Explicit continuation methods and preconditioning techniques for unconstrained optimization problems

Xin-long Luo · Hang Xiao · Jia-hui Lv · Sen Zhang

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Abstract This paper considers an explicit continuation method and the trust-region time-stepping scheme for the unconstrained optimization problem. Moreover, in order to improve its computational efficiency and robustness, the new method uses the switching preconditioning technique between the L-BFGS method and the inverse of the Hessian matrix. In the well-conditioned phase, the new method uses the L-BFGS method as the preconditioning technique in order to improve its computational efficiency. Otherwise, the new method uses the inverse of the Hessian matrix as the pre-conditioner in order to improve its robustness. We also analyze the global convergence analysis of the new method. According our numerical experiments, the new method is more robust and faster than the traditional optimization method such as the trust-region method and the line search method.
1 Introduction

In this article, we consider the following unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} f(x),$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is a differentiable function. For this problem, there are many efficient methods to solve it such as line search methods and the trust-region methods [12, 31, 37, 42]. The continuation method [2, 4, 17, 20, 23, 24, 39] is another method other than the traditional optimization methods for the problem (1). The advantage of the continuation method over the line search method or the trust-region method is capable of finding many local optimal points of the non-convex optimization problem by tracking its trajectory, and it is even possible to find the global optimal solution [7, 33, 41]. However, the consumed time of the continuation method may be higher than that of the traditional optimization method.

Recently, Luo, Xiao and Lv [27] consider the continuation Newton method with the adaptive time-stepping size based on the trust-region updating formula for the nonlinear system of equations. According to their numerical experiments, their method is robust and efficient to solve the nonlinear system of equations. In order to improve the computational efficiency and the robustness of their continuation method [27] further for the large-scale optimization problem, we consider the switching preconditioning technique for the ill-conditioned problem between the special L-BFGS method and the inverse of the Hessian matrix. That is to say, in the well-conditioned phase, the new method uses the L-BFGS method as the preconditioning technique in order to improve its computational efficiency. Otherwise, the new method uses the inverse of the Hessian matrix as the pre-conditioner in order to improve its robustness.

The rest of the paper is organized as follows. In section 2, we give a new continuation method with the trusty time-stepping scheme and the switching preconditioning technique for the unconstrained optimization problem (1). In section 3, we analyze the global convergence of this new method. In section 4, we report some promising numerical results of the new method, in comparison to the traditional trust-region method and the line search method (the quasi-Newton method, the built-in subroutine fminunc.m of the MATLAB environment) for some large-scale problems. Finally, we give some discussions and conclusions in section 5.
2 The explicit continuation method and preconditioning techniques

In this section, we construct an explicit continuation method with the new time-stepping scheme based on the trust-region updating strategy [42] for the unconstrained optimization problem (1). Firstly, we construct a generalized gradient flow for the stable point of the unconstrained optimization (1). Then, we construct an explicit continuation method with an adaptive time-stepping scheme for this special ordinary differential equations (ODEs) in order to improve the computational efficiency of the generalized gradient flow. Furthermore, we also consider a switching preconditioning technique between the L-BFGS method and the inverse of the Hessian matrix.

2.1 The generalized gradient flow

For the unconstrained optimization problem (1), we consider the damped Newton method [37] as follows:

\[
x_{k+1} = x_k - \alpha_k B(x_k)^{-1} g(x),
\]

where \( B(x) = \nabla^2 f(x) \) and \( g(x) = \nabla f(x) \). If we regard \( x_k = x(t_k) \), \( x_{k+1} = x(t_k + \alpha_k) \) and let \( \alpha_k \to 0 \), we obtain the continuous Newton flow [5, 14, 38] as follows:

\[
\frac{dx}{dt} = -B(x)^{-1} g(x), \quad x(0) = x_0.
\]

Actually, if we apply an iteration with the explicit Euler method [36] for the continuous Newton flow (3), we obtain the damped Newton method (2). Since \( B(x) \) may be singular, we reformulate the continuous Newton flow (3) as the following general formula:

\[
B(x) \frac{dx}{dt} + g(x) = 0, \quad x(0) = x_0.
\]

For the continuous Newton flow (4), we have the following property 1.

Property 1 (Brain [5] and Tanabe [38]) Assume that \( x(t) \) is the solution of the continuous Newton flow (4), then \( r(x(t)) = \|g(x(t))\|^2 \) converges to zero when \( t \to \infty \). That is to say, for every limit point \( x^* \) of \( x(t) \), it is also a stable point of the Newton flow (4). Furthermore, every element \( g_i(x(t)) \) of \( g(x(t)) \) has the same convergence rate \( \exp(-t) \) and \( x(t) \) can not converge to the stable point \( x^* \) of the continuous Newton flow (4) on the finite interval.

Proof. Assume that \( x(t) \) is the solution of the continuous Newton flow (4), then we have

\[
\frac{d}{dt} \langle e^t g(x) \rangle = e^t B(x) \frac{dx(t)}{dt} + e^t g(x) = 0.
\]
Consequently, we obtain
\[ g(x(t)) = g(x_0) e^{-t}. \]  

(5)

From equation (5), it is not difficult to know that every element \( g_i(x(t)) \) of \( g(x(t)) \) converges to zero with the linear convergence rate \( e^{-t} \) when \( t \to \infty \). Thus, if the solution \( x(t) \) of the continuous Newton flow (4) belongs to a compact set, it has a limit point \( x^\ast \) when \( t \to \infty \), and this limit point \( x^\ast \) is also its stable point.

If we assume that the solution \( x(t) \) of the continuous Newton flow (4) converges to its stable point \( x^\ast \) on the finite interval \((0, T]\), from equation (5), we have
\[ g(x^\ast) = g(x_0) e^{-T}. \]  

(6)

Since \( x^\ast \) is a stable point of the continuous Newton flow (4), we have \( g(x^\ast) = 0 \). By substituting it into equation (6), we obtain
\[ g(x_0) = 0. \]

which contradicts the assumption that \( x_0 \) is not a stable point of the continuous Newton flow (4). Therefore, the solution \( x(t) \) of the continuous Newton flow (4) can not converge to its stable point \( x^\ast \) on the finite interval. \( \Box \)

We can also regard the continuous Newton flow as the generalized gradient flow (p. 361, \cite{20}):
\[ \frac{dx}{dt} = -H(x)g(x), \quad x(0) = x_0, \]  

(7)

where \( H(x) \) equals the inverse of the Hessian matrix \( B(x)^{-1} \) or its quasi-Newton approximation. \( H(x) \) can be regarded as a pre-conditioner of \( g(x) \) to mitigate the stiffness of the ODEs (7). Consequently, we can adopt the explicit numerical method to compute the trajectory of the ODEs (7) efficiently \cite{27}.

Remark 1 If we assume that \( x(t) \) is the solution of the ODEs (7) and \( H(x) \) is a symmetric positive definite matrix, we obtain
\[ \frac{df(x)}{dt} = (g(x))^T \frac{dx}{dt} = -g(x)^T H(x)g(x) \leq 0. \]

That is to say, \( f(x) \) is monotonically decreasing along the solution curve \( x(t) \) of the dynamical system (7). Furthermore, the solution \( x(t) \) converges to \( x^\ast \) when \( f(x) \) is lower bounded and \( t \) tends to infinity \cite{20,24,33,39}, where \( x^\ast \) is the stable point of the generalized gradient flow (7). Thus, we can follow the trajectory \( x(t) \) of the ODEs (7) to obtain its stable point \( x^\ast \), which is also one stable point of the original optimization problem (1).
2.2 The explicit continuation method

The solution curve of the ordinary differential equations is not efficiently followed on an infinite interval by the traditional ODE method [3,8,21,36], so we need to construct the particular method for this problem (7). We apply the first-order implicit Euler method [3,36] to the ODEs (7), then we obtain

\[ x_{k+1} = x_k - \Delta t_k H(x_k)g(x_k), \]  

(8)

where \( \Delta t_k \) is the time-stepping size.

Since the system of equations (8) is a nonlinear system which cannot be directly solved, we seek for its explicit approximation formula. We denote

\[ s_k = x_{k+1} - x_k. \]

By using the first-order Taylor expansion, we have the linear approximation \( g(x_k) + B(x_k)s_k \) of \( g(x_{k+1}) \). By substituting it into equation (8) and using the zero-order approximation \( H(x_k) \) of \( H(x_{k+1}) \), we have

\[ s_k \approx -\Delta t_k H(x_k)(g(x_k) + B(x_k)s_k) = -\Delta t_k H(x_k)g(x_k) - \Delta t_k H(x_k)B(x_k)s_k. \]  

(9)

Let \( H(x_k) = (\nabla^2 f(x_k))^{-1} \). Then, we have \( H(x_k)B(x_k) = I \). By substituting it into equation (9), we obtain the explicit continuation method as follows:

\[ s_k = -\frac{\Delta t_k}{1 + \Delta t_k} H_k g_k, \]  

(10)

\[ x_{k+1} = x_k + s_k, \]  

(11)

where \( g_k = \nabla f(x_k) \) and \( H_k = (\nabla^2 f(x_k))^{-1} \) or its quasi-Newton approximation.

The explicit continuation method (10)-(11) equals the damped Newton method if we let \( \alpha_k = \Delta t_k / (1 + \Delta t_k) \) in equation (10). However, from the view of the ODE method, they are different. The damped Newton method (2) is derived from the explicit Euler method applied to the generalized gradient flow (7). Its time-stepping size \( \alpha_k \) is restricted by the numerical stability [36]. That is to say, for the linear test equation \( dx/dt = -\lambda x \), its time-stepping size \( \alpha_k \) is restricted by the stable region \( |1 - \lambda \alpha_k| \leq 1 \). Therefore, the large time-stepping size \( \alpha_k \) can not be adopted in the steady-state phase.

The explicit continuation method (10)-(11) is derived from the semi-implicit Euler scheme applied to the generalized gradient flow (7), and its time-stepping size \( \Delta t_k \) is not restricted by the numerical stability for the linear test equation. Therefore, the large time-stepping size \( \Delta t_k \) can be adopted in the steady-state phase, and the explicit continuation method (10)-(11) mimics the Newton method. Consequently, it has the fast convergence rate near the stable point \( x^* \) of the generalized gradient flow (7). The most of all, the new time-stepping size \( \alpha_k = \Delta t_k / (\Delta t_k + 1) \) is favourable to adopt the trust-region updating strategy for adaptively adjusting the time-stepping size \( \Delta t_k \) such that the explicit continuation method (10)-(11) accurately tracks the generalized gradient flow (7) in the transient-state phase and achieves the fast convergence rate in the steady-state phase.
Remark 2 Luo, Xiao and Lv [27] have considered the explicit continuation method for nonlinear equations when $H_k = g'(x_k)$. Here, we consider the quasi-Newton approximation $H_k$ in equation (11).

2.3 The trusty time-stepping scheme

Another issue is how to adaptively adjust the time-stepping size $\Delta t_k$ at every iteration. We borrow the adjustment method of the trust-region radius from the trust-region method due to its robustness and its fast convergence rate [12]. When we use the trust-region updating technique to adaptively adjust time-stepping size $\Delta t_k$ [22], we also need to construct a local approximation model of the objective $f(x)$ around $x_k$. Here, we adopt the following quadratic function as its approximation model:

\[
q_k(x_k + s) = f(x_k) + s^T g_k + \frac{1}{2} s^T B_k s,
\]  
(12)

where $B_k = \nabla^2 f(x_k)$ or its quasi-Newton approximation. In practical computation, we do not store the matrix $B_k$. Thus, we use the explicit continuation method (10)-(11) and regard $H_k = B_k^{-1}$ to simplify the quadratic model $q_k(x_k + s_k)$ as follows:

\[
m_k(s_k) = \nabla f(x_k)^T s_k - \frac{0.5 \Delta t_k}{1 + \Delta t_k} g_k^T s_k 
\approx q_k(x_k + s_k) - q_k(x_k).
\]  
(13)

where $g_k = \nabla f(x_k)$. We enlarge or reduce the time-stepping size $\Delta t_k$ at every iteration according to the following ratio:

\[
\rho_k = \frac{f(x_k) - f(x_{k+1})}{m_k(0) - m_k(s_k)}.
\]  
(14)

A particular adjustment strategy is given as follows:

\[
\Delta t_{k+1} = \begin{cases} 
\gamma_1 \Delta t_k, & \text{if } 0 \leq |1 - \rho_k| \leq \eta_1, \\
\Delta t_k, & \text{if } \eta_1 < |1 - \rho_k| < \eta_2, \\
\gamma_2 \Delta t_k, & \text{if } |1 - \rho_k| \geq \eta_2,
\end{cases}
\]  
(15)

where the constants are selected as $\eta_1 = 0.25$, $\gamma_1 = 2$, $\eta_2 = 0.75$, $\gamma_2 = 0.5$ according to numerical experiments. When $\rho_k \geq \eta_2$, we accept the trial step $s_k$ and let $x_{k+1} = x_k + s_k$, where $\eta_2$ is a small positive number such as $\eta_2 = 1.0 \times 10^{-6}$. Otherwise, we discard it and let $x_{k+1} = x_k$.

Remark 3 This new time-stepping size selection based on the trust-region strategy has some advantages compared to the traditional line search strategy. If we use the line search strategy and the damped Newton method (2) to track the trajectory $x(t)$ of the continuous Newton flow (4), in order to achieve the fast convergence rate in the steady-state phase, the time-stepping size $\alpha_k$ of the damped Newton method is tried from 1 and reduced by the half with many times at every iteration. Since the linear
model \( f(x_k) + g_k \) may not approximate \( f(x_k + s_k) \) well in the transient-state phase, the time-stepping size \( \alpha_k \) will be small. Consequently, the line search strategy consumes the unnecessary trial step in the transient-state phase. However, the selection of the time-stepping size \( \Delta t_k \) based on the trust-region strategy (14)-(15) can overcome this shortcoming.

2.4 The L-BFGS preconditioning technique

For the large-scale problem, the numerical evaluation of the Hessian matrix \( \nabla^2 f(x_k) \) consumes much time. In order to overcome this shortcoming, we use the limited-memory BFGS quasi-Newton formula (see [6, 15, 18, 30, 34] or pp. 222-230, [31]) to approximate \( (\nabla^2 f(x_k))^{-1} \). Recently, Ullah, Sabi and Shah [40] give an effective L-BFGS updating formula for the system of monotone nonlinear equations. In order to avoid the ill-conditioning of \( B_k \), they considered the revised BFGS updating formula [40] as follows:

\[
B_{k+1} = \lambda_k \left( I - \frac{s_k s_k^T}{y_k s_k} \right) + \sigma_k \frac{y_k y_k^T}{y_k^T s_k},
\]

(16)

where \( y_k = g_{k+1} - g_k \), \( s_k = x_{k+1} - x_k \) and \( \lambda_k, \sigma_k \) are two undetermined parameters. Then, they solved the minimizer of the measurement function \( \varphi [9] \) on the variables \( \lambda_k, \sigma_k \), where \( \varphi(B_{k+1}) \) is defined by

\[
\varphi(B_{k+1}) = \text{trace}(B_{k+1}) - \ln(\det(B_{k+1}))
\]

\[
= (n - 1)\lambda_k + \sigma_k \frac{\|y_k\|^2}{y_k^T s_k} - \ln \left( \lambda_k^{n-1} \sigma_k \frac{y_k y_k^T}{\|y_k\|^2} \right)
\]

\[
= (n - 1)(\lambda_k - \ln(\lambda_k)) + \sigma_k \frac{\|y_k\|^2}{y_k^T s_k} - \ln(\sigma_k) - \ln(y_k^T s_k) + \ln(\|s_k\|^2).
\]

(17)

Consequently, by solving \( \min_{\lambda_k, \sigma_k} \varphi(B_{k+1}) \), they obtained the optimal parameters \( \lambda_k = 1 \) and \( \sigma_k = \frac{y_k^T s_k}{\|y_k\|^2} \). By substituting them into equation (16), they obtained the revised LBFGS updating formula:

\[
B_{k+1} = I - \frac{s_k s_k^T}{y_k^T s_k} + \frac{y_k y_k^T}{\|y_k\|^2}.
\]

(18)

By using the Sherman-Morrison-Woodburg formula (P. 17, [37]), from equation (18), we obtain the inverse of \( B_{k+1} \):

\[
H_{k+1} = B_{k+1}^{-1} = I - \frac{y_k y_k^T}{y_k^T s_k} + \frac{y_k y_k^T}{(y_k^T s_k)^2} s_k s_k^T.
\]

(19)

The initial matrix \( H_0 \) can be simply selected by the inverse of the Hessian matrix \( \nabla^2 f(x_0) \). From equation (19), it is not difficult to verify

\[
H_{k+1} y_k = \frac{y_k y_k^T}{y_k^T s_k} s_k.
\]
That is to say, $H_{k+1}$ satisfies the scaling quasi-Newton property.

The L-BFGS updating formula (19) has some nice properties such as the symmetric positive definite property and the positive lower bound of its eigenvalues.

**Lemma 1** Matrix $H_{k+1}$ defined by equation (19) is symmetric positive definite and its eigenvalues are greater than 1/2.

**Proof.**

(i) For any nonzero vector $z \in \mathbb{R}^n$, from equation (19), we have

$$z^T H_{k+1} z = \|z\|^2 - 2(z^T y_k)(z^T s_k)/y_k^T s_k + 2(z^T s_k)^2 \|y_k\|^2/(y_k^T s_k)^2$$

$$= (\|z\| - |z^T s_k/y_k^T s_k| \|y_k\|)^2 + 2\|z\| |z^T s_k/y_k^T s_k| \|y_k\|$$

$$- 2(z^T y_k)(z^T s_k)/y_k^T s_k + \|y_k\|^2(z^T s_k/y_k^T s_k)^2 \geq 0.$$  \hspace{1cm} (20)

In the last inequality of equation (20), we use the Cauchy-Schwartz inequality $\|z^T y\|^2 \leq \|z\|\|y\|$ and its equality holds if only if $z = ty_k$. When $z = ty_k$, from equation (20), we have $z^T H_{k+1} z = t^2 \|y_k\|^2 = \|z\|^2 > 0$. When $z^T s_k = 0$, from equation (20), we also have $z^T H_{k+1} z = \|z\|^2 > 0$. Therefore, we conclude that $H_{k+1}$ is a symmetric positive definite matrix.

(ii) It is not difficult to know that it exists at least $n - 2$ linearly independent vectors $z_1, z_2, \ldots, z_{n-2}$ such that $z_i^T s_k = 0, z_i^T y_k = 0 (i = 1 : (n - 2))$ hold. That is to say, matrix $H_{k+1}$ defined by equation (19) has at least $(n - 2)$ linearly independent eigenvectors whose corresponding eigenvalues are 1. We denote the other two eigenvalues of $H_{k+1}$ as $\mu_{k+1}^i (i = 1 : 2)$ and their corresponding eigenvalues as $p_1$ and $p_2$, respectively. Then, from equation (19), we know that the eigenvectors $p_i (i = 1 : 2)$ can be represented as $p_i = y_k + \beta_i s_k$ when $\mu_{k+1}^i \neq 1 (i = 1 : 2)$. From equation (19) and $H_{k+1} p_i = \mu_{k+1} p_i$, $p_i (i = 1 : 2)$, we have

$$- \left( \mu_{k+1}^i + \beta_i y_k^T s_k/s_k^T y_k \right) y_k + \left( y_k^T y_k/y_k^T s_k + 2\beta_i (y_k^T y_k)(s_k^T s_k)/(y_k^T s_k)^2 - \mu_{k+1}^i \beta_i \right) s_k = 0, \quad i = 1 : n.$$  \hspace{1cm} (21)

When $y_k = ts_k$, from equation (19), we have $H_{k+1} = I$. In this case, we conclude that the eigenvalues of $H_{k+1}$ are greater than 1/2. When vectors $y_k$ and $s_k$ are linearly independent, from equation (21), we have

$$\mu_{k+1}^i + \beta_i y_k^T s_k/s_k^T y_k = 0,$$

$$y_k^T y_k/y_k^T s_k + 2\beta_i (y_k^T y_k)(s_k^T s_k)/(y_k^T s_k)^2 - \mu_{k+1}^i \beta_i = 0, \quad i = 1 : n.$$

That is to say, $\mu_{k+1}^i (i = 1 : 2)$ are the two solutions of the following equation:

$$\mu^2 - 2\mu (y_k^T y_k)(s_k^T s_k)/(s_k^T y_k)^2 + (y_k^T y_k)(s_k^T s_k)/(s_k^T y_k)^2 = 0.$$  \hspace{1cm} (22)

Consequently, from equation (22), we obtain

$$\mu_{k+1}^1 + \mu_{k+1}^2 = 2(y_k^T y_k)(s_k^T s_k)/(s_k^T y_k)^2, \quad \mu_{k+1}^1 \mu_{k+1}^2 = (y_k^T y_k)(s_k^T s_k)/(s_k^T y_k)^2.$$  \hspace{1cm} (23)
From equation (23), it is not difficult to obtain
\[ 1/\mu_{k+1}^1 + 1/\mu_{k+1}^2 = 2, \mu_{k+1}^i > 0, i = 1 : 2. \]  

(24)

Therefore, from equation (24), we conclude that
\[ \mu_{k+1}^i > \frac{1}{2} (i = 1 : 2). \]

Consequently, the eigenvalues of \( H_{k+1} \) are greater than 1/2. \( \square \)

According to our numerical experiments, the quasi-Newton updating method (19) works well for the most unconstrained optimization problems. However, for the very ill-conditioning problem, the quasi-Newton method (19) will fail to accurately obtain its minimizer \( x^\ast \). In order to improve the robustness of the method, we use the inverse of the Hessian matrix \( \nabla^2 f(x_k) \) as the pre-conditioner of the gradient \( g(x_k) \) in the ill-conditioned phase. Furthermore, we identify the ill-conditioning by the gap between \( f(x_k + s_k) \) and its approximation \( f(x_k) + g(x_k)^T s_k + \frac{1}{2} s_k^T B_k s_k \) when \( s_k \) is small. That is to say, we regard the problem as an ill-conditioning when the number of the indices \( k \) that satisfy \( |1 - \rho_k| \geq \eta_2 \) is greater than the threshold. Therefore, we give the following switching pre-conditioning strategy as follows:

\[
H_{k+1} = \begin{cases} 
I - \frac{y_k s_k + y_k s_k^T}{y_k^T y_k} + 2 \frac{y_k y_k^T s_k s_k^T}{y_k^T y_k}, & \text{if } K_{bad} \leq 5 \text{ & } |x_k^T y_k| > \theta \|s_k\|^2, \\
(\nabla^2 f(x_{k+1}))^{-1}, & \text{otherwise},
\end{cases}
\]

(25)

where \( K_{bad} \) represents the number of the indices \( k \geq 0 \) that satisfy \( |1 - \rho_k| \geq \eta_2 \), the ratio \( \rho_k \) is defined by equation (14), and \( \theta \) is a small positive constant such as \( \theta = 10^{-6} \).

For a real-world problem, the analytical Hessian \( \nabla^2 f(x) \) can not be offered. Thus, in equation (25), we replace the Hessian matrix \( \nabla^2 f(x_{k+1}) \) with its difference approximation in practice as follows:

\[
\nabla^2 f(x_{k+1}) \approx \left[ \frac{g(x_{k+1} + \varepsilon e_1) - g(x_{k+1})}{\varepsilon}, \ldots, \frac{g(x_{k+1} + \varepsilon e_n) - g(x_{k+1})}{\varepsilon} \right],
\]

(26)

where \( e_i \) represents the unit vector whose elements equal zeros except for the \( i \)-th element equals 1, and the parameter \( \varepsilon \) can be selected as \( 10^{-6} \) according to our numerical experiments.

According to the above discussions, we give the detailed implementation of the explicit continuation method with the trusty time-stepping scheme for the unconstrained optimization problem (1) in Algorithm 1.

3 Algorithm Analysis

In this section, we analyze the global convergence of the explicit continuation method (10)-(11) with the trusty time-stepping scheme and the preconditioning technique (25) for the unconstrained optimization problem (i.e. Algorithm 1). Firstly, we give a lower-bounded estimate of \( m_k(0) - m_k(s_k) \) (\( k = 1, 2, \ldots \)). This result is similar to
Algorithm 1 Explicit continuation methods and preconditioning techniques for unconstrained optimization problems (the Eptc method)

Input: 
the objective function \( f(x) \), the initial point \( x_0 \) (optional), the terminated parameter \( \varepsilon \) (optional).

Output: 
the optimal approximation solution \( x^* \).

1: Set \( x_0 = 2 \times \text{ones}(n,1) \) and \( \varepsilon = 10^{-8} \) as the default values.
2: Initialize the parameters: \( \eta_0 = 10^{-6}, \eta_1 = 0.25, \gamma_1 = 2, \eta_2 = 0.75, \gamma_2 = 0.5, \theta = 10^{-4} \).
3: Set \( k = 0 \). Evaluate \( f_0 = f(x_0), g_0 = \nabla f(x_0) \) and \( B_0 = \nabla^2 f(x_0) \).
4: Set \( y_{-1} = 0, s_{-1} = 0, K_{\text{bad}} = 0 \) and \( \Delta t_0 = 10^{-2} \).
5: while \( \| g_k \| > \varepsilon \) do
6: if \( \max(|x_k^T y_{-1}|, |s_k^T y_{-1}|) > \theta s_k^T y_{-1} \) then
7: \( s_k = - \nabla^2 f(x_k - \eta_1 s_k) \frac{g_k - \gamma_k y_k}{s_k - y_k} + \gamma_k g_k^2 y_k - y_k^2 s_k \).
8: else
9: \( s_k = - \nabla^2 f(x_k \mid B_k \setminus g_k) \).
10: end if
11: Compute \( s_{k+1} = s_k + s_k \).
12: Evaluate \( f_{k+1} = f(x_{k+1}) \) and compute the ratio \( \rho_k \) from equations (13)-(14).
13: if \( \rho_k \leq \eta_2 \) then
14: Set \( w_{k+1} = s_k, f_{k+1} = f_k, g_{k+1} = g_k, y_{k+1} = y_k - y_k \).
15: else
16: Evaluate \( g_{k+1} = \nabla f(x_{k+1}) \). Compute \( y_k = g_{k+1} - s_k \) and \( s_k = x_{k+1} - s_k \).
17: end if
18: if \( |1 - \rho_k| \geq \eta_2 \) then
19: \( K_{\text{bad}} = K_{\text{bad}} + 1; \Delta t_{k+1} = \eta_1 \Delta t_k \).
20: else if \( |1 - \rho_k| \geq \eta_1 \) then
21: \( \Delta t_{k+1} = \Delta t_k \).
22: else
23: \( \Delta t_{k+1} = \eta_1 \Delta t_k \).
24: end if
25: if \( \max(|x_k^T y_{-1}|, |s_k^T y_{-1}|) \leq \theta s_k^T y_{-1} \) or \( K_{\text{bad}} \geq 5 \) then
26: Evaluate \( B_{k+1} = \nabla^2 f(x_{k+1}) \) from the difference approximation (26).
27: end if
28: Set \( k \leftarrow k + 1 \).
29: end while

that of the trust-region method for the unconstrained optimization problem [32]. We denote the level set \( S_f \) as
\[
S_f = \{ x : f(x) \leq f(x_0) \}. \tag{27}
\]

Lemma 2 Assume that the Hessian matrix \( \nabla^2 f(x) \) of \( f(x) \) satisfies
\[
M\|z\|^2 \geq z^T \nabla^2 f(x) z \geq m\|z\|^2 > 0, \quad \forall x \in S_f \tag{28}
\]
holds for all \( z \in \mathbb{R}^n \), where \( m \) and \( M \) are two positive constants. Furthermore, we assume that the quadratic model \( q_k(x) \) is defined by equation (13) and \( s_k \) is computed by the explicit continuation method (10)-(11) and the preconditioning formula (25). Then, we have
\[
m_k(0) - m_k(s_k) \geq \frac{cm\Delta t_k}{2(1 + \Delta t_k)} \| s_k \|^2, \tag{29}
\]
where \( c_m \) is a positive constant.

**Proof.** When \( H_k \) is updated by the L-BFGS formula (19), from Lemma 1, we know that \( H_k \) is symmetric positive definite and its eigenvalues are greater than 1/2. When \( H_k \) is updated by the inverse of the Hessian matrix \( \nabla^2 f(x_k) \), from the assumption (28) of \( \nabla^2 f(x_k) \), we know that \( H_k \) is symmetric positive definite and its eigenvalues are greater than \( 1/M \). By combining these two cases, we know that the eigenvalues of \( H_k \) are greater than \( c_m = \min\{1/2, 1/M\} \).

By using the eigenvalue decomposition of \( H_k \), From the explicit continuation method (10)-(11) and the quadratic model (13), we have

\[
m_k(0) - m_k(s_k) \geq -\frac{1}{2} s_k^T H_k s_k = \frac{\Delta t_k}{2(1 + \Delta t_k)} g_k^T H_k g_k = \frac{c_m \Delta t_k}{2(1 + \Delta t_k)} \|g_k\|^2.
\]

In the first inequality in equation (30), we use the property \((1 + 0.5 \Delta t_k)/(1 + \Delta t_k) \geq 0.5 \) when \( \Delta t_k \geq 0 \). Consequently, we prove the result (29).

In order to prove that \( p_k \) converges to zero when \( k \) tends to infinity, we need to estimate the lower bound of time-stepping sizes \( \Delta t_k \) \((k = 1, 2, \ldots)\).

**Lemma 3** Assume that \( f: \mathbb{R}^n \rightarrow \mathbb{R} \) is twice continuously differentiable and its gradient \( g(x) \) satisfies the following Lipschitz continuity:

\[
\|g(x) - g(y)\| \leq L_c \|x - y\|, \forall x, y \in S_f.
\]

where \( L_c \) is the Lipschitz constant. The Hessian matrix \( \nabla^2 f(x) \) satisfies the strong convexity (28). We suppose that the sequence \( \{x_k\} \) is generated by Algorithm 1. Then, there exists a positive constant \( \delta_{\Delta t} \) such that

\[
\Delta t_k \geq \gamma_2 \delta_{\Delta t}
\]

holds for all \( k = 1, 2, \ldots \), where \( \Delta t_k \) is adaptively adjusted by the trust-region updating scheme (13)-(15).

**Proof.** When \( H_k \) is updated by the L-BFGS formula (19), from Lemma 1, we know that the eigenvalues of \( H_k \) is greater than 1/2 and it has at least \( n-2 \) eigenvectors which equal 1. When \(|s_{k-1}^T y_{k-1}| \geq \theta \|s_{k-1}\|^2 \), we denote the other two eigenvalues of \( H_k \) as \( \mu_1^k \) and \( \mu_2^k \). By substituting it into equation (23), we obtain

\[
\mu_1^k \mu_2^k = \frac{\|y_{k-1}\|^2 \|s_{k-1}\|^2}{(s_{k-1}^T y_{k-1})^2} \leq \frac{\|y_{k-1}\|^2 \|s_{k-1}\|^2}{\theta^2 \|s_{k-1}\|^4} = \frac{1}{\theta^2} \|y_{k-1}\|^2 \|s_{k-1}\|^2.
\]

From Lemma 2 and Algorithm 1, we know \( f(x_k) \leq f(x_0) \) \((k = 1, 2, \ldots)\). From the Lipschitz continuity (31) of \( g(x) \), we have

\[
\|y_{k-1}\| = \|g(x_k) - g(x_{k-1})\| \leq L_c \|x_k - x_{k-1}\| = L_c \|s_{k-1}\|.
\]
By substituting it into equation (33) and using $\mu^k_i > \frac{1}{2} (i = 1, 2)$, we obtain

$$
\frac{1}{2} < \mu^k_i < \frac{2L_c^2}{\theta^2}, \quad i = 1, 2.
$$

(35)

That is to say, the eigenvalues of $H_k$ are less than or equal to $\max\{1, 2L_c^2/\theta^2\}$.

When $H_k$ is updated by the inverse of the Hessian matrix $\nabla^2 f(x_k)$, from the assumption (28) of $\nabla^2 f(x_k)$, we know that $H_k$ is symmetric positive definite and its eigenvalues are less than or equal to $1/m$. That is to say, we obtain that the eigenvalues of $H_k$ are less than or equal to $M_H$ when $H_k$ is updated by the preconditioning formula (25), where $M_H = \max\{1, 2L_c^2/\theta^2, 1/m\}$. By using the property of the matrix norm, we have

$$
\|H_k g_k\| \leq M_H \|g_k\|.
$$

(36)

From the first-order Taylor expansion, we have

$$
f(x_k + s_k) = f(x_k) + \int_0^1 s_k^T g(x_k + ts_k) dt.
$$

(37)

Thus, from equations (13)-(14), (29), (37) and the Lipschitz continuity (31) of $g(x)$, we have

$$
|p_k - 1| = \left| \frac{(f(x_k) - f(x_k + s_k) - (m_k(0) - m_k(s_k)))}{m_k(0) - m_k(s_k)} \right|
\leq \frac{1 + \Delta t_k}{1 + 0.5 \Delta t_k} \left| \int_0^1 s_k^T (g(x_k + ts_k) - g(x_k)) dt \right|
\leq \frac{L c (1 + \Delta t_k)}{c_m \Delta t_k} \frac{\|s_k\|^2}{\|g_k\|^2} + \frac{0.5 \Delta t_k}{1 + 0.5 \Delta t_k}.
$$

(38)

By substituting equation (10) and equation (36) into equation (38), we have

$$
|p_k - 1| \leq \frac{L c M_H^2}{c_m (1 + \Delta t_k)} \frac{\|H_k g_k\|^2}{\|g_k\|^2} + \frac{0.5 \Delta t_k}{1 + 0.5 \Delta t_k}
\leq \frac{L c M_H^2}{c_m (1 + \Delta t_k)} \frac{\|H_k g_k\|^2}{\|g_k\|^2} + \frac{0.5 \Delta t_k}{1 + 0.5 \Delta t_k} \leq \frac{L c M_H^2 + 0.5 c_m \Delta t_k}{c_m (1 + 0.5 \Delta t_k)}.
$$

(39)

We denote

$$
\delta_{\Delta t} \triangleq \frac{c_m \eta_1}{L c M_H^2 + 0.5 c_m}.
$$

(40)

Then, from equation (39)-(40), when $\Delta t_k \leq \delta_{\Delta t}$, it is not difficult to verify

$$
|p_k - 1| \leq \frac{L c M_H^2 + 0.5 c_m \Delta t_k}{c_m} \eta_1 \leq \eta_1.
$$

(41)
We assume that $K$ is the first index such that $\Delta t_K \leq \delta_M$, where $\delta_M$ is defined by equation (40). Then, from equations (40)-(41), we know that $|\rho_K - 1| \leq \eta_1$. According to the time-stepping adjustment formula (15), $x_K + s_K$ will be accepted and the time-stepping size $\Delta t_{K+1}$ will be enlarged. Consequently, the time-stepping size $\Delta t_k$ holds $\Delta t_k \geq \gamma_2\delta_M$ for all $k = 1, 2, \ldots$. □

By using the results of Lemma 2 and Lemma 3, we prove the global convergence of Algorithm 1 for the unconstrained optimization problem (1) as follows.

**Theorem 1** Assume that $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable and its gradient $\nabla f(x)$ satisfies the Lipschitz continuity (31). The Hessian matrix $\nabla^2 f(x)$ satisfies the strong convexity (28). Furthermore, we suppose that $f(x)$ is lower bounded when $x \in S_f$, where the level set $S_f$ is defined by equation (27). The sequence $\{x_k\}$ is generated by Algorithm 1. Then, we have

$$\lim_{k \to \infty} \inf \|g_k\| = 0. \quad (42)$$

**Proof.** According to Lemma 3 and Algorithm 1, we know that there exists an infinite subsequence $\{x_k\}$ such that trial steps $s_k$ are accepted, i.e., $\rho_k \geq \eta_2, i = 1, 2, \ldots$. Otherwise, all steps are rejected after a given iteration index, then the time-stepping size will keep decreasing, which contradicts (32). Therefore, from equations (14) and (29), we have

$$f(x_0) - \lim_{k \to \infty} f(x_k) = \sum_{k=0}^{\infty} (f(x_k) - f(x_{k+1})) \geq \eta_2 \sum_{i=0}^{\infty} \frac{c_m\Delta t_k}{(\Delta t_k + 1)^2} \|g_k\|. \quad (43)$$

From the result (32) of Lemma 3, we know that $\Delta t_k \geq \gamma_2\delta_M (k = 1, 2, \ldots)$. By substituting it into equation (43), we have

$$f(x_0) - \lim_{k \to \infty} f(x_k) \geq \eta_2 \sum_{i=0}^{\infty} \frac{\gamma_2 c_m\delta_M}{(\gamma_2 \delta_M + 1)^2} \|g_k\|. \quad (44)$$

Since $f(x)$ is lower bounded when $x \in S_f$ and the sequence $\{f(x_k)\}$ is monotonically decreasing, we have $\lim_{k \to \infty} f(x_k) = f^\ast$. By substituting it into equation (44), we obtain the result (42). □

4 Numerical Experiments

In this section, some numerical experiments are performed to test the performance of Algorithm 1 (the Eptc method). The codes are executed by a HP notebook with the Intel quad-core CPU and 8Gb memory. We compare Eptc with the trust-region method and the quasi-Newton method (the built-in subroutine fminunc.m of the MATLAB environment) [6, 10, 11, 13, 16, 28] for 47 unconstrained optimization problems which can be found in [1, 35, 29]. The trust-region method and the quasi-Newton method
are two classical methods for solving unconstrained optimization problems and these two methods have been widely used until today. Therefore, we select these two typical methods as the basis for comparison. The termination conditions of the three compared methods are all set by

\[ \| \nabla f(x_k) \|_\infty \leq 1.0 \times 10^{-6}. \]

(45)

The initial points are set to \( x_0 = 2 \times \text{ones}(n, 1) \) for all test problems.

The numerical results are arranged in Table 1, Table 2 and Figure 1. From Tables 1-2, we find that Eptc works well for these 47 test problems. However, the trust-region method (fminunc.m is set by the trust-region method) and the quasi-Newton method (fminunc.m is set by the quasi-Newton method) fail to solve 2 problems and 7 problems, respectively. Thus, Eptc is more robust than the traditional optimization method such as the trust-region method or the line search method.

Moreover, from Table 1, we find that the consumed time of Eptc is about one percent of that of the trust-region method (fminunc.m) and one fifth of that of the quasi-Newton method (the line search method, fminunc.m) for the large-scale problems. One of the reasons is that the generalized gradient flow is non-stiff in the transient-state phase and Eptc uses the L-BFGS method as the preconditioning technique to follow their trajectories well for the most test problems. Consequently, Eptc only involves three pairs of the inner product of two vectors to obtain the trial step \( s_k \) at the transient-state phase iteration. However, the trust-region method at least needs to solve a linear system of equations and involves about \( \frac{1}{3} n^3 \) flops (p. 169, [19]) at every iteration. The quasi-Newton method involves one matrix-vector product to obtain the search direction \( d_k \) and involves about \( n^2 \) flops at every iteration.

### 5 Conclusion and Future Work

In this paper, we consider an explicit continuation method with the trust-region time-stepping scheme and the switching preconditioning technique between the L-BFGS method and the inverse of the Hessian matrix \( \nabla^2 f(x_k) \) (Eptc) for the unconstrained optimization problem. For the well-conditioned phase, Eptc uses the L-BFGS method (19) as the preconditioning technique. Otherwise, Eptc uses the inverse of the Hessian matrix \( \nabla^2 f(x_k) \) as the pre-conditioner. Consequently, for the well-conditioned phase, Eptc only involves the 6n flops to obtain its trial step \( s_k \) at every iteration. However, the trust-region method needs to solve a linear system of equations and involves \( \frac{1}{3} n^3 \) flops at every iteration. The quasi-Newton method (the line search method) involves one matrix-vector product to obtain the search direction \( d_k \) and involves about \( n^2 \) flops at every iteration. Numerical results also show that the consumed time of EPtc is about one percent of that of the trust-region method (fminunc.m) and one fifth of that of the quasi-Newton method (the line search method, fminunc.m) for the test problems with \( n = 1000 \), respectively. Moreover, Eptc is more robust than the traditional optimization method such as the trust-region method or the line search method.
Table 1: Numerical results of large-scale problems with $n = 1000$.

| Problems                         | Eptc (steps, time) | \(\|g(x^*)\|_\infty\)  | \(\|g^*\|_\infty\) | Eptc (steps, time) |
|---------------------------------|--------------------|----------------------|-----------------|--------------------|
| 1. Trid Function (n = 1000)     | 28 (0.2800)        | 7.7882E-07          | 0.0052          | 21 (147.3268)      |
| 2. Rosenbrock Function (n = 1000) | 57 (0.6280)        | 1.8925E-07          | 6.9663E-11      | 15 (208.36)        |
| 3. Ackley Function (n = 1000)   | 74 (1.1168)        | 2.1729E-08          | 6.9663E-11      | 2 (52.7352)        |
| 4. Dixon Pecu Function (n = 1000) | 57 (0.6220)        | 1.8582E-07          | 5.1937E-04      | 11 (78.2305)       |
| 5. Levy Function (n = 1000)     | 38 (0.1521)        | 7.6318E-08          | 4.9938E-07      | 6 (49.5847)        |
| 6. Molecular Energy Function (n = 1000) | 22 (0.3407)        | 6.9446E-07          | 3.1098E-09      | 4 (34.4602)        |
| 7. Powell Function (n = 1000)   | 44 (2.4665)        | 6.2593E-07          | 3.8521E-07      | 16 (110.4723)      |
| 8. Quartic With Noise Function (n = 1000) | 383 (0.2384)      | 3.1145E-06          | 5.4263E-07      | 13 (91.8643)       |
| 9. Rastrigin Function (n = 1000) | 9 (0.0712)         | 3.5796E-08          | 3.5728E-09      | 1 (21.1994)        |
| 10. Rotated Hyper Ellipsoid Function (n = 1000) | 28 (1.9075)      | 4.3481E-08          | 4.3032E-13      | 1 (176.9553)       |
| 11. Schwefel Function (n = 1000) | 36 (0.3373)        | 9.4745E-07          | 9.0242E-07      | 5 (40.8946)        |
| 12. Sphere Function (n = 1000)  | 14 (0.0231)        | 7.8407E-08          | 2.9779E-08      | 4 (33.5744)        |
| 13. Styblinski Tang Function (n = 1000) | 68 (1.6197)      | 2.6205E-06          | 1.0887E-06      | 8 (65.0469)        |
| 14. Sum squares Function (n = 1000) | 22 (0.0300)        | 7.9787E-07          | 1.0839E-20      | 4 (35.9020)        |
| 15. Schubert Function (n = 1000) | 16 (0.2256)        | 8.2217E-07          | 2.1316E-14      | 5 (41.7283)        |
| 16. Stretched V Function (n = 1000) | 14 (0.6951)        | 4.2645E-07          | 4.8375E-09      | 3 (73.4679)        |

Fig. 1: The Consumed time of each problem.
Table 2: Numerical results of small-scale problems with $n \leq 10$.

| Problems                          | Steps | fmin (s) | $\|g^i\|_\infty$ | $\|g^f\|_\infty$ | fmin (trust-region) | fmin (quasi-Newton) |
|----------------------------------|-------|----------|------------------|-----------------|---------------------|---------------------|
| 1. spheres function (n = 3)      | 94    | 0.0160   | 5.343E-08        | 3.691E-08       | 2.3924E-05          | 7.1145E-05          |
| 18. Beale Function (n = 2)       | 24    | 0.0060   | 4.147E-07        | 0.0005          | 0                   | 1.2666E-06          |
| 19. Griewank function (n = 10)   | 32    | 0.1275   | 1.653E-06        | 9.335E-06       | 7.102E-10           | 4.062E-08           |
| 21. Leaky Function (n = 2)       | 27    | 0.0092   | 9.932E-07        | 6.1055          | 2.639E-09           | 4.743E-09           |
| 27. Power Sum Function (n = 4)   | 48    | 0.0090   | 7.542E-07        | 0.0002          | 4.789E-08           | 2.113E-07           |
| 28. six hump camel Function (n = 2) | 61    | 0.0040   | 4.641E-07        | 1.1592          | 7.842E-06           | 9.677E-04           |
| 29. Zakharov Function (n = 10)   | 48    | 0.0042   | 2.771E-07        | 0.0363          | 5.917E-06           | 3.111               |
| 30. Bohachinsky Function (n = 2) | 32    | 0.0014   | 7.927E-07        | 0.0204          | 2.182E-06           | 9.983E-07           |
| 32. Drop Wave Function (n = 2)   | 37    | 0.0021   | 3.622E-07        | 0.0132          | 0.0047              | 5.031E-15           |
| 33. Schaffer Function (n = 2)    | 12    | 0.0016   | 7.051E-07        | 0.0040          | 7.051E-08           | 1.308E-06           |
| 34. Six Hump Camel Function (n = 2) | 32    | 0.0021   | 1.797E-07        | 0.0319          | 2.675E-06           | 7.543E-05           |
| 35. Three Hump Camel Function (n = 2) | 28    | 0.0015   | 2.900E-07        | 0.0110          | 1.084E-10           | 5.884E-06           |
| 36. Six Hump Camel Function (n = 2) | 27    | 0.0018   | 5.976E-07        | 0.0116          | 1.237E-10           | 2.101E-06           |
| 37. Ben bier exponential Quadratic Sum Function (n = 3) | 42    | 0.0042   | 8.597E-08        | 7.0255          | 8.740E-12           | 1.407E-07           |
| 38. Cinchrud Function (n = 2)    | 33    | 0.0036   | 2.131E-07        | 0.0300          | 1.407E-13           | 1.203E-05           |
| 39. Eleyhldt Function (n = 2)    | 78    | 0.0059   | 1.566E-05        | 0.0118          | 8.342E-07           | 6.094E-05           |
| 40. Exp Function (n = 2)         | 172   | 0.0093   | 2.027E-07        | 0.0406          | 3.421E-09           | 1.196E-06           |
| 41. Hansen Function (n = 2)      | 15    | 0.0014   | 7.111E-07        | 0.0517          | 2.878E-05           | 8.0229              |
| 42. Hartmann 3-D dimensional Function (n = 3) | 54    | 0.0051   | 6.188E-05        | 0.0698          | 1.659E-05           | 9.238E-07           |
| 43. Holder Table Function (n = 2) | 16    | 0.0021   | 3.620E-07        | 0.0430          | 2.675E-09           | 7.492E+37           |
| 44. Michalewicz Function (n = 2) | 31    | 0.0027   | 4.744E-07        | 0.0513          | 1.506E-08           | 2.705E-08           |
| 45. Schaffer Function N 4 (n = 2) | 2     | 0.0011   | 1.026E-07        | 0.1563          | 8.842E-07           | 6.076E-05           |
| 46. Trefethen 4 Function (n = 2) | 29    | 0.0018   | 2.441E-07        | 0.0443          | 1.282E-04           | 0.0052              |
| 47. Zettl Function (n = 2)       | 40    | 0.0017   | 5.186E-07        | 0.0438          | 3.740E-08           | 9.776E-06           |
Therefore, Ept is worth exploring further, and we will extend it to the constrained optimization problem in the future.

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