

Continuation Newton methods with the residual trust-region time-stepping scheme for nonlinear equations

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Abstract For nonlinear equations, the homotopy methods (continuation methods) are popular in engineering fields since their convergence regions are large and they are quite reliable to find a solution. The disadvantage of the classical homotopy methods is that their computational time is heavy since they need to solve many auxiliary nonlinear systems during the intermediate continuation processes. In order to overcome this shortcoming, we consider the special explicit continuation Newton method with the residual trust-region time-stepping scheme for this problem. According to our numerical experiments, the new method is more robust and faster to find the required solution of the real-world problem than the traditional optimization method (the built-in subroutine `fsolve.m` of the MATLAB environment) and the homotopy continuation methods (HOMPACK90 and NACLab). Furthermore, we analyze the global convergence and the local superlinear convergence of the new method.

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

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1 Introduction

In engineering fields, we often need to solve the equilibrium state of the differential equation [27, 39, 45, 51] as follows:

$$\frac{dx}{dt} = F(x), \quad x(t_0) = x_0. \quad (1)$$

That is to say, it requires to solve the following system of nonlinear equations:

$$F(x) = 0, \quad (2)$$

where $F : \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ is a vector function. For the nonlinear system (2), there are many popular traditional optimization methods [6, 10, 19, 42] and the classical homotopy continuation methods [1, 12, 43, 52] to solve it.

For the traditional optimization methods such as the trust-region methods [40, 53, 54] and the line search methods [22, 23], the solution x^* of the nonlinear system (2) is found via solving the following equivalent nonlinear least-squares problem

$$\min_{x \in \mathfrak{R}^n} f(x) = \frac{1}{2} \|F(x)\|^2, \quad (3)$$

where $\|\cdot\|$ denotes the Euclidean vector norm or its induced matrix norm. Generally speaking, the traditional optimization methods based on the merit function (3) are efficient for the large-scale problems since they have the local superlinear convergence near the solution x^* [6, 42].

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 $F(x^*)$ is singular or nearly singular, where $J(x) = \partial F(x)/\partial x$ (see p. 304, [42]). Furthermore, the termination condition

$$\|\nabla f(x_k)\| = \|J(x_k)^T F(x_k)\| < \varepsilon, \quad (4)$$

may lead these methods to early stop far away from the local minimum x^* . It can be illustrated as follows. We consider

$$F(x) = Ax = 0, \quad A = \begin{bmatrix} 1 & 0 \\ 0 & 10^{-6} \end{bmatrix}. \quad (5)$$

It is not difficult to know that the linear system (5) has a unique solution $x^* = (0, 0)$. If we set $\varepsilon = 10^{-6}$, the traditional optimization methods will early stop far away from x^* provided that $x_k = (0, c)$, $c < 10^6$.

For the classical homotopy methods, the solution x^* of the nonlinear system (2) is found via constructing the following homotopy function

$$H(x, \lambda) = (1 - \lambda)G(x) + \lambda F(x), \quad (6)$$

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], where the

zero point of the artificial smooth function $G(x)$ is known. Generally speaking, the homotopy continuation methods are more reliable than the merit-function methods and they are very popular in engineering fields [27]. The disadvantage of the classical homotopy methods is that they require significantly more function and derivative evaluations, and linear algebra operations than the merit-function methods since they need to solve many auxiliary nonlinear systems during the intermediate continuation processes.

In order to overcome this shortcoming of the traditional homotopy methods, we consider the special continuation method based on the following Newton flow [3, 4, 7, 50]

$$\frac{dx(t)}{dt} = -J(x)^{-1}F(x), \quad x(t_0) = x_0, \quad (7)$$

and construct a special ODE method with the new time-stepping scheme based on the trust-region updating strategy to follow the trajectory of the Newton flow (7). Consequently, we obtain its steady-state solution x^* , i.e. the required solution x^* of the nonlinear system (2).

The rest of this article is organized as follows. In the next section, we consider the explicit continuation Newton method with the trust-region updating strategy for nonlinear equations. In section 3, we prove the global convergence and the local super-linear convergence of the new method under some standard assumptions. In section 4, some promising numerical results of the new method are also reported, in comparison to the traditional trust-region method (the built-in subroutine `fsolve.m` of the MATLAB environment [37, 40]) and the classical homotopy continuation methods (HOMOPACK90 [52] and NAClab [25, 55, 56]). Finally, some conclusions and the future work are discussed in section 5. Throughout this article, we assume that $F(\cdot)$ exists the zero point x^* .

2 Continuation Newton methods

In this section, based on the trust-region updating strategy, we construct a new time-stepping scheme for the continuation Newton method to follow the trajectory of the Newton flow and obtain its steady-state solution x^* .

2.1 The continuous Newton flow

If we consider the damped Newton method with the line search strategy for the nonlinear system (2) [22, 42], we have

$$x_{k+1} = x_k - \alpha_k J(x_k)^{-1} F(x_k). \quad (8)$$

We denote $o(\alpha)$ as the higher-order infinitesimal of α , that is to say,

$$\lim_{\alpha \rightarrow 0} \frac{o(\alpha)}{\alpha} = 0.$$

In equation (8), if we let $x_k = x(t_k)$, $x_{k+1} = x(t_k + \alpha_k) + o(\alpha_k)$ and $\alpha_k \rightarrow 0$, we obtain the continuous Newton flow (7). Actually, if we apply an iteration with the explicit Euler method [15, 48] to the continuous Newton flow (7), we 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 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 backtracked to Davidenko's work [7] in 1953. After that, it was investigated by Branin [4], Deuffhard et al [9], Tanabe [50] and Kalaba et al [20] in 1970s, and applied to nonlinear boundary problems by Axelsson and Sysala [3] recently. The continuous and even growing interest in this method originates from its some nice properties. One of them is that the solution $x(t)$ of the continuous Newton flow converges to the steady-state solution x^* from any initial point x_0 , as described by the following property 1.

Property 1 (Branin [4] and Tanabe [50]) Assume that $x(t)$ is the solution of the continuous Newton flow (9), then $f(x(t)) = \|F(x)\|^2$ converges to zero when $t \rightarrow \infty$. That is to say, for every limit point x^* of $x(t)$, it is also a solution of the nonlinear system (2). Furthermore, every element $F^i(x)$ of $F(x)$ has the same convergence rate e^{-t} and $x(t)$ can not converge to the solution x^* of the nonlinear system (2) on the finite interval when the initial point x_0 is not a solution of the nonlinear system (2).

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

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

Consequently, we obtain

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

From equation (10), it is not difficult to know that every element $F^i(x)$ of $F(x)$ converges to zero with the linear convergence rate e^{-t} when $t \rightarrow \infty$. Thus, if the solution $x(t)$ of the continuous Newton flow (9) belongs to a compact set, it has a limit point x^* when $t \rightarrow \infty$, and this limit point x^* is also a solution of the nonlinear system (2).

If we assume that the solution $x(t)$ of the continuous Newton flow (9) converges to the solution x^* of the nonlinear system (2) on the finite interval $(0, T]$, from equation (10), we have

$$F(x^*) = F(x_0) e^{-T}. \quad (11)$$

Since x^* is a solution of the nonlinear system (2), we have $F(x^*) = 0$. By substituting it into equation (11), we obtain

$$F(x_0) = 0.$$

Thus, it contradicts the assumption that x_0 is not a solution of the nonlinear system (2). Consequently, the solution $x(t)$ of the continuous Newton flow (9) can not converge to the solution x^* of the nonlinear system (2) on the finite interval. \square

Remark 1 The inverse $J(x)^{-1}$ of the Jacobian matrix $J(x)$ can be regarded as the preconditioner of $F(x)$ such that the solution elements $x^i(t)$ ($i = 1, 2, \dots, n$) of the continuous Newton flow (7) have the roughly same convergence rates and it mitigates the stiff property of the ODE (7) (the definition of the stiff problem can be found in [16] and references therein). This property is very useful since it makes us adopt the explicit ODE method to follow the trajectory of the Newton flow.

Actually, if we consider $F(x) = Ax$, from the ODE (9), we have

$$A \frac{dx}{dt} = -Ax, x(0) = x_0. \quad (12)$$

By integrating the linear ODE (12), we obtain

$$x(t) = e^{-t}x_0. \quad (13)$$

From equation (13), we know that the solution $x(t)$ of the ODE (12) linearly converges to zero with the same rate e^{-t} when t tends to infinity.

2.2 Continuation Newton methods

From subsection 2.1, we know that the solution $x(t)$ of 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 (DAEs) and its trajectory can not be efficiently followed by the general ODE method such as the backward differentiation formulas (the built-in subroutine `ode15s.m` of the MATLAB environment [2, 5, 16, 37, 48]). Thus, we need to construct the special method to handle this problem. Furthermore, we expect that the new method has the global convergence as the homotopy continuation methods and the fast convergence rate near the solution x^* as the merit-function methods. In order to achieve these two aims, we construct the special continuous Newton method with the new step size $\alpha_k = \Delta t_k / (1 + \Delta t_k)$ and the time step Δt_k is adaptively adjusted by the trust-region updating strategy for problem (9).

Firstly, we apply the implicit Euler method to the continuous Newton flow (9) [2, 5], then we obtain

$$J(x_{k+1})(x_{k+1} - x_k) / \Delta t_k = -F(x_{k+1}). \quad (14)$$

The scheme (14) is an implicit method. Thus, 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 substitute $F(x_{k+1})$ with its linear approximation $F(x_k) + J(x_k)(x_{k+1} - x_k)$ in equation (14). Thus, we obtain the continuation Newton method as follows:

$$J(x_k)s_k = -(\Delta t_k / (1 + \Delta t_k))F(x_k), \quad (15)$$

$$x_{k+1} = x_k + s_k. \quad (16)$$

Remark 2 The explicit continuation Newton method (15)-(16) is similar to the damped Newton method (8) if we let $\alpha_k = \Delta t_k / (1 + \Delta t_k)$ in equation (15). However, from the view of the ODE method, they are different. The damped Newton method (8) is obtained by the explicit Euler method applied to the continuous Newton flow (9), and its time step α_k is restricted by the numerical stability [16,48]. That is to say, the large time step α_k can not be adopted in the steady-state phase. The explicit continuation Newton method (15)-(16) is obtained by the implicit Euler method and its linear approximation applied to the continuous Newton flow (9), and its time step Δt_k is not restricted by the numerical stability for the linear test equation $dx/dt = -\lambda x$, $\lambda > 0$. Therefore, the large time step Δt_k can be adopted in the steady-state phase for the explicit continuation Newton method (15)-(16), and it mimics the Newton method near the steady-state solution x^* such that it has the fast local convergence rate. The most of all, the new time step $\alpha_k = \Delta t_k / (\Delta t_k + 1)$ is favourable to adopt the trust-region updating strategy for adaptively adjusting the time step Δt_k such that the explicit continuation Newton method (15)-(16) accurately follows the trajectory of the continuous Newton flow in the transient-state phase and achieves the fast convergence rate near the steady-state solution x^* .

For the real-world problem, the Jacobian matrix $J(x)$ may be singular, which arises from the physical property. 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 [28]. A system is called to satisfy the linear conservation law ([46], or p. 35, [48]), if there is a constant vector $c \neq 0$ such that

$$c^T x(t) = c^T x(0) \quad (17)$$

holds for all $t \geq 0$. If there exists a constant vector c such that

$$c^T F(x) = 0, \quad \forall x \in \mathfrak{R}^n, \quad (18)$$

we have

$$c^T J(x) = 0, \quad \forall x \in \mathfrak{R}^n. \quad (19)$$

From equation (19), 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 (17).

For the isolated singularity of the Jacobian matrix $J(x)$, there are some efficient approaches to handle this problem [14]. Here, since the singularity set of the Jacobian matrix $J(x)$ may be connected, we adopt the regularization technique [17,21] to modify the explicit continuation Newton method (15)-(16) as follows:

$$(\mu_k I - J(x_k)) s_k^P = F(x_k), \quad (20)$$

$$s_k = (\Delta t_k / (1 + \Delta t_k)) s_k^P, \quad (21)$$

$$x_{k+1} = x_k + s_k, \quad (22)$$

where μ_k is a small positive number. In order to achieve the fast convergence rate near the solution x^* , the regularization continuation Newton method (20)-(22) is required

to approximate the Newton method $x_{k+1} = x_k - J(x_k)^{-1}F(x_k)$ near the solution x^* [11]. Thus, we select the regularization parameter μ_k as follows:

$$\mu_k = \begin{cases} c_\varepsilon, & \text{if } \Delta t_k \leq 1/c_\varepsilon, \\ 1/\Delta t_k, & \text{others,} \end{cases} \quad (23)$$

where c_ε 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 (20)-(22) preserves the linear conservation law (17) if it exists a constant vector $c \in \mathfrak{R}^n$ such that $c^T F(x) = 0$, $\forall x \in \mathfrak{R}^n$. Actually, from $c^T F(x) = 0$, we have $c^T J(x) = 0$. Therefore, from equations (20)-(22), we obtain

$$c^T x_{k+1} = c^T x_k + c^T s_k = c^T x_k + \frac{1}{\mu_k} c^T \left(\frac{\Delta t_k}{1 + \Delta t_k} F(x_k) + J(x_k) s_k \right) = c^T x_k. \quad (24)$$

That is to say, the regularization continuation Newton method (20)-(22) preserves the linear conservation law (17).

2.3 The residual trust-region time-stepping scheme

Another issue is how to adaptively adjust the time-stepping size Δt_k at every iteration. A popular way to control the time-stepping size is based on the trust-region technique [6, 8, 19, 30, 32]. For this time-stepping scheme, it needs to select suitable a merit function and construct an approximation model of the merit function. Here, we adopt the residual $\|F(x)\|$ as the merit function and adopt $\|F(x_k) + J(x_k)s_k\|$ as the approximation model of $\|F(x_k + s_k)\|$. Thus, according to the following ratio:

$$\rho_k = \frac{\|F(x_k)\| - \|F(x_k + s_k)\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|}, \quad (25)$$

we enlarge or reduce the time step Δt_k at every iteration. A particular adjustment strategy is given as follows:

$$\Delta t_{k+1} = \begin{cases} \gamma_1 \Delta t_k, & \text{if } |1 - \rho_k| \leq \eta_1, \\ \Delta t_k, & \text{else if } \eta_1 < |1 - \rho_k| < \eta_2, \\ \gamma_2 \Delta t_k, & \text{others,} \end{cases} \quad (26)$$

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

Remark 3 This new time-stepping scheme based on the trust-region updating strategy has some advantages compared to the traditional line search strategy [24]. If we use the line search strategy and the damped Newton method (8) to track the trajectory $z(t)$ of the continuous Newton flow (9), in order to achieve the fast convergence rate in the steady-state phase, the time step size α_k of the damped Newton method is tried from 1 and reduced by half with many times at every iteration. Since the linear model $F(x_k) + J(x_k)s_k$ may not approximate $F(x_k + s_k)$ well in the transient-state phase, the

time step size α_k will be small. Consequently, the line search strategy consumes the unnecessary trial steps in the transient-state phase. However, the selection scheme of the time step size based on the trust-region updating strategy (25)-(26) can overcome this shortcoming.

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

Algorithm 1 Continuation Newton methods with the residual trust-region time-stepping scheme (The CNMTr method)

Input:

Function $F : \mathfrak{R}^n \rightarrow \mathfrak{R}^n$, the initial point x_0 (optional), and the tolerance ε (optional).

Output:

An approximation solution x^* of nonlinear equations.

- 1: Set the default $x_0 = \text{ones}(n, 1)$ and $\varepsilon = 10^{-6}$ when x_0 or ε is not provided by the calling subroutine.
 - 2: Initialize the parameters: $\eta_a = 10^{-6}$, $\eta_1 = 0.25$, $\gamma_1 = 2$, $\eta_2 = 0.75$, $\gamma_2 = 0.5$, $\text{maxit} = 400$.
 - 3: Set $\Delta t_0 = 10^{-2}$, $\text{flag_success_trialstep} = 1$, $\text{itc} = 0$, $k = 0$.
 - 4: Evaluate $F_k = F(x_k)$ and $J_k = J(x_k)$. Compute the residual $\text{Res}_0 = \|F(x_0)\|_\infty$.
 - 5: **while** ($\text{itc} < \text{maxit}$) **do**
 - 6: **if** ($\text{flag_success_trialstep} == 1$) **then**
 - 7: Set $\text{itc} = \text{itc} + 1$.
 - 8: Compute $\text{Res}_k = \|F_k\|_\infty$.
 - 9: **if** ($\text{Res}_k < \varepsilon$) **then**
 - 10: **break**;
 - 11: **end if**
 - 12: Solve the linear system (20) to obtain the Newton step s_k^p .
 - 13: **end if**
 - 14: Compute $s_k = \Delta t_k / (1 + \Delta t_k) s_k^p$.
 - 15: Set $x_{k+1} = x_k + s_k$.
 - 16: Evaluate $F(x_{k+1})$.
 - 17: **if** $\|F(x_k)\| < \|F(x_k) + J(x_k)s_k\|$ **then**
 - 18: $\rho_k = -1$;
 - 19: **else**
 - 20: Compute the ratio ρ_k from equation (25).
 - 21: **end if**
 - 22: Adjust the time-stepping size Δt_{k+1} according to the trust-region updating strategy (26).
 - 23: **if** ($\rho_k \geq \eta_a$) **then**
 - 24: Accept the trial point x_{k+1} . Set $\text{flag_success_trialstep} = 1$.
 - 25: **else**
 - 26: Set $x_{k+1} = x_k$, $F_{k+1} = F_k$, $s_{k+1}^p = s_k^p$, $\text{flag_success_trialstep} = 0$.
 - 27: **end if**
 - 28: Set $k \leftarrow k + 1$.
 - 29: **end while**
-

3 Convergence analysis

In this section, we discuss some theoretical properties of Algorithm 1. Firstly, we estimate the lower bound of the predicted reduction $\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|$,

which is similar to the estimate of the trust-region method for the unconstrained optimization problem [44].

Lemma 1 *Assume that it exists a positive constant m such that*

$$\|J(x_k)y\| \geq m\|y\|, \forall y \in \mathfrak{R}^n, k = 0, 1, 2, \dots \quad (27)$$

Furthermore, we suppose that s_k is the solution of the regularization continuation Newton method (20)-(22), where the regularization parameter μ_k defined by equation (23) and the constant c_ε satisfy $\mu_k \leq c_\varepsilon < 0.5m$. Then, we have the following estimation

$$\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\| \geq c_r \|F(x_k)\| \Delta t_k / (1 + \Delta t_k), \quad (28)$$

where the positive constant c_r satisfies $0 < c_r < 1$.

Proof. From equations (20)-(21), we have

$$-J(x_k)s_k + \mu_k s_k = (\Delta t_k / (1 + \Delta t_k)) F(x_k). \quad (29)$$

Thus, from equation (29), we obtain

$$\begin{aligned} \|J(x_k)s_k + F(x_k)\| &= \|\mu_k s_k + F(x_k) / (1 + \Delta t_k)\| \\ &= \|\mu_k (\Delta t_k / (1 + \Delta t_k)) (-J(x_k) + \mu_k I)^{-1} F(x_k) + F(x_k) / (1 + \Delta t_k)\| \\ &\leq (1 / (1 + \Delta t_k)) \left(\Delta t_k \left\| (-J(x_k) / \mu_k + I)^{-1} \right\| + 1 \right) \|F(x_k)\|. \end{aligned} \quad (30)$$

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

$$\begin{aligned} \left\| (-J(x_k) / \mu_k + I)^{-1} \right\| &= \max_{z \neq 0} \left\| (-J(x_k) / \mu_k + I)^{-1} z \right\| / \|z\| \\ &= \max_{y \neq 0} \frac{\|y\|}{\|(-J(x_k) / \mu_k + I)y\|} = \frac{1}{\min_{\|y\|=1} \|(-J(x_k) / \mu_k + I)y\|}. \end{aligned} \quad (31)$$

On the other hand, when $\|y\| = 1$, from the nonsingular assumption (27) of matrix $J(x_k)$, we have

$$\begin{aligned} \|(-J(x_k) / \mu_k + I)y\| &= \|-J(x_k)y / \mu_k + y\| \\ &\geq \|J(x_k)y\| / \mu_k - \|y\| \geq m / \mu_k - 1. \end{aligned} \quad (32)$$

Thus, from the assumption $\mu_k \leq c_\varepsilon < 0.5m$ and equations (31)-(32), we have

$$\left\| (-J(x_k) / \mu_k + I)^{-1} \right\| \leq \mu_k / (m - \mu_k) \leq c_\varepsilon / (m - c_\varepsilon). \quad (33)$$

By substituting inequality (33) into inequality (30), we have

$$\|J(x_k)s_k + F(x_k)\| \leq ((1 + c_\varepsilon \Delta t_k / (m - c_\varepsilon)) / (1 + \Delta t_k)) \|F(x_k)\|.$$

That is to say, we obtain

$$\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\| \geq \left(\frac{m - 2c_\varepsilon}{m - c_\varepsilon} \right) \frac{\Delta t_k}{1 + \Delta t_k} \|F(x_k)\|. \quad (34)$$

We set $c_r = (m - 2c_\varepsilon)/(m - c_\varepsilon)$ in the above inequality (34). Then, we obtain the estimation (28). \square

In order to prove that the sequence $\{\|F(x_k)\|\}$ converges to zero when k tends to infinity, we also need to estimate the lower bound of the time step size Δt_k .

Lemma 2 Assume that $F : \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ is continuously differentiable and its Jacobian function J is Lipschitz continuous. That to say, it exists a positive number L such that

$$\|J(x) - J(y)\| \leq L\|x - y\| \quad (35)$$

holds for all $x, y \in \mathfrak{R}^n$. Furthermore, we suppose that the sequence $\{x_k\}$ is generated by Algorithm 1 and the nonsingular condition (27) of matrix $J(x_k)$ holds. Then, when the regularization parameter μ_k defined by equation (23) and the constant c_ε satisfy $\mu_k \leq c_\varepsilon < 0.5m$, it exists a positive number $\delta_{\Delta t}$ such that

$$\Delta t_k \geq \delta_{\Delta t} > 0, \quad k = 0, 1, 2, \dots, \quad (36)$$

where Δt_k is adaptively adjusted by formulas (25)-(26).

Proof. From the Lipschitz continuous assumption (35) of $J(\cdot)$, we have

$$\begin{aligned} \|F(x_{k+1}) - F(x_k) - J(x_k)s_k\| &= \left\| \int_0^1 J(x_k + ts_k)s_k dt - J(x_k)s_k \right\| \\ &= \left\| \int_0^1 (J(x_k + ts_k) - J(x_k))s_k dt \right\| \leq \int_0^1 \| (J(x_k + ts_k) - J(x_k))s_k \| dt \\ &\leq \int_0^1 \|J(x_k + ts_k) - J(x_k)\| \|s_k\| dt \leq \int_0^1 L \|s_k\|^2 t dt = 0.5L \|s_k\|^2. \end{aligned} \quad (37)$$

On the other hand, from equations (20)-(21), we have

$$\begin{aligned} \|s_k\| &= (\Delta t_k / (1 + \Delta t_k)) \left\| (-J(x_k) + \mu_k I)^{-1} F(x_k) \right\| \\ &\leq (\Delta t_k / (1 + \Delta t_k)) \left\| (-J(x_k) + \mu_k I)^{-1} \right\| \|F(x_k)\|. \end{aligned} \quad (38)$$

Similarly to the estimation (33), from the assumption $\mu_k \leq c_\varepsilon < 0.5m$ and the nonsingular assumption (27) of $J(x_k)$, we have

$$\left\| (-J(x_k) + \mu_k I)^{-1} \right\| \leq 1/(m - \mu_k) \leq 1/(m - c_\varepsilon). \quad (39)$$

Thus, from inequalities (37)-(39), we obtain

$$\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\| \leq \frac{L}{2(m - c_\varepsilon)^2} \left(\frac{\Delta t_k}{1 + \Delta t_k} \right)^2 \|F(x_k)\|^2. \quad (40)$$

From the definition (25) of ρ_k , the estimation (34), and inequality (40), we have

$$\begin{aligned} |\rho_k - 1| &= \left| \frac{\|F(x_k)\| - \|F(x_{k+1})\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} - 1 \right| \\ &\leq \frac{\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} \leq \frac{L}{2(m-2c_\varepsilon)^2} \left(\frac{\Delta t_k}{1 + \Delta t_k} \right) \|F(x_k)\|. \end{aligned} \quad (41)$$

According to Algorithm 1, we know that the sequence $\{\|F(x_k)\|\}$ is monotonically decreasing. Consequently, we have $\|F(x_k)\| \leq \|F(x_0)\|$, $k = 1, 2, \dots$. We set

$$\bar{\delta}_{\Delta t} \triangleq 2(m-2c_\varepsilon)^2 \eta_1 / (\|F(x_0)\|L). \quad (42)$$

Assume that K is the first index such that $\Delta t_K \leq \bar{\delta}_{\Delta t}$. Then, from inequalities (41)-(42), we obtain $|\rho_K - 1| < \eta_1$. Consequently, Δt_{K+1} will be greater than Δt_K according to the adaptive adjustment scheme (26). We set $\delta_{\Delta t} = \min\{\Delta t_K, \bar{\delta}_{\Delta t}\}$. Then, $\Delta t_k \geq \delta_{\Delta t}$ holds for all $k = 0, 1, 2, \dots$. \square

By using the estimation results of Lemma 1 and Lemma 2, we can prove that the sequence $\{\|F(x_k)\|\}$ converges to zero when k tends to infinity.

Theorem 1 Assume that $F : \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ is continuously differentiable and its Jacobian function J satisfies the Lipschitz condition (35). Furthermore, we suppose that the sequence $\{x_k\}$ is generated by Algorithm 1 and $J(x_k)$ satisfies the nonsingular assumption (27). Then, when the regularization parameter μ_k defined by equation (23) and the constant c_ε satisfy $\mu_k \leq c_\varepsilon < 0.5m$, we have

$$\liminf_{k \rightarrow \infty} \|F(x_k)\| = 0. \quad (43)$$

Proof. According to Algorithm 1 and inequality (41), we know that there exists an infinite subsequence $\{x_{k_l}\}$ such that

$$\frac{\|F(x_{k_l})\| - \|F(x_{k_l} + s_{k_l})\|}{\|F(x_{k_l})\| - \|F(x_{k_l}) + J(x_{k_l})s_{k_l}\|} \geq \eta_a, \quad l = 1, 2, \dots \quad (44)$$

Otherwise, all steps are rejected after a given iteration index, then the time step size Δt_k will keep decreasing, which contradicts equation (36).

From inequalities (28), (36) and (44), we have

$$\|F(x_{k_l})\| - \|F(x_{k_l} + s_{k_l})\| \geq \frac{\eta_a c_r \Delta t_{k_l}}{(1 + \Delta t_{k_l})} \|F(x_{k_l})\| \geq \frac{\eta_a c_r \delta_{\Delta t}}{(1 + \delta_{\Delta t})} \|F(x_{k_l})\|. \quad (45)$$

Therefore, from equation (45) and $\|F(x_{k+1})\| \leq \|F(x_k)\|$, we have

$$\begin{aligned} \|F(x_0)\| &\geq \|F(x_0)\| - \lim_{k \rightarrow \infty} \|F(x_k)\| = \sum_{k=0}^{\infty} (\|F(x_k)\| - \|F(x_{k+1})\|) \\ &\geq \sum_{l=0}^{\infty} (\|F(x_{k_l})\| - \|F(x_{k_l} + s_{k_l})\|) \geq \frac{\eta_a c_r \delta_{\Delta t}}{1 + \delta_{\Delta t}} \sum_{l=0}^{\infty} \|F(x_{k_l})\|. \end{aligned} \quad (46)$$

Consequently, from inequality (46), we obtain

$$\lim_{k_l \rightarrow \infty} \|F(x_{k_l})\| = 0. \quad (47)$$

That is to say, the result (43) is true. Furthermore, from $\|F(x_{k+1})\| \leq \|F(x_k)\|$ and equation (47), it is not difficult to know $\lim_{k \rightarrow \infty} \|F(x_k)\| = 0$. \square

Under the nonsingular assumption of $J(x^*)$ and the local Lipschitz continuity (35) of $J(\cdot)$, we analyze the local superlinear convergence rate of Algorithm 1 near the solution x^* as follows. For convenience, we define the neighbourhood $B_\delta(x^*)$ of x^* as

$$B_\delta(x^*) = \{x : \|x - x^*\| \leq \delta\}.$$

Theorem 2 *Assume that $F : \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ is continuously differentiable and $F(x^*) = 0$. Furthermore, we suppose that J satisfies the local Lipschitz continuity (35) around x^* and the nonsingular condition (27) when $x \in B_\delta(x^*)$. Then, when the regularization parameter μ_k defined by equation (23) and the constant c_ε satisfy $\mu_k \leq c_\varepsilon < 0.5m$, there exists a neighborhood $B_r(x^*)$ such that the sequence $\{x_k\}$ generated by Algorithm 1 with $x_0 \in B_r(x^*)$ superlinearly converges to x^* .*

Proof. The framework of its proof can be roughly described as follows. Firstly, we prove that the sequence $\{x_k\}$ linearly converges to x^* when x_0 gets close enough to x^* . Then, we prove $\lim_{k \rightarrow \infty} \Delta t_k = \infty$. Finally, we prove that the search step s_k approximates the Newton step s_k^N . Consequently, the sequence $\{x_k\}$ superlinearly converges to x^* .

Firstly, similarly to the estimation (33), from the assumption $\mu_k \leq c_\varepsilon < 0.5m$, we obtain

$$\|(\mu_k I - J(x_k))^{-1}\| \leq 1/(m - c_\varepsilon), \quad \forall x_k \in B_\delta(x^*), \quad k = 0, 1, 2, \dots \quad (48)$$

We denote $e_k = x_k - x^*$. From equations (20)-(21), we have

$$\begin{aligned} e_{k+1} &= e_k + s_k = e_k + \frac{\Delta t_k}{1 + \Delta t_k} (\mu_k I - J(x_k))^{-1} (F(x_k) - F(x^*)) \\ &= e_k + \frac{\Delta t_k}{1 + \Delta t_k} (\mu_k I - J(x_k))^{-1} \int_0^1 J(x^* + te_k) e_k dt. \end{aligned} \quad (49)$$

By rearranging the above equation (49), we obtain

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

By using the Lipschitz continuous assumption (35) of $J(\cdot)$, the estimation (48), and the assumption $\mu_k \leq c_\varepsilon < 0.5m$, we have

$$\begin{aligned} \|e_{k+1}\| &\leq \|e_k\|/(1 + \Delta t_k) \\ &+ (\Delta t_k/(1 + \Delta t_k)) \left\| (\mu_k I - J(x_k))^{-1} \right\| \int_0^1 (\|J(x^* + te_k) - J(x_k)\| + \mu_k) \|e_k\| dt \\ &\leq \|e_k\|/(1 + \Delta t_k) + (\Delta t_k/((1 + \Delta t_k)(m - \mu_k))) (\mu_k + 0.5L\|e_k\|) \|e_k\| \\ &= \frac{1 + \frac{1}{m - \mu_k} (\mu_k + 0.5L\|e_k\|) \Delta t_k}{1 + \Delta t_k} \|e_k\| \leq \frac{1 + \frac{1}{m - c_\varepsilon} (c_\varepsilon + 0.5L\|e_k\|) \Delta t_k}{1 + \Delta t_k} \|e_k\|. \end{aligned} \quad (50)$$

We denote

$$q_k \triangleq \frac{1 + (c_\varepsilon + 0.5L\|e_k\|) \Delta t_k / (m - c_\varepsilon)}{1 + \Delta t_k}, \quad (51)$$

and select $x_0 \in B_\delta(x^*)$ to satisfy

$$\|e_0\| < (m - 2c_\varepsilon)/L. \quad (52)$$

We set $r = \min\{\delta, (m - 2c_\varepsilon)/L\}$. When $x_0 \in B_r(x^*)$, from equations (50)-(52) and the assumption $c_\varepsilon < 0.5m$, by induction, we have

$$\|e_{k+1}\| \leq q_k \|e_k\|, \quad q_k < \frac{1 + 0.5\Delta t_k m / (m - c_\varepsilon)}{1 + \Delta t_k} < 1, \quad k = 0, 1, \dots \quad (53)$$

It is not difficult to know that $f(t) \triangleq (1 + \alpha t)/(1 + t)$ is monotonically decreasing when $0 \leq \alpha < 1$. Thus, from the estimation (36) of the time step size Δt_k and inequality (53), we obtain

$$\|e_{k+1}\| \leq q_k \|e_k\| \leq q \|e_k\|, \quad q \triangleq \frac{1 + 0.5\delta_{\Delta t} m / (m - c_\varepsilon)}{1 + \delta_{\Delta t}} < 1.$$

Therefore, we have

$$\|e_{k+1}\| \leq q^k \|e_0\| \rightarrow 0, \quad \text{when } k \rightarrow \infty. \quad (54)$$

That is to say, we obtain $\lim_{k \rightarrow \infty} x_k = x^*$.

Secondly, from equations (20)-(21) and inequality (48), we have

$$\begin{aligned} \|s_k\| &= (\Delta t_k / (1 + \Delta t_k)) \left\| (-J(x_k) + \mu_k I)^{-1} F(x_k) \right\| \\ &\leq \frac{\Delta t_k}{1 + \Delta t_k} \left\| (-J(x_k) + \mu_k I)^{-1} \right\| \|F(x_k)\| \leq \frac{1}{m - c_\varepsilon} \frac{\Delta t_k}{1 + \Delta t_k} \|F(x_k)\|. \end{aligned} \quad (55)$$

Similarly to the estimation (41), from the definition (25) of ρ_k , inequalities (34) and (55), we have

$$\begin{aligned} |\rho_k - 1| &= \left| \frac{\|F(x_k)\| - \|F(x_{k+1})\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} - 1 \right| \\ &\leq \frac{0.5L}{(m - 2c_\varepsilon)^2} \left(\frac{\Delta t_k}{1 + \Delta t_k} \right) \|F(x_k)\| \leq \frac{0.5L}{(m - 2c_\varepsilon)^2} \|F(x_k)\|. \end{aligned} \quad (56)$$

Since $\{\|F(x_k)\|\}$ is monotonically decreasing and $\lim_{k \rightarrow \infty} x_k = x^*$, $F(x^*) = 0$, we can select a sufficiently large number K such that

$$\|F(x_k)\| \leq \frac{2\eta_1(m-2c_\varepsilon)^2}{L}, \text{ when } k \geq K. \quad (57)$$

From inequalities (56)-(57), we have

$$|\rho_k - 1| \leq \eta_1, \text{ when } k \geq K.$$

This means $\Delta t_{k+1} = \gamma_1 \Delta t_k$ when $k \geq K$, according to the time-stepping scheme (26). That is to say, we have

$$\lim_{k \rightarrow \infty} \Delta t_k = \infty. \quad (58)$$

Finally, since $\lim_{k \rightarrow \infty} \Delta t_k = \infty$, we can select a sufficiently large number K_μ such that $1/\Delta t_k < c_\varepsilon$ when $k \geq K_\mu$. Consequently, from the definition (23) of the regularization parameter μ_k , we obtain $\mu_k = 1/\Delta t_k$ when $k \geq K_\mu$. By substituting it into inequality (50), we have

$$\begin{aligned} \frac{\|e_{k+1}\|}{\|e_k\|} &\leq \frac{1}{1+\Delta t_k} + \frac{\Delta t_k}{1+\Delta t_k} \frac{1}{m-\mu_k} (\mu_k + 0.5L\|e_k\|) \\ &= \frac{1}{1+\Delta t_k} + \frac{\Delta t_k}{1+\Delta t_k} \frac{1}{m-1/\Delta t_k} (1/\Delta t_k + 0.5L\|e_k\|), \text{ when } k \geq K_\mu. \end{aligned} \quad (59)$$

From equations (54) and (58), we know $\lim_{k \rightarrow \infty} \|e_k\| = 0$ and $\lim_{k \rightarrow \infty} \Delta t_k = \infty$, respectively. Therefore, by combining them with inequality (59), we obtain

$$\lim_{k \rightarrow \infty} \frac{\|e_{k+1}\|}{\|e_k\|} = 0.$$

That is to say, the sequence $\{x_k\}$ superlinearly converges to x^* . \square

For the real-world problem, the singularity of $J(x)$ may arise from the linear conservation law such as the conservation of mass or the conservation of charge [31, 46, 47, 48]. In the rest of this section, we analyze convergence properties of Algorithm 1 when $J(x)$ is singular. Similarly to the standard assumption of the nonlinear dynamical system, we suppose that $J(\cdot)$ satisfies the one-sided Lipschitz condition (see p. 303, [8] or p. 180, [16]) as follows:

$$y^T J(x)y \leq -\nu \|y\|^2, \text{ for } y \in S_c = \{y | c^T y = 0\}, \nu > 0, \quad (60)$$

where the constant vector c satisfies $c^T F(x) = 0$, $\forall x \in \mathfrak{R}^n$. The positive number ν is called the one-sided Lipschitz constant. Under the assumption of the one-sided Lipschitz condition (60), we know that matrix $(\mu I - J(x))$ is nonsingular when $\mu > 0$. We state it as the following property 2.

Property 2 Assume that $J(\cdot)$ satisfies the one-sided Lipschitz condition (60). Then, matrix $(\mu I - J(x))$ is nonsingular when $\mu > 0$, and the solution s_k of equations (20)-(21) satisfies $c^T s_k = 0$.

Proof. We prove it by contradiction. If we assume that matrix $(\mu I - J(x))$ is singular, there exists a nonzero vector y such that

$$(\mu I - J(x))y = 0. \quad (61)$$

Consequently, from the assumption $c^T F(x) = 0$, we have

$$c^T y = c^T (J(x)y)/\mu = (c^T J(x))y/\mu = 0.$$

Thus, from the one-sided Lipschitz condition (60) and $\mu > 0$, $\nu > 0$, we obtain

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

which contradicts the assumption (61). Therefore, matrix $(\mu I - J(x))$ is nonsingular.

From equations (20)-(21), we have

$$(\mu_k I - J(x_k))s_k = (\Delta t_k / (1 + \Delta t_k))F(x_k). \quad (62)$$

By combining it with the assumption $c^T F(x_k) = 0$, we obtain

$$c^T (\mu_k I - J(x_k))s_k = (\Delta t_k / (1 + \Delta t_k))c^T F(x_k) = 0. \quad (63)$$

Therefore, by substituting $c^T J(x_k) = 0$ into equation (63), we have

$$\mu_k c^T s_k = c^T J(x_k)s_k = (c^T J(x_k))s_k = 0. \quad (64)$$

That is to say, we obtain $c^T s_k = 0$. \square

Similarly to the estimation (28) of $\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|$ for the nonsingular Jacobian matrix $J(x_k)$, we also have its lower-bounded estimation when $J(x_k)$ is singular, $k = 0, 1, 2, \dots$

Lemma 3 Assume that $J(x_k)$ satisfies the one-sided Lipschitz condition (60) and s_k is the solution of equations (20)-(22). Then, we have

$$\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\| \geq c_s (\Delta t_k / (1 + \Delta t_k)) \|F(x_k)\|, \quad (65)$$

where the positive constant c_s satisfies $0 < c_s < 1$.

Proof. From Property 2, we know that matrix $(\mu I - J(x_k))$ is nonsingular and s_k satisfies $c^T s_k = 0$. From equations (20)-(21) and the Cauchy-Schwartz inequality $|x^T y| \leq \|x\| \|y\|$, we have

$$\mu_k \|s_k\|^2 - s_k^T J(x_k)s_k = s_k^T F(x_k) \Delta t_k / (1 + \Delta t_k) \leq (\Delta t_k / (1 + \Delta t_k)) \|s_k\| \|F(x_k)\|. \quad (66)$$

By substituting one-sided Lipschitz condition (60) into equation (66), we obtain

$$(\mu_k + \nu) \|s_k\|^2 \leq \mu_k \|s_k\|^2 - s_k^T J(x_k)s_k \leq (\Delta t_k / (1 + \Delta t_k)) \|s_k\| \|F(x_k)\|.$$

Consequently, we have

$$\|s_k\| \leq \frac{1}{\mu_k + \nu} \frac{\Delta t_k}{1 + \Delta t_k} \|F(x_k)\|. \quad (67)$$

From equations (20)-(21) and (67), we have

$$\begin{aligned} \|F(x_k) + J(x_k)s_k\| &= \left\| \mu_k s_k + \frac{1}{1 + \Delta t_k} F(x_k) \right\| \leq \mu_k \|s_k\| + \frac{1}{1 + \Delta t_k} \|F(x_k)\| \\ &\leq \frac{\mu_k}{\mu_k + \nu} \frac{\Delta t_k}{1 + \Delta t_k} \|F(x_k)\| + \frac{1}{1 + \Delta t_k} \|F(x_k)\|. \end{aligned} \quad (68)$$

From the definition (23) of the parameter μ_k , we know $\mu_k \leq c_\varepsilon$. By substituting it into inequality (68), we obtain

$$\begin{aligned} \|F(x_k)\| - \|F(x_k) + J(x_k)s_k\| &\geq \frac{\nu}{\mu_k + \nu} \frac{\Delta t_k}{1 + \Delta t_k} \|F(x_k)\| \\ &\geq \frac{\nu}{c_\varepsilon + \nu} \frac{\Delta t_k}{1 + \Delta t_k} \|F(x_k)\|. \end{aligned} \quad (69)$$

We set $c_s = \nu/(c_\varepsilon + \nu)$. Then, from equation (69), we obtain the estimation (65). \square

Similarly to the lower-bounded estimation (36) of the time step size Δt_k for the nonsingular Jacobian matrix $J(x_k)$, we also have its lower-bounded estimation when $J(x_k)$ is singular, $k = 0, 1, 2, \dots$

Lemma 4 *Assume that $F : \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ is continuously differentiable and $J(\cdot)$ satisfies the Lipschitz continuity (35) and the one-sided Lipschitz condition (60). The sequence $\{x_k\}$ is generated by Algorithm 1. Then, there exists a positive δ_s such that*

$$\Delta t_k \geq \delta_s > 0, \quad k = 1, 2, \dots, \quad (70)$$

where Δt_k is adaptively updated by the trust-region updating strategy (25)-(26).

Proof. From the Lipschitz continuity (35) of $J(\cdot)$, we have

$$\begin{aligned} \|F(x_{k+1}) - F(x_k) - J(x_k)s_k\| &= \left\| \int_0^1 (J(x_k + ts_k) - J(x_k))s_k dt \right\| \\ &\leq \int_0^1 \|J(x_k + ts_k) - J(x_k)\| \|s_k\| dt \leq \int_0^1 L \|s_k\|^2 t dt = 0.5L \|s_k\|^2. \end{aligned} \quad (71)$$

By substituting the estimation (67) of s_k into inequality (71), we obtain

$$\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\| \leq \frac{0.5L}{(\mu_k + \nu)^2} \left(\frac{\Delta t_k}{1 + \Delta t_k} \right)^2 \|F(x_k)\|^2. \quad (72)$$

Thus, from the definition (25) of ρ_k , inequalities (69) and (72), we obtain

$$\begin{aligned} |\rho_k - 1| &= \left| \frac{\|F(x_k)\| - \|F(x_{k+1})\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} - 1 \right| \leq \frac{\|F(x_{k+1}) - F(x_k) - J(x_k)s_k\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} \\ &\leq \frac{L}{2\nu(\mu_k + \nu)} \left(\frac{\Delta t_k}{1 + \Delta t_k} \right) \|F(x_k)\| \leq \frac{L}{2\nu^2} \left(\frac{\Delta t_k}{1 + \Delta t_k} \right) \|F(x_k)\|. \end{aligned} \quad (73)$$

According to Algorithm 1, we know that the sequence $\{\|F(x_k)\|\}$ is monotonically decreasing. Consequently, we have $\|F(x_k)\| \leq \|F(x_0)\|$, $k = 1, 2, \dots$. We set

$$\bar{\delta}_s = 2v^2\eta_1/(\|F(x_0)\|L). \quad (74)$$

If we assume that K is the first index such that $\Delta t_K \leq \bar{\delta}_s$, then, from inequalities (73)-(74), we obtain $|\rho_K - 1| < \eta_1$. Consequently, Δt_{K+1} will be greater than Δt_K according to the time-stepping scheme (26). Set $\delta_s = \min\{\Delta t_K, \bar{\delta}_s\}$. Then, we have $\Delta t_k \geq \delta_s$, $k = 0, 1, 2, \dots$. \square

Now, from 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 the proof of Theorem 1. We state it as the following theorem 3 and omit its proof.

Theorem 3 Assume that $F : \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ is continuously differentiable and its Jacobian function $J(\cdot)$ satisfies the Lipschitz continuity (35) and the one-sided Lipschitz condition (60). The sequence $\{x_k\}$ is generated by Algorithm 1. Then, we have

$$\liminf_{k \rightarrow \infty} \|F(x_k)\| = 0. \quad (75)$$

Theorem 4 Assume that $F : \mathfrak{R}^n \rightarrow \mathfrak{R}^n$ is continuously differentiable and its Jacobian function $J(\cdot)$ satisfies the Lipschitz continuity (35) and the one-sided Lipschitz condition (60). Furthermore, we suppose that the sequence $\{x_k\}$ is generated by Algorithm 1 and its subsequence $\{x_{k_i}\}$ converges to x^* . Then, the sequence $\{x_k\}$ superlinearly converges to x^* .

Proof. The framework of its proof can be roughly described as follows. Firstly, we prove $\lim_{k \rightarrow \infty} \Delta t_k = \infty$. Then, we prove that the sequence $\{x_k\}$ linearly converges to x^* . Finally, we prove that the search step s_k approximates the Newton step s_k^N . Consequently, the sequence $\{x_k\}$ superlinearly converges to x^* .

From Property 2, we know that matrix $(\mu I - J(x_k))$ is nonsingular and s_k satisfies $c^T s_k = 0$, where the constant vector c satisfies $c^T F(x) = 0$ for all $x \in \mathfrak{R}^n$ and s_k is the solution of equations (20)-(21).

Firstly, we prove that there exists an index K such that Δt_k will be enlarged at every iteration when $k \geq K$. Consequently, we have $\lim_{k \rightarrow \infty} \Delta t_k = \infty$. From the lower-bounded estimation (69) of $F(x_k) - F(x_k + s_k)$ and inequality (73), we have

$$\begin{aligned} |\rho_k - 1| &= \left| \frac{\|F(x_k)\| - \|F(x_{k+1})\|}{\|F(x_k)\| - \|F(x_k) + J(x_k)s_k\|} - 1 \right| \\ &\leq \frac{L}{2v(\mu_k + v)} \left(\frac{\Delta t_k}{1 + \Delta t_k} \right) \|F(x_k)\| \leq \frac{L}{2v^2} \|F(x_k)\|. \end{aligned} \quad (76)$$

Since the subsequence $\{x_{k_i}\}$ converges to x^* , there exists an index K_F such that

$$\|F(x_{K_F})\| \leq 2\eta_1 v^2 / L. \quad (77)$$

Furthermore, according to Algorithm 1, we know that the sequence $\{\|F(x_k)\|\}$ is monotonically decreasing. Consequently, we have $\|F(x_k)\| \leq \|F(x_{K_F})\|$ when $k \geq K_F$. Thus, from inequalities (76)-(77), we have

$$|\rho_k - 1| \leq \eta_1, \text{ when } k \geq K_F. \quad (78)$$

Consequently, according to the time-stepping scheme (26), we know that $\Delta t_{k+1} = \gamma_1 \Delta t_k$ when $k \geq K_F$. Therefore, we obtain $\lim_{k \rightarrow \infty} \Delta t_k = \infty$.

Secondly, we prove that the sequence $\{x_k\}$ linearly converges to x^* as follows. We denote

$$e_k = x_k - x^*. \quad (79)$$

From equations (20)-(21) and (79), we have

$$e_{k+1} = e_k + s_k = e_k + (\Delta t_k / (1 + \Delta t_k)) (\mu_k I - J(x_k))^{-1} F(x_k). \quad (80)$$

By rearranging inequality (80), we obtain

$$\begin{aligned} (\mu_k I - J(x_k)) e_{k+1} &= (\mu_k I - J(x_k)) e_k + (\Delta t_k / (1 + \Delta t_k)) (F(x_k) - F(x^*)) \\ &= \mu_k e_k - J(x_k) e_k / \Delta t_k + (\Delta t_k / (1 + \Delta t_k)) \int_0^1 (J(x^* + t e_k) - J(x_k)) e_k dt. \end{aligned} \quad (81)$$

Since $c^T s_k = 0$ and the subsequence $\{x_{k_i}\}_{i=1}^{+\infty}$ converges to x^* , from equation (80), we have

$$c^T e_{k+1} = c^T e_k + c^T s_k = c^T e_k = \dots = c^T e_{k_i} \rightarrow 0, \text{ when } i \rightarrow \infty.$$

That is to say, we have $c^T e_k = 0$, $k = 0, 1, \dots$. Thus, from the one-sided Lipschitz condition (60) and the Cauchy-Schwartz inequality $|x^T y| \leq \|x\| \|y\|$, we have

$$\begin{aligned} \|e_{k+1}\| \|(\mu_k I - J(x_k)) e_{k+1}\| &\geq e_{k+1}^T (\mu_k I - J(x_k)) e_{k+1} \\ &= \mu_k e_{k+1}^T e_{k+1} - e_{k+1}^T J(x_k) e_{k+1} \geq (\mu_k + \nu) \|e_{k+1}\|^2. \end{aligned} \quad (82)$$

By rearranging inequality (82), we obtain

$$\|e_{k+1}\| \leq \|(\mu_k I - J(x_k)) e_{k+1}\| / (\mu_k + \nu). \quad (83)$$

From the continuity of J at x^* , there exists the positive constants M and ε such that

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

Since the subsequence $\{x_{k_i}\}$ converges to x^* , there exists K_1 such that $\|x_{K_1} - x^*\| < \varepsilon$. By combining it with $\lim_{k \rightarrow \infty} \Delta t_k = \infty$, we can select a sufficiently large number K_2 such that $\Delta t_{K_2} \geq 4M/\nu$ and $\|e_{K_2}\| \leq 0.5\nu/L$. We set $K = \max\{K_1, K_2\}$.

From equation (81) and the Lipschitz continuity (35), we have

$$\begin{aligned} \|(\mu_K I - J(x_K))e_{K+1}\| &\leq \mu_K \|e_K\| + \|J(x_K)\| \|e_K\| / \Delta t_K \\ &+ \int_0^1 \|J(x^* + te_K) - J(x_K)\| \|e_K\| dt \Delta t_K / (1 + \Delta t_K) \\ &\leq (\mu_K + M/\Delta t_K) \|e_K\| + \int_0^1 L \|e_K\|^2 dt \leq (\mu_K + M/\Delta t_K + 0.5L\|e_K\|) \|e_K\|. \end{aligned}$$

By combining it with inequality (83), $\Delta t_K \geq (4M)/\nu$, and $\|e_K\| \leq \nu/(2L)$, we obtain

$$\|e_{K+1}\| \leq \frac{\mu_K + M/\Delta t_K + 0.5L\|e_K\|}{\mu_K + \nu} \|e_K\| \leq \frac{\mu_K + 0.5\nu}{\mu_K + \nu} \|e_K\| < \|e_K\| < \varepsilon. \quad (84)$$

Therefore, by induction, we obtain

$$\|e_{k+1}\| \leq \frac{\mu_k + M/\Delta t_k + 0.5L\|e_k\|}{\mu_k + \nu} \|e_k\| \leq \frac{\mu_k + 0.5\nu}{\mu_k + \nu} \|e_k\|, \text{ when } k \geq K. \quad (85)$$

Furthermore, from the definition (23), we know that $\mu_k < c_\varepsilon$. By substituting it into inequality (85), we have

$$\|e_{k+1}\| \leq q \|e_k\| \leq \dots \leq q^{(k-K+1)} \|e_K\|, \quad q \triangleq \frac{c_\varepsilon + 1/2\nu}{c_\varepsilon + \nu} < 1, \text{ when } k \geq K.$$

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

Finally, we prove that the sequence $\{x_k\}$ superlinearly converges to x^* . Since $\lim_{k \rightarrow \infty} \Delta t_k = \infty$, we can select a sufficiently large number K_μ such that $1/\Delta t_k < c_\varepsilon$ when $k \geq K_\mu$. Thus, from the definition (23) of the regularization parameter μ_k , we know $\mu_k = 1/\Delta t_k$ when $k \geq K_\mu$. By substituting it into equation (85), we obtain

$$\frac{\|e_{k+1}\|}{\|e_k\|} \leq \frac{\mu_k + M/\Delta t_k + 0.5L\|e_k\|}{\mu_k + \nu} = \frac{1/\Delta t_k + M/\Delta t_k + 0.5L\|e_k\|}{1/\Delta t_k + \nu}. \quad (86)$$

Consequently, from $\lim_{k \rightarrow \infty} \Delta t_k = \infty$, $\lim_{k \rightarrow \infty} \|e_k\| = 0$, and equation (86), we have $\lim_{k \rightarrow \infty} \|e_{k+1}\|/\|e_k\| = 0$. That is to say, the sequence $\{x_k\}$ superlinearly converges to x^* . \square

4 Numerical Experiments

In this section, for some real-world 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 [37, 40]) and the homotopy methods (HOMPACK90 [52], and NAClab [25, 55, 56]).

HOMPACK90 [52] 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

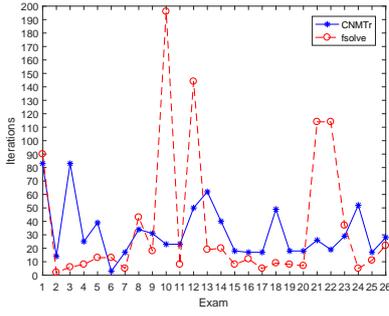


Fig. 1: The number of iterations.

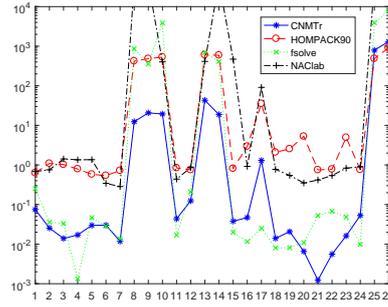


Fig. 2: The computational time.

[25,55]. 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, 45, 51], and some of which come from the classical test problems [8, 10, 29, 41, 42]. Their simple descriptions are given by Table 1. Their dimensions vary from 1 to 3000. The Jacobian matrix $J(\cdot)$ of $F(\cdot)$ is singular for some test problems. The codes are executed by a HP Pavilion notebook with an Intel quad-core CPU. The termination condition is given by

$$\|F(x^{it})\|_{\infty} \leq 10^{-12}. \quad (87)$$

The numerical results are arranged in Table 3 and Table 2. The number of iterations of CNMTr and `fsolve` is illustrated by Figure 1. The computational time of these four methods (CNMTr, HOMPACK90, `fsolve` and NAClab) is illustrated by Figure 2. From Table 3 and Table 2, we find that CNMTr performs well for those test problems. However, the trust-region method (`fsolve`) and the classical homotopy methods (HOMPACK90 and NAClab) fail to solve some problems, which especially come from the real-world 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 has the same fast convergence property as the traditional optimization method (`fsolve`).

5 Conclusions

In this article, we consider the continuation Newton method with the new time-stepping scheme (CNMTr) based on the trust-region updating strategy. We also analyze its local and global convergence for the nonsingular Jacobian and singular Jacobian problems. Finally, for some classical test problems, we compare it with the classical homotopy methods (HOMPACK90 and `psolve.m`) and the traditional optimization method (`fsolve.m`). Numerical results show that CNMTr is more robust and

Table 1: Test problems.

Problems	dimension	problem descriptions
Exam 1	$n = 3$	Robertson problem, an autocatalytic reaction [16,45]
Exam 2	$n = 4$	E5, the chemical pyrolysis [16]
Exam 3	$n = 20$	The pollution problem [51]
Exam 4	$n = 5$	The stability problem of an aircraft (p. 279, [42])
Exam 5	$n = 1$	$F(x) = \sin(5x) - x$ (p. 279, [42])
Exam 6	$n = 2$	$e^{x^2+y^2} - 3 = 0,$ $x + y - \sin(3(x+y)) = 0$ (p. 149, [8])
Exam 7	$n = 2$	$x = 0, -2y = 0$
Exam 8	$n = 3000$	Extended Rosenbrock function (p. 362, [10] or [41])
Exam 9	$n = 3000$	Extended Powell singular function (p. 362, [10] or [41])
Exam 10	$n = 3000$	Trigonometric function (p. 362, [10] or [41])
Exam 11	$n = 3$	Helical valley function (p. 362, [10])
Exam 12	$n = 4$	Wood function (p. 362, [10])
Exam 13	$n = 3000$	Extended Cragg and Levy function [29]
Exam 14	$n = 3000$	Singular Broyden problem [29]
Exam 15	$n = 10$	The tridiagonal system [29]
Exam 16	$n = 10$	The discrete boundary-value problem [29]
Exam 17	$n = 100$	Broyden tridiagonal problem [29]
Exam 18	$n = 5$	The asymptotic boundary value problem [9]
Exam 19	$n = 3$	The box problem [41]
Exam 20	$n = 2$	$f_1(x) = x_1^2 + x_2^2 - 2,$ $f_2(x) = e^{x_1-1} + x_2^2 - 2$ (p.149, [10])
Exam 21	$n = 2$	Powell badly scaled function [41]
Exam 22	$n = 2$	Chemical equilibrium problem 1 [18]
Exam 23	$n = 6$	Chemical equilibrium problem 2 [18]
Exam 24	$n = 10$	Brown almost linear function [41]
Exam 25	$n = 3000$	$a = 2 * \text{ones}(n, 1), b = \text{ones}((n-1), 1),$ $A = \text{diag}(a, 1) + \text{diag}(b, 1) + \text{diag}(b, -1),$ $Ax - \lambda x = 0, x^T x = 1$
Exam 26	$n = 3000$	$a = \text{ones}(n, 1), b = \text{ones}((n-1), 1), c = 2 * b,$ $A = \text{diag}(a, 1) + \text{diag}(b, 1) + \text{diag}(c, -1),$ $Ax - \lambda x = 0, x^T x = 1$

faster than the traditional optimization method. From our point of view, the continuation Newton method with the trust-region updating strategy (Algorithm 1) is worth investigating further as a special continuation method. We have also extended it to the linear programming problem [33], the unconstrained optimization problem [35] and the underdetermined system of nonlinear equations [36]. The promising results are reported for those problems therein.

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Table 2: Numerical results.

Exam	CNMTr		HOMPACK90		fsolve		NAClab (psolve)	
	CPU (s)	$\ F(x^d)\ _\infty$	CPU (s)	$\ F(x^d)\ _\infty$	CPU (s)	$\ F(x^d)\ _\infty$	CPU (s)	$\ F(x^d)\ _\infty$
1	7.46E-02	4.87E-13	6.31E-01	5.01E-04 (failed)	2.52E-01	1.64E-07	6.84E-01	0 (failed)
2	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)
3	1.39E-02	9.61E-14	1.02	3.12 (failed)	3.32E-02	9.24E-05 (far sol.)	1.42	0 (failed)
4	1.71E-02	1.17E-15	7.94E-01	0.74 (failed)	1.34E-03	1.93 (failed)	1.35	1.40E+01 (failed)
5	2.98E-02	4.66E-15	5.87E-01	2.60E-12	4.67E-02	5.51E-01 (failed)	1.36	1.96 (failed)
6	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)
7	1.18E-02	3.05E-13	7.52E-01	0	1.36E-02	2.34E-09	2.85E-01	0
8	1.24E+01	3.91E-13	4.21E+02	5.12E-13	8.64E+02	3.20E-13	3.65E+04	7.12E-12
9	2.07E+01	4.10E-13	4.83E+02	6.84E-12	3.55E+02	7.50E-13	3.97E+04	5.21E-13
10	1.94E+01	4.05E-13	5.31E+02	6.31E-15	3.85E+03	6.75 (failed)	4.02E+03	1.20E+04 (failed)
11	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)
12	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
13	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)
14	1.87E+01	6.31E-13	5.91E+02	8.41E-13	4.12E+02	1.48E-06	4.10E+04	8.13E-12
15	3.80E-02	1.42E-14	8.06E-01	3.84E-14	1.99E-02	5.72E-13	4.71E+02	5.18E-13
16	4.67E-02	2.44E-14	2.94	6.57E-14	1.16E-02	6.76E-13	9.20E-01	4.15E-13
17	1.30	6.17E-13	3.54E+01	5.71E-13	2.51E-02	8.88E-16	9.13E+01	3.16E-12
18	1.40E-02	3.81E-16	2.09	6.14E-16	8.02E-03	7.19E-12	7.74E-01	1 (failed)
19	2.07E-02	5.84E-15	2.54	6.58E-12	8.13E-03	4.96E-13	5.45E-01	0
20	6.57E-03	2.66E-15	5.28	5.14E-13	1.09E-02	2.22E-16	3.51E-01	8.53 (failed)
21	1.23E-03	8.77E-15	7.53E-01	1.22E-02 (failed)	5.29E-02	3.55E-05	4.17E-01	1 (failed)
22	5.58E-03	0	7.79E-01	0	6.73E-02	2.73 (failed)	5.41E-01	0
23	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)
24	5.30E-02	1.24E-14	7.63E-01	6.26E-13	9.83E-03	4.23E-12	9.00E-01	2.22E-16
25	7.94E+02	6.09E-13	4.87E+02	4.13E-13	3.91E+03	3.55E-15	4.07E+04	1.45E-12
26	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 3: Statistical results.

	CNMTr	HOMPACK90	fsolve	NAClab
number of failed problems	0	7	9	13
number of the minimum time	19	0	7	0

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