27]

The extended Cragg and Levy function has the following form:

\[
f(x) = \exp \left( \sum_{i=1}^{n} (x_i - x_{i-1})^2 \right)
\]

We set \( n = 3000 \). The initial point is \((10, 20, 20, 20, \ldots, 10, 20, 20, 20)\).

Example 14. The singular Broyden problem [27]

The singular Broyden function has the following form:

\[
f(x) = \left( (3 - 2x_1)x_1 - 2x_2 + 1 \right)^2,
\]

for \( i = 2, \ldots, n - 1 \)

\[
f(x) = \left( (3 - 2x_1)x_1 - 2x_2 + 1 \right)^2,
\]

end

We set \( n = 3000 \). The initial point is \((-10, -10, \ldots, -10, -10)\).

Example 15. The tridiagonal system [27]

The tridiagonal function has the following form:

\[
f(x) = 4(x_1 - x_2^2),
\]

for \( i = 2, \ldots, n - 1 \)

\[
f(x) = 8x_i (x_i^2 - x_{i-1}) - 2(1 - x_i) + 4 (x_i - x_{i+1}^2);
\]

end

\[
f(x) = 8x_n (x_n^2 - x_{n-1}) - 2(1 - x_n).
\]
The initial point is \((1.3, 1, 3, \ldots, 1.3)\).

**Example 16. The discrete boundary-value problem [27]**

The discrete boundary-value problem has the following form:

\[ n = 10, \]
\[ h = 1/(n+1), \]
\[ f_i(x) = 2x_1 + h^2(x_1 + 1 + h)^3 / 2 - x_2, \]

for \(i = 2, \ldots, n-1\)

\[ f_n(x) = 2x_n + h^2(x_n + 1 + nh)^3 / 2 - x_{n-1}. \]

The initial point is \((10h(h-1), \ldots, 10hn(h-1))\).

**Example 17. The Broyden tridiagonal problem [27]**

The Broyden tridiagonal function has the following form:

\[ n = 100, \]
\[ f_i(x) = (3 - 2x_i)x_i - 2x_i + 1, \]

for \(i = 2, \ldots, n-1\)

\[ f_n(x) = (3 - 2x_n)x_n - x_{n-1} + 2x_{n-1} + 1; \]

end

\[ f(x) = (3 - 2x_n)x_n - x_{n-1} + 1. \]

The initial point is \((-1, \ldots, -1)\).

**Example 18. The asymptotic boundary value problem [9]**

The asymptotic boundary value problem with final time \(\tau = \infty\) has the following form:

\[ r = -0.1, \]
\[ s = 0.2, \]
\[ x_1' = x_2, \]
\[ x_2' = x_3, \]
\[ x_3' = -0.5(3 - r)x_1x_3 - rx_3^2 + 1 - x_2 + xx_3, \]
\[ x_4' = x_5, \]
\[ x_5' = -0.5(3 - r)x_1x_5 - (r - 1)x_2x_4 + s(x_4 - 1), \]

with 5 boundary conditions

\[ x_1(0) = x_2(0) = x_3(0) = 0, \]
\[ x_2(\tau) = 0, \]
\[ x_3(\tau) = 1. \]

The initial point is \((1, \ldots, 1)\).

**Example 19. The box problem [33]**

The function of this test problem has the following form:

\[ f_1(x) = \exp(-0.1x_1) - \exp(-0.1x_2) - x_3(\exp(-0.1) + \exp(-1)), \]
\[ f_2(x) = \exp(-0.2x_1) - \exp(-0.2x_2) - x_3(\exp(-0.2) + \exp(-2)), \]
\[ f_3(x) = \exp(-0.3x_1) - \exp(-0.3x_2) - x_3(\exp(-0.3) + \exp(-3)). \]
The initial point is (0, 10, 20).

**Example 20. The simple problem (p.149, [10])**

The function of this test problem has the following form:

\[
\begin{align*}
    f_1(x) &= x_1^2 + x_2^2 - 2, \\
    f_2(x) &= \exp(x_1 - 1) + x_2^2 - 2.
\end{align*}
\]

It has two zero points located at (1, 1) and (1, -1). Since the Jacobian matrix is singular along the line \(x_2 = 0\), Newton’s method jumps back and forth across the symmetry line and terminates near the line \(x_2 = 0\). The initial point is (2, 2).

**Example 21. The Powell badly scaled function [34]**

The function of this test problem has the following form:

\[
\begin{align*}
    f_1(x) &= 10^4 x_1 x_2 - 1, \\
    f_2(x) &= \exp(-x_1) + \exp(-x_2) - 1.0001.
\end{align*}
\]

The initial point is (0, 1).

**Example 22. The chemical equilibrium problem 1 [18]**

The function of this test problem has the following form:

\[
\begin{align*}
    f_1(x) &= x_2 - 10, \\
    f_2(x) &= x_1 x_2 - 5 \times 10^4.
\end{align*}
\]

The initial point is \(10^4, 1\).

**Example 23. Chemical equilibrium problem 2 [18]**

This problem is badly scaled and its function has the following form:

\[
\begin{align*}
    f_1(x) &= x_1 + x_2 + x_4 - 0.001, \\
    f_2(x) &= x_5 + x_6 - 55, \\
    f_3(x) &= x_1 + x_2 + x_3 + 2x_5 + x_6 - 110.001, \\
    f_4(x) &= x_1 - 0.1x_2, \\
    f_5(x) &= x_1 - 10^4 x_3 x_4, \\
    f_6(x) &= x_5 - 55 \times 10^{14} x_3 x_6.
\end{align*}
\]

The initial point is \(1, 0, \ldots, 0\).

**Example 24. The Brown almost linear function [31]**

The function of this test problem has the following form:

\[
\begin{align*}
    n &= 10, \\
    f_i &= x_i + \sum_{j=1}^{n} x_j - (n + 1), \quad 1 \leq i \leq n, \\
    f_n &= \left( \prod_{j=1}^{n} x_j \right) - 1.
\end{align*}
\]

The initial point is \(1/2, \ldots, 1/2\).

**Example 25. The symmetric eigenvalue problem**
We construct a symmetric eigenvalue problem as the test problem of nonlinear equations and its matrix $A \in \mathbb{R}^{n \times n}$ has the following tridiagonal form:

$$A = \begin{bmatrix}
2 & 1 & 0 & \cdots & 0 & 0 \\
1 & 2 & 1 & \cdots & 0 & 0 \\
0 & 1 & 2 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 2 & 1 \\
0 & 0 & 0 & \cdots & 1 & 2 \\
0 & 0 & 0 & \cdots & 2 & 1
\end{bmatrix}.$$  

We calculate its eigenvalue and the corresponding eigenvector via solving the following nonlinear equations:

$$Ax - \lambda x = 0,$$

$$x^T x = 1.$$  

We set $n = 3000$ and the initial point $x_0 = (1, \ldots, 1, 2)$.

**Example 26. The asymmetric eigenvalue problem**

We construct an asymmetric eigenvalue problem as the test problem of nonlinear equations and its matrix $A \in \mathbb{R}^{n \times n}$ has the following tridiagonal form:

$$A = \begin{bmatrix}
1 & 1 & 0 & \cdots & 0 & 0 \\
2 & 1 & 1 & \cdots & 0 & 0 \\
0 & 2 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & 1 \\
0 & 0 & 0 & \cdots & 2 & 1 \\
0 & 0 & 0 & \cdots & 0 & 2
\end{bmatrix}.$$  

We calculate its eigenvalue and the corresponding eigenvector via solving the following nonlinear equations:

$$Ax - \lambda x = 0,$$

$$x^T x = 1.$$  

We set $n = 3000$ and the initial point $x_0 = (1, \ldots, 1, 2)$.

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