

Adaptive Conic Trust-Region Method for Nonlinear Least Squares Problems

Yang Yang¹, Sun Wenyu²

(1 School of Mathematics and Physics Science, Xuzhou Institute of Technology Xuzhou 221008 China)

(2 School of Mathematics and Computer Science, Nanjing Normal University, Nanjing 210097, China)

Abstract In this paper, a new method for nonlinear least-squares problems is presented. The method uses the quasi-Newton update of the Gauss-Newtonian based on a conic model. A method with adaptive trust region strategy is constructed. The method needs to solve the trust region subproblem with a conic model, which can be transformed to the trust region subproblem with a quadratic model. So the algorithm is easily implemented. The new algorithm is analyzed and its global and local superlinear convergence results are established. Numerical tests are presented that confirm the efficiency of the new algorithm.

Key words nonlinear least squares problems trust region method conic model global convergence superlinear convergence

CLC number O221.2 **Document code** A **Article ID** 1001-4616(2007)01-0013-09

求解非线性最小二乘问题的自适应锥模型信赖域算法

杨 扬¹, 孙文瑜²

(1 徐州工程学院数学与物理科学学院, 江苏 徐州 221008)

(2 南京师范大学数学与计算机科学学院, 江苏 南京 210097)

[摘要] 针对非线性最小二乘问题, 利用锥模型算法思想, 给出了海赛矩阵中二阶信息项的割线近似的不同校正公式, 并利用自适应信赖域技术给出了求解非线性最小二乘问题的自适应锥模型信赖域算法。算法中我们允许使用非精确方法近似求解信赖域子问题。文中给出了新算法的全局收敛性和超线性收敛性分析以及数值试验结果。

[关键词] 非线性最小二乘问题, 信赖域方法, 锥模型, 自适应, 总体收敛性, 超线性收敛性

0 Introduction

We consider the following nonlinear least squares problem

$$\min_{x \in R^n} f(x), \quad (1)$$

where the objective function f has the following special form

$$f(x) = \frac{1}{2} \sum_{j=1}^m r_j^2(x), \quad (2)$$

where each $r_j(x)$ is a smooth function from R^n to \mathbf{R} . We refer to each r_j as a residual, and we assume throughout this paper that $m \geq n$.

Received date 2005-09-28. **Revised date** 2006-01-20

Foundation item: Supported by the National Natural Science Foundation of China (10231060), the Special Research Found of Doctoral Program of Higher Education of China (20040319003), the Research Project of Xuzhou Institute of Technology (XKY200622).

Biography Yang Yang born in 1981, female, teaching assistant majored in numerical mathematics E-mail yangyoung600@sina.com.

Corresponding author Sun Wenyu, born in 1949, professor majored in numerical mathematics E-mail wysun@njnu.edu.cn

Nonlinear least squares problems have been a fruitful study area mainly because of their applications to various practical problems for instance the solution of nonlinear equations and data fitting. We can see that the nonlinear least squares problem (1) ~ (2) is a kind of unconstrained optimization problems. However, it has its special structure. So it is intelligent to exploit the special structure in and its derivatives form in minimizing problem (1) ~ (2).

We first define $\kappa: R^n \rightarrow R^m$ by

$$\mathbf{r}(\mathbf{x}) = (r_1(\mathbf{x}), r_2(\mathbf{x}), \dots, r_m(\mathbf{x}))^\top. \quad (3)$$

Using this notation, we have

$$\mathbf{g}(\mathbf{x}) = \nabla f(\mathbf{x}) = J(\mathbf{x})^\top \mathbf{r}(\mathbf{x}), \quad (4)$$

$$\mathbf{H}(\mathbf{x}) = \nabla^2 f(\mathbf{x}) = J(\mathbf{x})^\top J(\mathbf{x}) + \sum_{j=1}^m r_j(\mathbf{x}) \nabla^2 r_j(\mathbf{x}), \quad (5)$$

where $J(\mathbf{x})_{j,i} = \frac{\partial r_j}{\partial x_i}$. We denote $\mathbf{S}(\mathbf{x}) = \sum_{j=1}^m r_j(\mathbf{x}) \nabla^2 r_j(\mathbf{x})$. In many applications, it is possible to calculate $J(\mathbf{x})$ explicitly then the gradient $\mathbf{g}(\mathbf{x})$ and the first part of Hessian $\mathbf{H}(\mathbf{x})$ can be easily obtained. However, the computation of the second part $\mathbf{S}(\mathbf{x})$ may cost expensively.

In the following paper, we denote $f_k = f(\mathbf{x}_k)$, $\mathbf{J}_k = J(\mathbf{x}_k)$, $\mathbf{S}_k = \mathbf{S}(\mathbf{x}_k)$, $\mathbf{g}_k = \mathbf{g}(\mathbf{x}_k)$ and $\mathbf{H}_k = \mathbf{H}(\mathbf{x}_k)$.

At the current iterate \mathbf{x}_k , the Gauss-Newton method uses the approximation $\mathbf{H}_k \approx \mathbf{J}_k^\top \mathbf{J}_k$, and employs the following quadratic model at \mathbf{x}_k

$$q(\mathbf{d}) = f_k + \mathbf{g}_k^\top \mathbf{d} + \frac{1}{2} \mathbf{d}^\top \mathbf{J}_k^\top \mathbf{J}_k \mathbf{d} \quad (6)$$

A lot of numerical experiments show that this model is effective for zero-residual and small-residual case. However, for large-residual case, the model (6) is inadequate because \mathbf{S}_k is too significant to be ignored. Thus, we can get a secant approximation of \mathbf{S}_k by using the quasi-Newton updating formula and then we get a better approximation of \mathbf{H}_k . We assume that at \mathbf{x}_k , symmetric matrix \mathbf{A}_k is the approximation of \mathbf{S}_k , then we can employ such a quadratic model

$$q(\mathbf{d}) = f_k + \mathbf{g}_k^\top \mathbf{d} + \frac{1}{2} \mathbf{d}^\top (\mathbf{J}_k^\top \mathbf{J}_k + \mathbf{A}_k) \mathbf{d} \quad (7)$$

In Dennis et al^[1,2], the update formula for \mathbf{A}_k is given as follows

$$\mathbf{A}_{k+1} = \mathbf{A}_k + \frac{(\hat{\mathbf{y}}_k - \mathbf{A}_k \mathbf{d}_k) \mathbf{y}_k^\top + \mathbf{y}_k (\hat{\mathbf{y}}_k - \mathbf{A}_k \mathbf{d}_k)^\top}{\mathbf{y}_k^\top \mathbf{d}_k} - \frac{\mathbf{d}_k^\top (\hat{\mathbf{y}}_k - \mathbf{A}_k \mathbf{d}_k) \mathbf{y}_k \mathbf{y}_k^\top}{(\mathbf{y}_k^\top \mathbf{d}_k)^2}, \quad (8)$$

where $\mathbf{A}_0 = 0$, $\hat{\mathbf{y}}_k = (\mathbf{J}_{k+1} - \mathbf{J}_k)^\top \mathbf{r}(\mathbf{x}_{k+1})$, $\mathbf{y}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$, $\mathbf{d}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$.

Since Davidon^[3] proposed the conic method for the unconstrained optimization, various scholars have studied this topic. The conic model method with more degree of freedom can incorporate more information in iterations and it is more effective. Moreover, the conic model has the rapid convergence property near the minimizer point as the quadratic model.

In the next section, we describe our new algorithm. We discuss its global and local superlinear convergence results in section 2. In section 3, the numerical results are reported. The final remarks are given in section 4.

1 Our Algorithm

In this section we describe our new algorithm for nonlinear least squares problems. At the k th iteration, the local conic model for (1) ~ (2) is as follows

$$\phi_k(\mathbf{d}) = f_k + \frac{\mathbf{g}_k^\top \mathbf{d}}{1 + \mathbf{h}_k^\top \mathbf{d}} + \frac{1}{2} \frac{\mathbf{d}^\top \mathbf{B}_k \mathbf{d}}{(1 + \mathbf{h}_k^\top \mathbf{d})^2} \quad (9)$$

where $\mathbf{h}_k \in R^n$ is a horizon vector satisfying $1 + \mathbf{h}_k^\top \mathbf{d} > 0$. It is easy to get

$$\nabla \phi_k(\mathbf{d}) = \frac{1}{1 + \mathbf{h}_k^\top \mathbf{d}} \left(I - \frac{\mathbf{h}_k \mathbf{h}_k^\top}{1 + \mathbf{h}_k^\top \mathbf{d}} \right) \left(\mathbf{g}_k + \frac{\mathbf{B}_k \mathbf{d}}{1 + \mathbf{h}_k^\top \mathbf{d}} \right), \quad (10)$$

$$\nabla^2 \phi_k(\mathbf{d}) = \frac{\mathbf{B}_k - \mathbf{h}_k \mathbf{g}_k^\top - \mathbf{g}_k \mathbf{h}_k^\top}{(1 + \mathbf{h}_k^\top \mathbf{d})^2} - \frac{2\mathbf{B}_k \mathbf{d} \mathbf{h}_k^\top + 2\mathbf{h}_k \mathbf{d}^\top \mathbf{B}_k}{(1 + \mathbf{h}_k^\top \mathbf{d})^3} - \frac{\mathbf{h}_k \mathbf{h}_k^\top}{(1 + \mathbf{h}_k^\top \mathbf{d})^3} \left(2\mathbf{g}_k^\top \mathbf{d} + \frac{3\mathbf{d}^\top \mathbf{B}_k \mathbf{d}}{1 + \mathbf{h}_k^\top \mathbf{d}} \right). \quad (11)$$

Obviously, we have that $\phi_k(\mathbf{0}) = f_k$, $\nabla \phi_k(\mathbf{0}) = \mathbf{g}_k$, $\nabla^2 \phi_k(\mathbf{0}) = \mathbf{B}_k - \mathbf{h}_k \mathbf{g}_k^\top - \mathbf{g}_k \mathbf{h}_k^\top$.

Assume that we get the next iteration point $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{d}_k$ (how to get \mathbf{d}_k will be given later), and the conic model at \mathbf{x}_{k+1} is

$$\phi_{k+1}(\mathbf{d}) = f_{k+1} + \frac{\mathbf{g}_{k+1}^\top \mathbf{d}}{1 + \mathbf{h}_{k+1}^\top \mathbf{d}} + \frac{1}{2} \frac{\mathbf{d}^\top \mathbf{B}_{k+1} \mathbf{d}}{(1 + \mathbf{h}_{k+1}^\top \mathbf{d})^2}. \quad (12)$$

As the analysis in [4], we want the above conic model to satisfy the following conditions

$$\phi_{k+1}(\mathbf{0}) = f_{k+1}, \quad \nabla \phi_{k+1}(\mathbf{0}) = \mathbf{g}_{k+1}, \quad (13)$$

$$\phi_{k+1}(-\mathbf{d}_k) = f_k, \quad \nabla \phi_{k+1}(-\mathbf{d}_k) = \mathbf{g}_k, \quad (14)$$

$$\nabla^2 \phi_{k+1}(\mathbf{0}) = \mathbf{J}_{k+1}^\top \mathbf{J}_{k+1} + \mathbf{A}_{k+1}. \quad (15)$$

We can find that (13) obviously holds. It is easy to show that (14) are satisfied by choosing $\gamma_k > 0$, \mathbf{h}_{k+1} and \mathbf{B}_{k+1} to satisfy

$$\mathbf{h}_{k+1}^\top \mathbf{d}_k = 1 - \gamma_k \quad (16)$$

$$(\mathbf{g}_k^\top \mathbf{d}_k) \gamma_k^2 + 2(f_k - f_{k+1}) \gamma_k + \mathbf{g}_{k+1}^\top \mathbf{d}_k = 0 \quad (17)$$

$$\mathbf{B}_{k+1} \mathbf{d}_k = \gamma_k \mathbf{g}_{k+1} - \gamma_k^2 \mathbf{g}_k + \gamma_k^2 \mathbf{h}_{k+1} \mathbf{d}_k^\top \mathbf{g}_k \quad (18)$$

Let

$$D_k = (f_k - f_{k+1})^2 - \mathbf{g}_{k+1}^\top \mathbf{d}_k \mathbf{g}_k^\top \mathbf{d}_k, \quad (19)$$

if $D_k \geq 0$, set $\theta_k = \sqrt{D_k}$ and $\gamma_k = \frac{f_k - f_{k+1} + \theta_k}{-\mathbf{g}_k^\top \mathbf{d}_k}$. Once γ_k is determined, note that

$$\mathbf{h}_{k+1} = \frac{(1 - \gamma_k) \mathbf{b}_k}{\mathbf{d}_k^\top \mathbf{b}_k} \quad (20)$$

for any $\mathbf{b}_k \in R^n$ such that $\mathbf{d}_k^\top \mathbf{b}_k \neq 0$ will satisfy (16). In particular, since $\mathbf{g}_k^\top \mathbf{d}_k < 0$, we can use $\mathbf{b}_k = \mathbf{g}_k$, so that

$$\mathbf{h}_{k+1} = \frac{(1 - \gamma_k) \mathbf{g}_k}{\mathbf{g}_k^\top \mathbf{d}_k}. \quad (21)$$

Since $\nabla^2 \phi_{k+1}(\mathbf{0}) = \mathbf{B}_{k+1} - \mathbf{h}_{k+1} \mathbf{g}_{k+1}^\top - \mathbf{g}_{k+1} \mathbf{h}_{k+1}^\top$, from (15) we have that

$$(\mathbf{J}_{k+1}^\top \mathbf{J}_{k+1} + \mathbf{A}_{k+1}) \mathbf{d}_k = \mathbf{B}_{k+1} \mathbf{d}_k - \mathbf{h}_{k+1} \mathbf{g}_{k+1}^\top \mathbf{d}_k - \mathbf{g}_{k+1} \mathbf{h}_{k+1}^\top \mathbf{d}_k.$$

Then according to (16) and (18), we get that

$$(\mathbf{J}_{k+1}^\top \mathbf{J}_{k+1} + \mathbf{A}_{k+1}) \mathbf{d}_k = (2\gamma_k - 1) \mathbf{g}_{k+1} - \gamma_k^2 \mathbf{g}_k + \mathbf{h}_{k+1} (\gamma_k^2 \mathbf{d}_k^\top \mathbf{g}_k - \mathbf{d}_k^\top \mathbf{g}_{k+1}). \quad (22)$$

From (22), we know that \mathbf{A}_{k+1} needs to satisfy the following generalized quasi-Newton equation

$$\mathbf{A}_{k+1} \mathbf{d}_k = \tilde{\mathbf{y}}_k, \quad (23)$$

where $\tilde{\mathbf{y}}_k = (2\gamma_k - 1) \mathbf{g}_{k+1} - \gamma_k^2 \mathbf{g}_k + \mathbf{h}_{k+1} (\gamma_k^2 \mathbf{d}_k^\top \mathbf{g}_k - \mathbf{d}_k^\top \mathbf{g}_{k+1}) - \mathbf{J}_{k+1}^\top \mathbf{J}_{k+1} \mathbf{d}_k$.

Remark 1.1 If $D_k < 0$, we set $\gamma_k = 1$, and then we get $\mathbf{h}_{k+1} = \mathbf{0}$ and $\tilde{\mathbf{y}}_k = \mathbf{g}_{k+1} - \mathbf{g}_k - \mathbf{J}_{k+1}^\top \mathbf{J}_{k+1} \mathbf{d}_k$. The conic model is reduced to the quadratic one.

To determine \mathbf{A}_{k+1} uniquely, we impose the additional condition that among all symmetric matrices satisfying the secant equation (23), \mathbf{A}_{k+1} is in some sense closest to the current matrix \mathbf{A}_k . In other words, \mathbf{A}_{k+1} is the solution to the following problem

$$\text{min} \|\mathbf{A} - \mathbf{A}_k\| \quad (24)$$

$$\text{s.t. } \mathbf{A} = \mathbf{A}^\top, \quad \mathbf{A} \mathbf{d}_k = \tilde{\mathbf{y}}_k. \quad (25)$$

Many matrix norms can be used in (24), and each norm gives rise to a different quasi-Newton method. Now, we use the weighted Frobenius norm to produce a quasi-Newton updating formula of \mathbf{A}_{k+1} .

Theorem 1.2 Assume that $\mathbf{v}_k \in R^n$ satisfies $\mathbf{v}_k^\top \mathbf{d}_k > 0$ and $\mathbf{W} \in R^{n \times n}$ is the nonsingular symmetric matrix satisfying the relation $\mathbf{W} \mathbf{v}_k = \mathbf{W}^{-1} \mathbf{d}_k$, then the updating

$$\mathbf{A}_{k+1} = \mathbf{A}_k + \frac{(\tilde{\mathbf{y}}_k - \mathbf{A}_k \mathbf{d}_k) \mathbf{v}_k^\top + \mathbf{v}_k (\tilde{\mathbf{y}}_k - \mathbf{A}_k \mathbf{d}_k)^\top}{\mathbf{v}_k^\top \mathbf{d}_k} - \frac{(\tilde{\mathbf{y}}_k - \mathbf{A}_k \mathbf{d}_k)^\top \mathbf{d}_k}{(\mathbf{v}_k^\top \mathbf{d}_k)^2} \mathbf{v}_k \mathbf{v}_k^\top \quad (26)$$

is the unique solution to the minimizing problem

$$\min \{ \|A - A_k\|_{W,F} : A d_k = \tilde{y}_k A^T = A \},$$

where $\|A\|_{W,F} = \|WA W\|_F$.

Proof See Theorem 5.1.7 in [5].

In particular if we set $v_k = d_k$, we get PSB analogue update

$$A_{k+1} = A_k + \frac{(\tilde{y}_k - A_k d_k) d_k^T + d_k (\tilde{y}_k - A_k d_k)^T}{d_k^T d_k} - \frac{(\tilde{y}_k - A_k d_k)^T d_k}{(d_k^T d_k)^2} d_k d_k^T, \quad (27)$$

and if we set $v_k = y_k = g_{k+1} - g_k$, then we get the DFP analogue update

$$A_{k+1} = A_k + \frac{(\tilde{y}_k - A_k d_k) y_k^T + y_k (\tilde{y}_k - A_k d_k)^T}{y_k^T d_k} - \frac{(\tilde{y}_k - A_k d_k)^T d_k}{(y_k^T d_k)^2} y_k y_k^T. \quad (28)$$

According to the different values of v_k , we can get other different updates.

Once A_{k+1} is determined we get the update of B_{k+1} ,

$$B_{k+1} = J_{k+1}^T J_{k+1} + A_{k+1} + h_{k+1} g_{k+1}^T + g_{k+1} h_{k+1}^T.$$

We know that B_k is symmetric but we cannot keep the positive definiteness of B_k for these updates. Since the trust region approach does not need B_k to be positive definite to obtain global convergence, we construct an algorithm with trust region strategy.

In the following paper the notation $\|\cdot\|$ denotes the Euclidean norm on R^n . At the k th iteration we add a constraint $\left\| \frac{d}{1+h_k^T d} \right\| \leq \Delta_k$ to the local conic model (9), that is we can get d_k by solving the following subproblem

$$\begin{aligned} \min \phi_k(d) &= f_k + \frac{g_k^T d}{1+h_k^T d} + \frac{1}{2} \frac{d^T B_k d}{(1+h_k^T d)^2} \\ \text{s.t. } &\left\| \frac{d}{1+h_k^T d} \right\| \leq \Delta_k. \end{aligned} \quad (29)$$

If we set $w = \frac{d}{1+h_k^T d}$, then the trust region subproblem with a conic model (29) is transformed to the following

general trust region subproblem with a quadratic model

$$\begin{aligned} \min \phi_k(w) &= f_k + g_k^T w + \frac{1}{2} w^T B_k w \\ \text{s.t. } &\|w\| \leq \Delta_k. \end{aligned} \quad (30)$$

The choice of the trust region radius is important to the efficiency of the trust region method so we use the adaptive trust region method given by Zhang et al^[6] to implement our algorithm. That is in (30), $\Delta_k = c^p \|g_k\| \cdot \|B_k^{-1}\|$, where $0 < c < 1$, and p is a nonnegative integer. B_k is a safely positive definite matrix based on Schnabel and Eskow modified Cholesky factorization^[7]. We get w_k and set the trial step $d_k = \frac{w_k}{1-h_k^T w_k}$. Then the actual reduction of $f(x)$ is defined by

$$aread_k = f_k - f(x_k + d_k) \quad (31)$$

and the predictive reduction of $f(x)$ is defined by

$$pred_k = \phi_k(\mathbf{0}) - \phi_k(d_k) = \phi(\mathbf{0}) - \phi(w_k) = -g_k^T w_k - \frac{1}{2} w_k^T B_k w_k. \quad (32)$$

Further we define $r_k = aread_k / pred_k$ to be a measure of the improvement. If $aread_k$ is satisfactory compared with $pred_k$, the trial step d_k is accepted and $x_{k+1} = x_k + d_k$. Otherwise we reduce the trust region radius (increasing p by one) to solve the subproblem (30) again until a satisfactory trial step is obtained.

Remark 1.3 We will not solve the subproblem (30) exactly to get w_k , instead we can use some inexact methods to solve it. No matter which inexact method is used we want w_k to satisfy the following condition

$$pred_k \geq \beta \|\mathbf{g}_k\| \min \left\{ \Delta_k, \frac{\|\mathbf{g}_k\|}{\|\mathbf{B}_k\|} \right\}, \quad (33)$$

where $\beta \in (0, 1]$.

Now we describe our new algorithm as follows

Algorithm 1.4

Step 0 Given \mathbf{x}_0 , \mathbf{h}_0 , \mathbf{A}_0 , $\varepsilon > 0$, $0 < \eta < 1$. Set $k = 0$, $p = 0$.

Step 1 Compute $r(\mathbf{x}_k)$, \mathbf{J}_k and set $\mathbf{g}_k = \mathbf{J}_k^T r(\mathbf{x}_k)$. If $\|\mathbf{g}_k\| \leq \varepsilon$, then stop.

Step 2 Set $f_k = \frac{1}{2} r(\mathbf{x}_k)^T r(\mathbf{x}_k)$, $\mathbf{B}_k = \mathbf{J}_k^T \mathbf{J}_k + \mathbf{A}_k + \mathbf{h}_k \mathbf{g}_k^T + \mathbf{g}_k \mathbf{h}_k^T$.

Step 3 Solve the subproblem (30) to get \mathbf{w}_k , and set $\mathbf{d}_k = \frac{\mathbf{w}_k}{1 - \mathbf{h}_k^T \mathbf{w}_k}$.

Step 4 Compute $ared_k$, $pred_k$ and \mathbf{r}_k .

Step 5 If $\mathbf{r}_k \geq \eta$, set $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{d}_k$, generate \mathbf{h}_{k+1} , \mathbf{A}_{k+1} , set $k = k + 1$, $p = 0$, go to step 1. Otherwise set $p = p + 1$, go to step 3.

Remark 1.5 Generally we set $\mathbf{h}_0 = \mathbf{0}$ and $\mathbf{A}_0 = \mathbf{0}$, that is we use Gauss-Newton iteration to get \mathbf{x}_1 .

Remark 1.6 In order to keep $1 + \mathbf{h}_k^T \mathbf{d}_k > 0$ we just need to keep $1 - \mathbf{h}_k^T \mathbf{w}_k > 0$. So we need to keep

$\|\mathbf{h}_k\| \Delta_k < 1$. If the trust region radius Δ_k satisfies $\|\mathbf{h}_k\| \Delta_k \geq 1$, we will set $\Delta_k = \frac{\alpha}{\|\mathbf{h}_k\|}$ where $0 < \alpha < 1$.

2 Convergence Property

In this section, we discuss the global and local superlinear convergence properties of our algorithm. First of all we would like to make the following assumptions.

Assumption 2.1 (i) The level set $L(\mathbf{x}_0) = \{\mathbf{x} \mid f(\mathbf{x}) \leq f(\mathbf{x}_0)\}$ is bounded for any given $\mathbf{x}_0 \in R^n$; $r_i(\mathbf{x})$ ($i = 1, 2, \dots, m$) is twice continuously differentiable in $L(\mathbf{x}_0)$ and bounded; (ii) $\|\mathbf{B}_k\|$ and $\|\mathbf{h}_k\|$ are both uniformly bounded, that is there exist $K_1 > 0$ and $K_2 > 0$ such that $\|\mathbf{B}_k\| \leq K_1$ and $\|\mathbf{h}_k\| \leq K_2$ for all k .

Remark 2.2 If Assumption 2.1 holds and \mathbf{B}_k is invertible, since $\|\mathbf{B}_k^{-1}\| \|\mathbf{B}_k\| \geq 1$, we know that there exists a positive number $K_3 > 0$ such that for all k

$$\|\mathbf{B}_k^{-1}\| \geq K_3 \quad (34)$$

Lemma 2.3 Suppose that Assumption 2.1 holds and that \mathbf{w}_k is an inexact solution of the subproblem (30) such that (33) holds. Then Algorithm 1.4 cannot cycle infinitely between Step 3 and Step 5.

Proof Suppose that Algorithm 1.4 cycles infinitely between Step 3 and Step 5 at iteration k . We define the cycling index at iteration k by $k(i)$, then we have

$$r_{k(i)} < \eta, \quad i = 1, 2, \dots \quad (35)$$

and $\Delta_{k(i)} = c^i \|\mathbf{g}_k\| \|\mathbf{B}_k^{-1}\| \rightarrow 0$ as $i \rightarrow \infty$. On the other hand when $\Delta_{k(i)} \rightarrow 0$, we have $\mathbf{w}_{k(i)} \rightarrow 0$. Then when $\|\mathbf{w}_k\|$ is sufficiently close to zero since $\|\mathbf{h}_k\|$ is bounded we have $1/(1 - \mathbf{h}_k^T \mathbf{w}_k) = 1 + O(\|\mathbf{w}_k\|)$. Since $r_i(\mathbf{x})$ ($i = 1, 2, \dots, m$) is twice continuously differentiable in $L(\mathbf{x}_0)$, then there exists $K_4 > 0$ such that $\|\mathbf{H}(\mathbf{x})\| \leq K_4$ holds for all $\mathbf{x} \in L(\mathbf{x}_0)$. Then from the boundedness of $\|\mathbf{B}_k\|$ and $\|\mathbf{H}(\mathbf{x})\|$, we obtain

$$\mathbf{g}_k^T \mathbf{d}_k = \frac{\mathbf{g}_k^T \mathbf{w}_k}{1 - \mathbf{h}_k^T \mathbf{w}_k} = \mathbf{g}_k^T \mathbf{w}_k + O(\|\mathbf{w}_k\|^2), \quad (36)$$

$$\mathbf{d}_k^T \mathbf{H}(\mathbf{x}) \mathbf{d}_k = \frac{\mathbf{w}_k^T \mathbf{H}(\mathbf{x}) \mathbf{w}_k}{(1 - \mathbf{h}_k^T \mathbf{w}_k)^2} = \mathbf{w}_k^T \mathbf{H}(\mathbf{x}) \mathbf{w}_k + o(\|\mathbf{w}_k\|^2), \quad (37)$$

$$\begin{aligned} |ared_k - pred_k| &= |f(\mathbf{x}_k) - f(\mathbf{x}_k + \mathbf{d}_k) + \mathbf{g}_k^T \mathbf{w}_k + \frac{1}{2} \mathbf{w}_k^T \mathbf{B}_k \mathbf{w}_k| \\ &= |- \mathbf{g}_k^T \mathbf{d}_k - \frac{1}{2} \mathbf{d}_k^T \mathbf{H}(\mathbf{x}_k + \theta_k \mathbf{d}_k) \mathbf{d}_k + \mathbf{g}_k^T \mathbf{w}_k + \frac{1}{2} \mathbf{w}_k^T \mathbf{B}_k \mathbf{w}_k| \\ &= |- \frac{1}{2} \mathbf{w}_k^T \mathbf{H}(\mathbf{x}_k + \theta_k \mathbf{d}_k) \mathbf{w}_k + \frac{1}{2} \mathbf{w}_k^T \mathbf{B}_k \mathbf{w}_k + O(\|\mathbf{w}_k\|^2)| \end{aligned}$$

$$\leq \frac{1}{2}(K_1 + K_4) \|\mathbf{w}_k\|^2 + O(\|\mathbf{w}_k\|^2) = O(\|\mathbf{w}_k^2\|). \quad (38)$$

Then we have

$$|r_{k(i)} - 1| = \frac{|ared_{k(i)} - pred_{k(i)}|}{|pred_{k(i)}|} \leq \frac{O(\|\mathbf{w}_{k(i)}\|^2)}{\beta \|\mathbf{g}_k\| \max \left\{ \|\mathbf{w}_{k(i)}\|, \frac{\|\mathbf{g}_k\|}{\|\mathbf{B}_k\|} \right\}}. \quad (39)$$

Since $\|\mathbf{w}_{k(i)}\| \rightarrow 0$ as $i \rightarrow \infty$, then from (39) we have $|r_{k(i)} - 1| \rightarrow 0$ as $i \rightarrow \infty$, which implies that $r_{k(i)} \geq \eta$ holds for sufficiently large i . This is a contradiction to (35).

Lemma 2.4 If \mathbf{B}_k is uniformly bounded there exist two positive scalars c_1 and c_2 such that $c_1 \leq \|\mathbf{B}_k^{-1}\| \leq c_2$.

Proof In the sense of modified Cholesky factorization, we have $\mathbf{B}_k = \mathbf{B}_k + \mathbf{E}_k$ is safely positive definite. Since \mathbf{B}_k is uniformly bounded there exist two positive scalars $\mu_1 \leq \mu_2$ such that

$$0 < \mu_1 \leq \lambda_i(\mathbf{B}_k) \leq \mu_2, \quad k = 1, 2, \dots$$

Then $c_1 \leq \|\mathbf{B}_k^{-1}\| \leq c_2$ for $k = 1, 2, \dots$, where $c_1 = \frac{1}{\mu_2}$, $c_2 = \frac{1}{\mu_1}$.

Theorem 2.5 Suppose that the conditions of Lemma 2.3 hold. If $\varepsilon = 0$ Algorithm 1.4 either stops in finitely many steps or generates an infinite sequence $\{\mathbf{x}_k\}$ such that

$$\lim_{k \rightarrow \infty} \|\mathbf{g}_k\| = 0 \quad (40)$$

Proof Suppose that (40) is not true, then there exists a positive scalar ε and an infinite set T , such that $\forall k \in T$, $\|\mathbf{g}_k\| \geq \varepsilon$. Since by Lemma 2.3 and Lemma 2.4, we have c and $\|\mathbf{B}_k^{-1}\|$ are both bounded away from zero, then we have Δ_k is bounded away from zero $\forall k \in T$. On the other hand, we have

$$f(\mathbf{x}_k) - f(\mathbf{x}_{k+1}) \geq \eta \cdot pred_k \geq \eta \cdot \beta \cdot \|\mathbf{g}_k\| \max \left\{ \Delta_k, \frac{\|\mathbf{g}_k\|}{\|\mathbf{B}_k\|} \right\} \geq \eta \cdot \beta \cdot \min \inf_{k \in T} \Delta_k \frac{\varepsilon}{K_1}. \quad (41)$$

Since $\{f(\mathbf{x}_k)\}$ is monotonically decreasing and bounded below, then from (41) we have $\lim_{k \in T} \Delta_k = 0$. This is a contradiction.

Next we establish the local superlinear convergence for our algorithm.

Theorem 2.6 Suppose that Assumption 2.1 holds and the sequence $\{\mathbf{x}_k\}$ generated by Algorithm 1.4 converges to \mathbf{x}^* , where $\mathbf{H}(\mathbf{x}^*)$ is positive definite. If \mathbf{B}_k is positive definite for k sufficiently large and the following condition

$$\lim_{k \rightarrow \infty} \frac{\|(\mathbf{B}_k - \mathbf{H}(\mathbf{x}^*))\hat{\mathbf{w}}_k\|}{\|\hat{\mathbf{w}}_k\|} = 0 \quad (42)$$

holds where $\hat{\mathbf{w}}_k = -\mathbf{B}_k^{-1}\mathbf{g}_k$, then \mathbf{x}_k converges to \mathbf{x}^* superlinearly.

Proof From the assumption we know that $\mathbf{B}_k = \mathbf{B}_k$ when k is sufficiently large. Moreover, $\hat{\mathbf{w}}_k = -\mathbf{B}_k^{-1}\mathbf{g}_k$ is the solution of the following subproblem

$$\begin{aligned} \text{min } \phi_k(\mathbf{w}) &= f_k + \mathbf{g}_k^T \mathbf{w} + \frac{1}{2} \mathbf{w}^T \mathbf{B}_k \mathbf{w} \\ \text{s.t. } \|\mathbf{w}\| &\leq \|\mathbf{g}_k\| \|\mathbf{B}_k^{-1}\| \end{aligned} \quad (43)$$

First of all we show that for k sufficiently large, we have

$$\frac{f(\mathbf{x}_k) - f(\mathbf{x}_k + \mathbf{d}_k)}{\phi(\mathbf{0}) - \phi(\mathbf{d}_k)} > \eta, \quad (44)$$

where $\mathbf{d}_k = \frac{\hat{\mathbf{w}}_k}{1 - \mathbf{h}_k^T \hat{\mathbf{w}}_k}$. It follows from (42) that

$$\mathbf{g}_k + \mathbf{H}(\mathbf{x}^*)\hat{\mathbf{w}}_k = o(\|\hat{\mathbf{w}}_k\|),$$

i.e.

$$\hat{\mathbf{w}}_k = -\mathbf{H}(\mathbf{x}^*)^{-1}\mathbf{g}_k + o(\|\hat{\mathbf{w}}_k\|),$$

then

$$\|\hat{w}_k\| \leq \|H(x^*)^{-1}\| \|\mathbf{g}_k\| + o(\|\hat{w}_k\|), \quad \frac{\|\mathbf{g}_k\|}{\|\hat{w}_k\|} \geq \frac{1}{\|H(x^*)^{-1}\|} + \frac{o(\|\hat{w}_k\|)}{\|\hat{w}_k\|}.$$

Since $H(x^*)$ is positive definite, we have that $\|\hat{w}_k\| = O(\|\mathbf{g}_k\|)$.

From Theorem 2.5, we know that $\mathbf{g}_k \rightarrow \mathbf{0}$ so we have $\hat{w}_k \rightarrow \mathbf{0}$.

$$\begin{aligned} f(\mathbf{x}_k + \mathbf{d}_k) - \phi(\mathbf{d}_k) &= \frac{\mathbf{g}_k^\top \hat{w}_k}{1 - \mathbf{h}_k^\top \hat{w}_k} + \frac{1}{2} \frac{1}{(1 - \mathbf{h}_k^\top \hat{w}_k)^2} \hat{w}_k^\top \mathbf{M}_k \hat{w}_k - \mathbf{g}_k^\top \hat{w}_k - \frac{1}{2} \hat{w}_k^\top \mathbf{B}_k \hat{w}_k \\ &= \frac{1}{1 - \mathbf{h}_k^\top \hat{w}_k} \mathbf{g}_k^\top \hat{w}_k \mathbf{h}_k^\top \hat{w}_k + \frac{1}{2} \hat{w}_k^\top (H(x^*) - \mathbf{B}_k) \hat{w}_k \\ &\quad + \frac{1}{2} \hat{w}_k^\top (\mathbf{M}_k - H(x^*)) \hat{w}_k + \frac{1}{2} \left(\frac{1}{(1 - \mathbf{h}_k^\top \hat{w}_k)^2} - 1 \right) \hat{w}_k^\top \mathbf{M}_k \hat{w}_k, \end{aligned} \quad (45)$$

where $\mathbf{M}_k = H(x_k + \frac{\theta \hat{w}_k}{1 - \mathbf{h}_k^\top \hat{w}_k})$ for some $\theta \in (0, 1)$. Since \mathbf{h}_k is uniformly bounded, we have

$$\frac{1}{1 - \mathbf{h}_k^\top \hat{w}_k} = 1 + O(\|\hat{w}_k\|). \quad (46)$$

Moreover, from $\mathbf{g}_k \rightarrow \mathbf{0}$, $\hat{w}_k \rightarrow \mathbf{0}$ and (42), we know that

$$\frac{|f(\mathbf{x}_k + \mathbf{d}_k) - \phi(\mathbf{d}_k)|}{\|\hat{w}_k\|^2} \rightarrow 0 \text{ as } k \rightarrow \infty. \quad (47)$$

From Remark 2.2, we know that

$$\phi(\mathbf{0}) - \phi(\mathbf{d}_k) = -\mathbf{g}_k^\top \hat{w}_k - \frac{1}{2} \hat{w}_k^\top \mathbf{B}_k \hat{w}_k = \mathbf{g}_k^\top \mathbf{B}_k^{-1} \mathbf{g}_k - \frac{1}{2} \mathbf{g}_k^\top \mathbf{B}_k^{-1} \mathbf{g}_k = \frac{1}{2} \mathbf{g}_k^\top \mathbf{B}_k^{-1} \mathbf{g}_k \geq \frac{1}{2} K_3 \|\mathbf{g}_k\|^2. \quad (48)$$

Therefore

$$\begin{aligned} \lim_{k \rightarrow \infty} \left| \frac{f(\mathbf{x}_k) - f(\mathbf{x}_k + \mathbf{d}_k)}{\phi(\mathbf{0}) - \phi(\mathbf{d}_k)} - 1 \right| &= \lim_{k \rightarrow \infty} \frac{|f(\mathbf{x}_k + \mathbf{d}_k) - \phi(\mathbf{d}_k)|}{|\phi(\mathbf{0}) - \phi(\mathbf{d}_k)|} \\ &\leq \lim_{k \rightarrow \infty} \frac{|f(\mathbf{x}_k + \mathbf{d}_k) - \phi(\mathbf{d}_k)|}{\frac{1}{2} K_3 \|\mathbf{g}_k\|^2} = \lim_{k \rightarrow \infty} \frac{|f(\mathbf{x}_k + \mathbf{d}_k) - \phi(\mathbf{d}_k)|}{\|\hat{w}_k\|^2}. \end{aligned} \quad (49)$$

The last equation of (49) holds because of $\|\hat{w}_k\| = O(\|\mathbf{g}_k\|)$. From (49) and (47), we know that (44) holds for k sufficiently large, so $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{d}_k$ when k is sufficiently large. Since $\mathbf{g}_{k+1} = \mathbf{g}_{k+1} - \mathbf{g}_k - \mathbf{B}_k \hat{w}_k$, then by the way to prove (45), we have

$$\frac{\|\mathbf{g}_{k+1}\|}{\|\hat{w}_k\|} = \frac{\|\mathbf{g}_{k+1} - \mathbf{g}_k - \mathbf{B}_k \hat{w}_k\|}{\|\hat{w}_k\|} \rightarrow 0 \quad (50)$$

From $\mathbf{d}_k = \hat{w}_k / (1 - \mathbf{h}_k^\top \hat{w}_k)$ and (46) we have

$$\frac{\|\mathbf{d}_k\|}{\|\hat{w}_k\|} \rightarrow 1 \text{ as } k \rightarrow \infty. \quad (51)$$

Then from (50) and (51), we obtain

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{g}_{k+1}\|}{\|\mathbf{x}_{k+1} - \mathbf{x}_k\|} = 0 \quad (52)$$

Since $f(\mathbf{x})$ is twice continuously differentiable and $H(x^*)$ is positive definite, it is easy to show that

$$\lim_{k \rightarrow \infty} \frac{\|\mathbf{x}_{k+1} - \mathbf{x}^*\|}{\|\mathbf{x}_k - \mathbf{x}^*\|} = 0 \quad (53)$$

Thus \mathbf{x}_k converges to \mathbf{x}^* superlinearly.

3 Numerical Results

In this section, we test our Algorithm 1.4 on a set of standard nonlinear least-squares problems given in [8]. In the following, we use *cls* to stand for our new algorithm. In order to show the performance of *cls*, we compare *cls* with the quasi-Newton trust region algorithm using the quadratic model (7), which is denoted by *qls*

in the remainder. All the programs are written in MATLAB with double precision. For comparison, *qls* also uses the adaptive trust region strategy.

In this paper, we use the conjugate gradient method proposed by Steihaug^[9] to solve the quadratic trust region subproblems (30). It can be proved that this inexact method can keep (33) hold with $\beta = \frac{1}{2}$. For comparison, *cls* and *qls* use the same subroutine to solve the quadratic trust region subproblem.

The parameters are chosen as follows: $\eta = 0.1$, $\varepsilon = 10^{-8}$, $c = 0.25$, $\alpha = 1 - \varepsilon$. We denote the number of gradient evaluations by *ng*, the number of function evaluations by *nf*. *L* is the common logarithm of parameter factor to the standard initial point according to the rule given in [8]. *f* is the final objective function value that we obtain. Note that in the following tables, f^* denotes the optimal objective function value.

From the numerical results, we have the following conclusions:

1. From the numerical results in Table 2 and Table 3, we can see that for most of the problems, *cls* performs better than *qls*, and for some problems, *cls* reaches the minimum, but *qls* fails.

2. From the numerical results about *cls* in Table 2 and Table 3, we can see that the numbers *nf* and *ng* for the update (28) are smaller than those required for the update (27) for most of the problems considered.

3. Also, we have compared our results about *cls* in Table 2 with the results in [4], we find that our algorithm performs better.

Table 1 List of test problems

No	Name of Problem	<i>n</i>	<i>m</i>
1	Rosenbrock function	2	2
2	Helical valley function	3	3
3	Powell singular function	4	4
4	Freudenstein and Roth function	2	2
5	Bard function	3	15
6	Kowalewski and Osborne function	4	11
7	Waston function	6	31
8	Watson function	9	31
9	Watson function	12	31
10	Box three-dimensional function	3	10
11	Jennrich and Sampson function	2	10
12	Brown and Dennis function	4	20
13	Brown alnost linear function	40	40
14	Osborne 1 function	5	33

Table 2 Numerical results

No(L)	f^*	<i>cls</i>				<i>qls</i>		
		<i>nf</i>	<i>ng</i>	<i>f</i>	<i>nf</i>	<i>ng</i>	<i>f</i>	
1(0)	0	74	44	9.6387e-026	55	15	1.7808e-021	
1(1)	0	96	58	3.6108e-023	103	27	1.7289e-024	
2(0)	0	27	15	4.6396e-022	54	18	6.7311e-021	
2(1)	0	30	16	1.3756e-020	77	32	4.2974e-019	
3(0)	0	36	24	3.2330e-013	46	23	4.0327e-012	
3(1)	0	46	29	1.6360e-013	67	29	6.6495e-013	
4(0)	22.4921...	38	15	22.4921	23	10	22.4921	
4(1)	22.4921...	43	23	22.4921	61	20	22.4921	
5(0)	4.10743... 10^{-3}	26	15	0.0041	70	21	1.1815 †	
5(1)	8.7143...	501*	490	8.7280	501*	440	8.7225	
6(0)	1.53752... 10^{-4}	36	20	2.1184e-004	54	23	2.1184e-004	
7(0)	1.14383... 10^{-3}	44	19	0.0011	83	21	0.0011	
8(0)	6.9988... 10^{-7}	56	37	6.9988e-007	75	16	6.9988e-007	
9(0)	2.36119... 10^{-10}	114	95	6.7949e-009	501*	464	9.8524e-009	
10(0)	0	26	11	2.8298e-015	22	9	2.7072e-020	
10(1)	0	83	31	9.1362e-018	409	88	7.5518e-013	
11(0)*	62.181...	26	17	62.1811	292	212	62.1811	
11(1)*	62.181...	87	55	62.1811	299	89	129.7901 †	
12(0)*	42.9111...	40	21	4.2911e+004	62	30	4.2911e+004	
12(1)*	42.9111...	45	22	4.2911e+004	66	31	4.2911e+004	
13(0)*	0	12	8	4.2383e-023	44	32	2.9228e-010	
13(1)*	0	158	108	2.4891e-012	345	235	1.1289e-011	
14(0)*	2.7324... 10^{-5}	94	70	2.7324e-005	187	48	2.7324e-005	

* : We stop *cls* or *qls* when *nf* > 500 †: *cls* reaches the minimum, but *qls* fails * : For these problems we stop *cls* and *qls* when $\frac{\|d_k\|}{\|\mathbf{x}_{k+1}\| + \|\mathbf{x}_k\|} \leq \varepsilon$

Table 3 Numerical results

No(L)	f^*	cls				qls		
		nf	ng	f	nf	ng	f	
1(0)	0	53	23	1.7770e-022	86	38	8.1963e-023	
1(1)	0	129	76	7.0885e-016	200	63	1.0095e-023	
2(0)	0	61	19	1.7182e-019	74	27	2.1683e-018	
2(1)	0	24	14	1.1677e-009	52	28	5.9902e-023	
3(0)	0	42	27	4.1661e-013	57	30	2.3738e-012	
3(1)	0	74	38	2.4180e-014	126	46	1.5797e-012	
4(0)	22.4921...	72	22	22.4921	216	37	22.4921	
4(1)	22.4921...	75	27	22.4921	274	48	22.4921	
5(0)	4.10743...10 ⁻³	25	12	0.0041	47	16	0.0041	
5(1)	8.7143...	501*	481	8.7617	501*	465	8.7363	
6(0)	1.53752...10 ⁻⁴	41	23	2.1184e-004	86	27	2.1184e-004	
7(0)	1.14383...10 ⁻³	48	18	0.0011	79	21	0.0011	
8(0)	6.9988...10 ⁻⁷	64	42	6.9988e-007	54	16	6.9988e-007	
9(0)	2.36119...10 ⁻¹⁰	501*	484	2.3336e-008	501*	453	3.9592e-007	
10(0)	0	29	13	4.5729e-024	33	11	3.2819e-021	
10(1)	0	83	35	1.0169e-017	245	42	3.3626e-023	
11(0)*	62.181...	29	19	62.1811	35	21	62.1811	
11(1)*	62.181...	95	56	62.1811	346	119	129.7901†	
12(0)*	42.9111...	58	24	4.2911e+004	79	25	4.2911e+004	
12(1)*	42.9111...	39	26	4.2911e+004	82	38	4.2911e+004	
13(0)*	0	11	6	1.0197e-011	10	7	1.0239e-027	
13(1)*	0	154	105	3.5613e-011	313	229	0	
14(0)*	2.7324...10 ⁻⁵	158	114	2.7324e-005	160	46	2.7324e-005	

4 Conclusions

An adaptive conic trust region method for nonlinear least-squares problems has been presented. Under certain mild conditions, we establish the global and local superlinear convergence results for the proposed method. The numerical results show that the conic model in connection with the adaptive trust region strategy and approximation solution of subproblem is competitive.

[References]

- [1] Dennis J E, Gay D M, Welsch R E. An adaptive nonlinear least-squares algorithm [J]. ACM Transactions on Math Software 1981(7): 348-368.
- [2] Dennis J E, Gay D M, Welsch R E. Algorithms 573 NL2SOL—an adaptive nonlinear least algorithm E4[J]. ACM Transactions on Math Software 1981(7): 369-383.
- [3] Davilon W C. Conic approximation and collinear scaling for optimizers[J]. SIAM J Numer Anal 1980(17): 268-281.
- [4] Han Q M, Sheng S B. Conic model algorithms for nonlinear least-squares problems[J]. Numerical Mathematics: A Journal of Chinese Universities 1995(1): 48-59.
- [5] Yuan Y, Sun W. Optimization Theory and Methods[M]. Beijing: Science Press, 1997.
- [6] Zhang X S, Zhang J L, Liao L Z, et al. An adaptive trust region method and its convergence[J]. Science in China (Series A), 2002, 45: 620-631.
- [7] Schnabel R B, Eskow E. A new modified Cholesky factorization[J]. SIAM Journal on Scientific Computing 1990(11): 1136-1158.
- [8] More J J, Garbow B S, Hillstrom K E. Testing unconstrained optimization software[J]. ACM Trans Math Software 1981(7(1)): 17-41.
- [9] Steihaug T. The conjugate gradient method and trust region in large scale optimization[J]. SIAM J Numer Anal 1983(20): 626-637.

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