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A HYBRID METHOD FOR SOLVING THE NONLINEAR LEAST SQUARES PROBLEM WITH LINEAR INEQUALITY CONSTRAINTS

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Abstract This paper presents a new method with trust region technique for solving the nonlinear least squares problem with linear inequality constraints. The method proposed in this paper stems from the one presented in a recent paper by the authors. The method successively constructs trust region constraints, which are ellipsoids centered at the iterative points, in such a way that they lie in the relative interior of the feasible region. Thus the method belongs to the class of interior point methods, and hence we may expect that the generated sequence approaches a solution smoothly without the combinatorial complications inherent to traditional active set methods. We establish a convergence theorem for the proposed method and show its practical efficiency by numerical experiments.

1. Introduction

In [16], we have proposed an algorithm for solving nonlinear least squares problems with simple bounds. The purpose of this paper is to generalize the results of [16] to problems with linear constraints. Although the constrained linear least squares problem has extensively been studied [1, 2, 3, 6, 8, 12, 17], less attention has been paid on the constrained nonlinear least squares problem. Holt and Fletcher [9] consider the nonlinear least squares problem with simple bounds and monotonicity constraints on the variables. Wright and Holt [20] extend the results of [9] to general linearly constrained problems by utilizing the structure of the sum of squares objective function. For the problem with nonlinear equality constraints, Knoth [11] gives a generalized Gauss-Newton method with stepsize strategy based on an exact penalty function. Mahdavi-Amiri and Bartels [13] consider an exact penalty method to solve the problem with nonlinear constraints and use quasi-Newton updates that take into account the structure of nonlinear least squares Hessians. Schittkowski [18] considers SQP methods to solve nonlinearly constrained least squares problems.

In this paper, we consider the following nonlinear least squares problem with linear inequality constraints:

$$\begin{aligned} \text{minimize} \quad & \frac{1}{2}\sum_{i=1}^{\ell} F_i(x)^2 \\ \text{subject to} \quad & A^T x \leq b, \quad x \geq 0, \end{aligned} \tag{1.1}$$

where $x \in R^n$, $b \in R^m$, $A \in R^{n\times m}$ and $F_i : R^n \to R$, $i = 1, \cdots, \ell$, are continuously differentiable. We define the functions $F : R^n \to R^\ell$ and $f : R^n \to R$ by $F(x) = (F_1(x), \cdots, F_\ell(x))^T$ and $f(x) = \frac{1}{2} \| F(x) \|^2$, respectively, where $\| \cdot \|$ denotes the Euclidean norm.

Using slack variables $y \in R^m$, we may rewrite problem (1.1) as

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & A^T x + y = b, \\ & x \geq 0, \quad y \geq 0. \end{array} \tag{1.2}$$

The method proposed in this paper stems from the one presented in [16]. Specifically, the method constructs trust region constraints, which are ellipsoids centered at the iterative points, in such a way that they lie in the relative interior $\{(x, y) \mid A^T x + y = 0, x > 0, y > 0\}$ of the feasible region of (1.2). Thus the method belongs to the class of interior point methods. However, since solutions of the problem are usually on the boundary of the feasible region, the trust region ellipsoids may become extremely thin, which causes numerical instability. To avoid this difficulty, we incorporate an active set strategy into the method. With such a modification, we may still expect that the method retains the advantage of the interior point method, as observed in [16] for the case of problems with simple bound constraints on the variables.

The paper is organized as follows. Section 2 presents motivation and description of the algorithm. In Section 3, we establish a global convergence theorem. Finally, in Section 4, we report some computational results with the proposed algorithm compared with the successive quadratic programming method.

2. Algorithm

First, we describe a basic idea of the algorithm. Suppose that (x, y) is a relative interior point of the feasible region of (1.2), i.e., $A^T x + y = b$, $x > 0, y > 0$. Let p and q denote the vectors which determine the next points (x^+, y^+) from the current point (x, y), that is $x^+ = x + p$ and $y^+ = y + q$. We consider the following Gauss-Newton type subproblem with an additional trust region constraint:

$$\begin{array}{ll} \text{minimize}_{p,q} & \dfrac{1}{2} \parallel F(x) + \nabla F(x)^T p \parallel^2 \\ \text{subject to} & A^T p + q = 0, \\ & \parallel D(x)p \parallel^2 + \|D(y)q\|^2 \leq \Delta^2, \end{array}$$

where $D(x) = diag(1/x_i)$, $D(y) = diag(1/y_i)$ and Δ is a constant such that $0 < \Delta < 1$.

This problem can be rewritten as

$$\begin{array}{ll} \text{minimize}_{p,q} & g(x)^T p + \dfrac{1}{2} p^T H(x) p \\ \text{subject to} & A^T p + q = 0, \\ & \|D(x)p\|^2 + \|D(y)q\|^2 \leq \Delta^2, \end{array} \tag{2.1}$$

where $H(x) = \nabla F(x) \nabla F(x)^T$ and $g(x) = \nabla F(x) F(x)$. Note that if (p, q) satisfies $A^T p + q = 0$, then $(x^+, y^+) = (x, y) + (p, q)$ also satisfies $A^T x^+ + y^+ = b$. Also, if (p, q) satisfies $\|D(x)p\|^2 + \|D(y)q\|^2 \leq \Delta^2$, then x^+ and y^+ remain in the relative interior of the feasible region, i.e., $x^+ > 0$ and $y^+ > 0$. In fact, if $x_k^+ \leq 0$ for some k, then it follows that

$$0 < x_k = x_k^+ - p_k \leq -p_k.$$

This implies that

$$\begin{aligned} \|D(x)p\|^2 + \|D(y)q\|^2 &= \sum_{i=1}^{n} \left(\frac{p_i}{x_i}\right)^2 + \sum_{j=1}^{m} \left(\frac{q_j}{y_j}\right)^2 \\ &\geq \left(\frac{p_k}{x_k}\right)^2 \geq 1, \end{aligned}$$

contradicting $\|D(x)p\|^2 + \|D(y)q\|^2 \leq \Delta^2 < 1$. Hence, $x^+ > 0$ must hold. In a similar manner, we can show $y^+ > 0$. To guarantee convergence of the method, we control the size Δ of the trust region according to the ratio of the actual and predicted reductions caused by the step (p, q) chosen to determine the next iterate.

The trust region constraint $\|D(x)p\|^2 + \|D(y)q\|^2 \leq \Delta^2$ in (2.1) represents an ellipsoid, which is centered at the current point (x, y) and strictly contained in the nonnegative orthant $\{(x, y) \mid x \geq 0, y \geq 0\}$. However, when the current point is close to the boundary of the nonnegative orthant, the trust region ellipsoid becomes thin and solution of (2.1) suffers from numerical instability. To overcome this difficulty, we modify (2.1) using the idea of active set strategy [5] in constrained optimization.

For the current point (x, y), we define the sets of indices

$$I = \{i \mid x_i \geq \epsilon_1\}, \quad J = \{j \mid y_j \geq \epsilon_1\}, \tag{2.2}$$

where ϵ_1 is a sufficiently small positive constant. We also denote $\overline{I} = \{1, 2, \cdots, n\} - I$ and $\overline{J} = \{1, 2, \cdots, m\} - J$. According to the above definition, we partition vectors and matrices as

$$x = \begin{bmatrix} x_I \\ x_{\overline{I}} \end{bmatrix}, \quad y = \begin{bmatrix} y_J \\ y_{\overline{J}} \end{bmatrix}, \quad p = \begin{bmatrix} p_I \\ p_{\overline{I}} \end{bmatrix}, \quad q = \begin{bmatrix} q_J \\ q_{\overline{J}} \end{bmatrix},$$

$$g(x) = \begin{bmatrix} g_I(x) \\ g_{\overline{I}}(x) \end{bmatrix}, \quad H(x) = \begin{bmatrix} H_{II}(x) & H_{I\overline{I}}(x) \\ H_{\overline{I}I}(x) & H_{\overline{I}\overline{I}}(x) \end{bmatrix}, \quad A = \begin{bmatrix} A_{IJ} & A_{I\overline{J}} \\ A_{\overline{I}J} & A_{\overline{I}\overline{J}} \end{bmatrix}.$$

By adding the extra constraints $p_{\overline{I}} = 0$ and $q_{\overline{J}} = 0$ to (2.1), we get the following problem:

$$\text{minimize}_{p_I, q_J} \quad g_I(x)^T p_I + \frac{1}{2} p_I^T H_{II}(x) p_I \tag{2.3-a}$$

$$\text{subject to} \quad A_{I\overline{J}}^T p_I = 0, \tag{2.3-b}$$

$$A_{IJ}^T p_I + q_J = 0, \tag{2.3-c}$$

$$\|D_I(x)p_I\|^2 + \|D_J(y)q_J\|^2 \leq \Delta^2, \tag{2.3-d}$$

where $D_I(x)$ and $D_J(y)$ are the diagonal submatrices of $D(x)$ and $D(y)$ with elements $1/x_i$, $i \in I$, and $1/y_j$, $j \in J$, respectively. Note that by the definition (2.2) of I and J, the following inequalities are always satisfied:

$$p_I^T D_I(x)^2 p_I \leq \frac{1}{\epsilon_1^2} \| p_I \|^2, \quad q_J^T D_J(y)^2 q_J \leq \frac{1}{\epsilon_1^2} \| q_J \|^2 .$$

Thus any (p_I, q_J) satisfying

$$\| p_I \|^2 + \| q_J \|^2 \leq \epsilon_1^2 \Delta^2$$

also satisfies the inequality (2.3-d). This fact implies that the ellipsoid determined by (2.3-d) contains the sphere with radius $\epsilon_1 \Delta$. So the ellipsoid never becomes thin as long as the

value of Δ does not approach zero. (The latter property will be shown to hold in the proof of Theorem 3.1.)

Now, as $q_J = -A_{IJ}^T p_I$ by (2.3-c), from (2.3-d) we have

$$p_I^T D_I(x)^2 p_I + q_J^T D_J(y)^2 q_J = p_I^T \left(D_I(x)^2 + A_{IJ} D_J(y)^2 A_{IJ}^T \right) p_I \leq \Delta^2.$$

Thus, we can rewrite (2.3) as

$$\begin{aligned} &\text{minimize}_{p_I} \quad g_I(x)^T p_I + \frac{1}{2} p_I^T H_{II}(x) p_I \\ &\text{subject to} \quad A_{I\bar{J}}^T p_I = 0, \quad p_I^T E(x) p_I \leq \Delta^2, \end{aligned} \tag{2.4}$$

where $E(x)$ is defined by

$$\begin{aligned} E(x) &= D_I(x)^2 + A_{IJ} D_J(y)^2 A_{IJ}^T \\ &= D_I(x)^2 + A_{IJ} D_J(b - A^T x)^2 A_{IJ}^T, \end{aligned} \tag{2.5}$$

where the last equation follows from the fact that (x, y) is feasible to (1.2). In the remainder of the paper, we suppose that the following two conditions are always satisfied:

$$\text{rank } A_{I\bar{J}} = |\bar{J}|, \tag{2.6}$$

$$Z^T H_{II}(x) Z \text{ is positive definite}, \tag{2.7}$$

where Z is a $| I | \times (|I| - |\bar{J}|)$ matrix whose columns span the null space of $A_{I\bar{J}}^T$. Note that (2.6) is satisfied when (1.2) enjoys the primal nondegeneracy condition, provided that ϵ_1 is chosen sufficiently small.

Let a solution p_I^* of (2.4) be obtained. Suppose that $\|p_I^*\| \geq \epsilon_2$ is satisfied, where ϵ_2 is a predetermined positive number significantly smaller than ϵ_1. If the value $f(x + p^*)$ is sufficiently smaller than $f(x)$, then we accept p^* to determine the next point. Otherwise, we halve Δ and solve subproblem (2.4) again. More precisely, let $0 < \mu < \eta < 1$, $\gamma > 1$ and $0 < \Delta_{max} < 1$ be given constants. Compute the ratio

$$\rho \equiv \frac{f(x + p^*) - f(x)}{\psi(x, p^*)}, \tag{2.8}$$

where $\psi(x, p) = g(x)^T p + \frac{1}{2} p^T H(x) p$. If $\rho < \mu$, then put $x^+ := x$ and $\Delta^+ := \frac{1}{2}\Delta$; if $\mu \leq \rho < \eta$, then put $x^+ := x + p^*$ and $\Delta^+ := \Delta$; if $\rho \geq \eta$, then put $x^+ := x + p^*$ and $\Delta^+ := \min(\gamma\Delta, \Delta_{max})$. When x is updated, i.e., $x^+ = x + p^*$, we compute $y^+ := y + q^* \geq 0$, where $q_J^* = -A_{IJ}{}^T p_I^*$ and $q_{\bar{J}}^* = 0$. With the next iterative point (x^+, y^+), we update the index sets I and J by (2.2). As a result, we have problem (2.4) corresponding to the new index sets I and J. In this manner, we repeatedly solve subproblems (2.4) while updating the index sets I and J as long as $\|p_I^*\| \geq \epsilon_2$ holds.

On the other hand, if $\|p_I^*\| < \epsilon_2$ is satisfied, then we may regard the current point x as an approximate optimal solution of the problem

$$\begin{aligned} &\text{minimize} \quad f(x) \\ &\text{subject to} \quad A^T x + y = b, \\ &\qquad\qquad x_{\bar{I}} = 0, y_{\bar{J}} = 0. \end{aligned} \tag{2.9}$$

This can be verified as follows. When p_I^* is small, so is $q_J^* = -A_{IJ}^T p_I^*$ by (2.3-c). Since the ellipsoid determined by (2.3-d) contains the sphere with radius $\epsilon_1\Delta$ as noted earlier, we may

think that the constraint (2.3-d) is inactive at the solution (p_I^*, q_J^*) of problem (2.3), when Δ is not too small. (Recall that ϵ_2 was chosen significantly smaller than ϵ_1.) Therefore, (p_I^*, q_J^*) satisfies the following optimality condition for problem (2.3) with constraint (2.3-d) being ignored:

$$g_I(x) + H_{II}(x)p_I + A_{I\bar{J}}\lambda_{\bar{J}} + A_{IJ}\lambda_J = 0, \quad (2.10\text{-a})$$
$$\lambda_J = 0, \quad (2.10\text{-b})$$
$$A_{I\bar{J}}^T p_I = 0, \quad (2.10\text{-c})$$
$$A_{IJ}^T p_I + q_J = 0, \quad (2.10\text{-d})$$

where λ is the Lagrange multiplier vector and $(\lambda_J, \lambda_{\bar{J}})$ is the partition of λ corresponding to the index set J defined by (2.2). If (p_I^*, q_J^*) satisfying (2.10) is sufficiently small, then the point x may be considered to approximately satisfy

$$g_I(x) + A_{I\bar{J}}\lambda_{\bar{J}} = 0, \quad (2.11)$$

which is actually the optimality condition for problem (2.9).

So in the case where $\| p_I^* \| < \epsilon_2$ is satisfied, we have to further examine optimality of the point x for the original problem (1.2). Namely, we compute Lagrange multipliers $\lambda_{\bar{J}}$ by solving the equation

$$A_{I\bar{J}}^T A_{I\bar{J}}\lambda_{\bar{J}} = -A_{I\bar{J}}^T g_I(x) \quad (2.12)$$

and check if $\lambda_{\bar{J}}$ satisfies the inequalities

$$g_{\bar{I}}(x) + A_{\bar{I}\bar{J}}\lambda_{\bar{J}} \geq -\epsilon_3 e, \quad (2.13)$$
$$\lambda_{\bar{J}} \geq -\epsilon_3 e, \quad (2.14)$$

where ϵ_3 is a sufficiently small positive constant and e is a vector of appropriate dimension whose components are all unity. Note that, by assumption (2.6), equation (2.12) has the unique solution $\lambda_{\bar{J}}$. If (2.13) and (2.14) hold, then we terminate the iteration, since the definition of I and J implies that (x, y) satisfies approximate optimality conditions for problem (1.1), which depend on ϵ_1, ϵ_2 and ϵ_3.

To see this, note that the Kuhn-Tucker conditions for problem (1.2) are given by

$$g(x) + A\lambda \geq 0, \quad x \geq 0, \quad x^T(g(x) + A\lambda) = 0,$$
$$\lambda \geq 0, \quad y \geq 0, \quad \lambda^T y = 0,$$

which imply

$$g_{I_0}(x) + A_{I_0\bar{J}_0}\lambda_{\bar{J}_0} = 0, \quad x_{I_0} \geq 0, \quad (2.15\text{-a})$$
$$g_{\bar{I}_0}(x) + A_{\bar{I}_0\bar{J}_0}\lambda_{\bar{J}_0} \geq 0, \quad x_{\bar{I}_0} = 0, \quad (2.15\text{-b})$$
$$\lambda_{J_0} = 0, \quad y_{J_0} \geq 0, \quad (2.15\text{-c})$$
$$\lambda_{\bar{J}_0} \geq 0, \quad y_{\bar{J}_0} = 0, \quad (2.15\text{-d})$$

for some partitions $(I_0, \bar{I}_0)$ and $(J_0, \bar{J}_0)$ of $\{1, 2, \cdots, n\}$ and $\{1, 2, \cdots, m\}$, respectively. In view of the definition (2.2) of I and J, we see that (2.13) and (2.14) are relaxations of conditions (2.15-b) and (2.15-d), respectively. Moreover, (2.15-a) and (2.15-c) correspond to (2.10-a) and (2.10-b), which approximately represent condition (2.11) when (p_I^*, q_J^*) is

sufficiently small. In the following, conditions (2.13) and (2.14) will simply be referred to as ϵ-*optimality conditions* for problem (1.1), with $\epsilon = (\epsilon_1, \epsilon_2, \epsilon_3)$.

When any of the conditions (2.13) and (2.14) is violated, we try to improve the current solution by solving subproblem (2.4), in which the index set I or J is modified. Specifically, if (2.13) is violated, we let the currently active variable x_{i^*} be inactive, where index i^* is determined by

$$i^* := \arg\max \left\{ \left| (g_{\overline{I}}(x) + A_{\overline{I}\overline{J}}\lambda_{\overline{J}})_i \right| \;\middle|\; (g_{\overline{I}}(x) + A_{\overline{I}\overline{J}}\lambda_{\overline{J}})_i < -\epsilon_3,\ i \in \overline{I} \right\},$$

namely, we let

$$\overline{I} := \overline{I} - \{i^*\}, \quad I := I \cup \{i^*\}.$$

Similarly, if (2.14) is violated, we let the currently active variable y_{j^*} be inactive, where index j^* is determined by

$$j^* := \arg\max \left\{ |\lambda_j| \;\middle|\; \lambda_j < -\epsilon_3,\ j \in \overline{J} \right\},$$

namely, we let

$$\overline{J} := \overline{J} - \{j^*\}, \quad J := J \cup \{j^*\}.$$

By means of this manipulation, we may expect to improve the current solution by solving subproblem (2.4) with the revised active sets. In fact, let the condition (2.13) be violated and the index set I be augmented by i^*. To be precise, we denote $\hat{I} = I \cup \{i^*\}$. Then, since $\|p_I^*\|$ is small, the current solution x approximately satisfies (2.11), i.e.,

$$g_I(x) + A_{I\overline{J}}\lambda_{\overline{J}} = 0 \tag{2.16}$$

and i^* is such that

$$g_{i^*}(x) + A_{i^*\overline{J}}\lambda_{\overline{J}} < 0. \tag{2.17}$$

Now suppose that, on the next iteration, the solution x fails to be improved by solving (2.4) with the revised active set $\hat{I}$. Then we must have $\|p_{\hat{I}}^*\| \simeq 0$ again for the current solution x, so that x approximately satisfies

$$g_{\hat{I}}(x) + A_{\hat{I}\overline{J}}\hat{\lambda}_{\overline{J}} = 0$$

for some $\hat{\lambda}_{\overline{J}}$, i.e., we have approximately

$$g_I(x) + A_{I\overline{J}}\hat{\lambda}_{\overline{J}} = 0, \tag{2.18}$$

$$g_{i^*}(x) + A_{i^*\overline{J}}\hat{\lambda}_{\overline{J}} = 0. \tag{2.19}$$

However, since $A_{I\overline{J}}$ has full column rank, (2.16) and (2.18) imply that the vector $\hat{\lambda}_{\overline{J}}$ is approximately equal to $\lambda_{\overline{J}}$, which contradicts (2.17) and (2.19). So when (2.13) is violated, an improvement will be obtained on the next iteration. The case where the condition (2.14) is violated can be argued similarly.

We are now ready to state an algorithm for finding an ϵ-optimal solution of (1.1). An outline of the algorithm is shown in Figure 1.

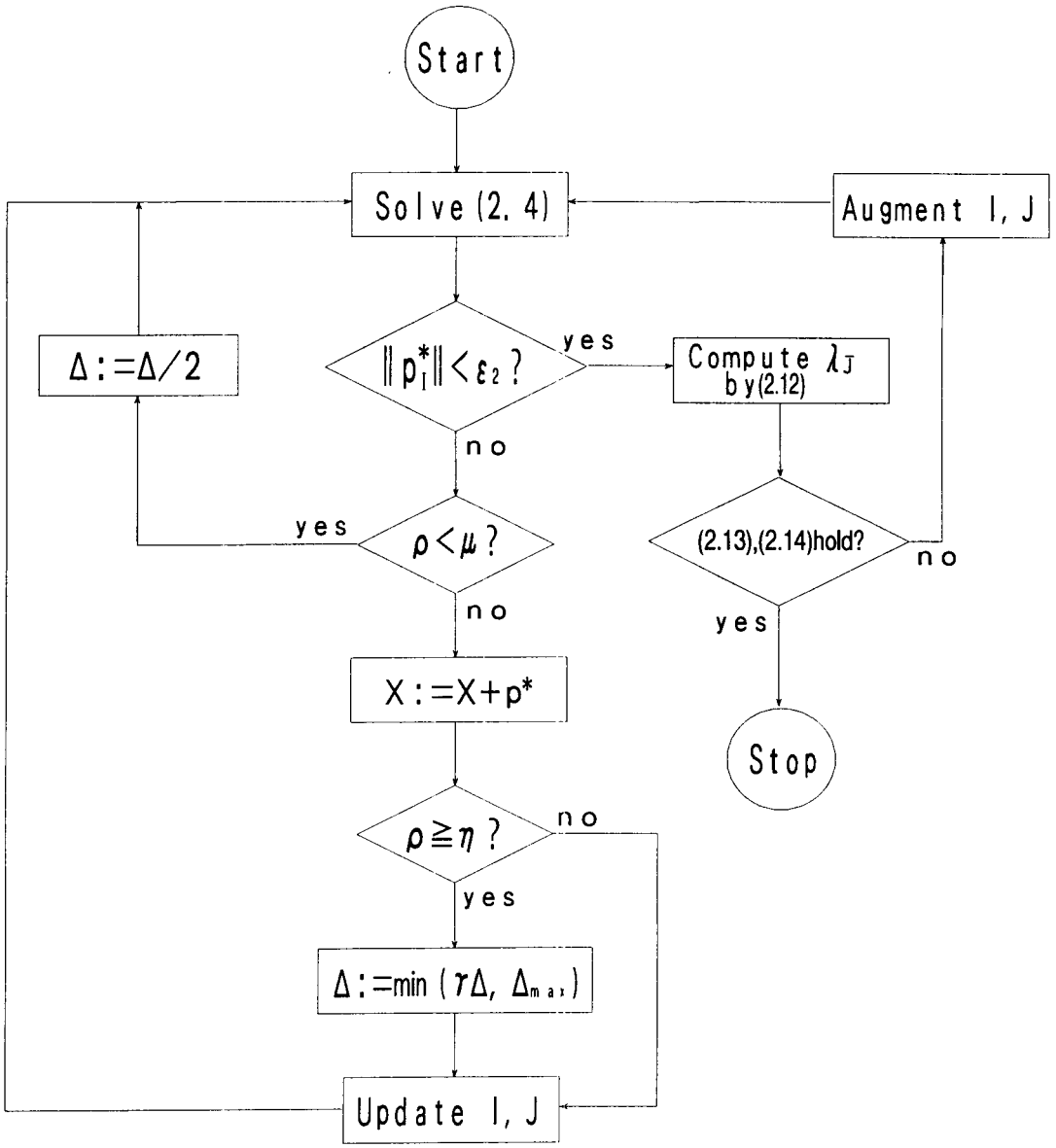

Figure 1: Flowchart of the algorithm

Algorithm

Initialize: Choose sufficiently small positive constants ϵ_i, $i = 1, 2, 3$, and parameters $\mu, \gamma, \Delta_{max}$ and η such that $0 < \mu < \eta < 1, \gamma > 1$ and $0 < \Delta_{max} < 1$. Choose an initial point (x, y) such that $A^T x + y = b, x > 0, y > 0$, and an initial trust region radius $\Delta \in (0, 1)$. Let I and J be the index sets defined by (2.2).
Comment. The complements of I and J will always be denoted by $\overline{I}$ and $\overline{J}$, respectively.

while (x, y) is not ϵ-optimal **do**

begin

while $\|p_I^*\| \geq \epsilon_2$ **do**

begin
Solve subproblem (2.4) with $\overline{I}$ and $\overline{J}$ to find p_I^*;
$p_{\overline{I}}^* := 0$;
compute ρ using (2.8)
if $\rho \geq \mu$ **then**
begin
$x := x + p^*$
if $\rho \geq \eta$ **then**
$\Delta := \min(\gamma\Delta, \Delta_{max})$
endif
end
$I := I - \{i \in I | x_i < \epsilon_1\}$;
$J := J - \{j \in J | y_j < \epsilon_1\}$
else
$\Delta := \frac{1}{2}\Delta$
endif
end

endwhile

if (2.13) is violated **then**

begin
$i^* := \arg\max \left\{ | (g_{\overline{I}}(x) + A_{\overline{I}\overline{J}}\lambda_{\overline{J}})_i | \;\middle|\; (g_{\overline{I}}(x) + A_{\overline{I}\overline{J}}\lambda_{\overline{J}})_i < -\epsilon_3,\ i \in \overline{I} \right\}$;
$I := I \cup \{i^*\}$
end

elseif (2.14) is violated **then**

begin
$j^* := \arg\max \left\{ |\lambda_j| \;\middle|\; \lambda_j < -\epsilon_3,\ j \in \overline{J} \right\}$;
$J := J \cup \{j^*\}$
end

endif

end

endwhile

3. Convergence

In this section, we prove that the proposed algorithm finitely obtains an ϵ-optimal solution of problem (1.1) under appropriate conditions. In particular, we shall assume throughout this section that the level set $\{x \mid f(x) \leq f(x^0)\}$ of function f is bounded, where x^0 is an initial point of the algorithm.

Proposition 3.1 *Let x be an arbitrary point in the level set $\{x \mid f(x) \leq f(x^0)\}$. Suppose that assumptions (2.6) and (2.7) are satisfied. Let p_I^* be a solution of (2.4) and let $p^* = (p_I^*, 0)$. If $\|p_I^*\| \geq \epsilon_2$, then there are some constants $\kappa > 0$ and $\beta > 0$, independent of x and p^*, such that the following inequality is satisfied:*

$$-\psi(x, p^*) \geq \frac{1}{2}\kappa \min\{\Delta, \kappa/\beta\}, \tag{3.1}$$

where $\psi(x,p) = g(x)^T p + \frac{1}{2}p^T H(x)p$ is the objective function of (2.1).

Proof. Recall that any p_I satisfying $A_{I\bar{J}}^T p_I = 0$ can be expressed as $p_I = Z\hat{p}_I$ for some $\hat{p}_I \in R^{|I|-|\bar{J}|}$, where Z is a $|I| \times (|I| - |\bar{J}|)$ matrix whose columns span the null space of $A_{I\bar{J}}^T$. Thus, problem (2.4) may be rewritten as

$$\begin{array}{ll} \text{minimize}_{\hat{p}_I \in R^{|I|-|\bar{J}|}} & g_I(x)^T Z\hat{p}_I + \dfrac{1}{2}(Z\hat{p}_I)^T H_{II}(x) Z\hat{p}_I, \\ \text{subject to} & \hat{p}_I^T Z^T E(x) Z\hat{p}_I \leq \Delta^2. \end{array}$$

Furthermore, there exists a nonsingular matrix $C(x) \in R^{(|I|-|\bar{J}|)\times(|I|-|\bar{J}|)}$, which depends on x, such that

$$Z^T E(x) Z = C(x)^T C(x). \tag{3.2}$$

Therefore, (2.4) may be rewritten as

$$\text{minimize}_{\hat{p}_I \in R^{|I|-|\bar{J}|}} \quad \hat{g}_I(x)^T \hat{p}_I + \frac{1}{2}\hat{p}_I^T \hat{H}_{II}(x)\hat{p}_I \tag{3.3}$$

$$\text{subject to} \quad \|C(x)\hat{p}_I\| \leq \Delta, \tag{3.4}$$

where $\hat{g}_I(x) = Z^T g_I(x) \in R^{|I|-|\bar{J}|}$ and $\hat{H}_{II}(x) = Z^T H_{II}(x) Z \in R^{(|I|-|\bar{J}|)\times(|I|-|\bar{J}|)}$.

We define $\hat{\psi} : R^{|I|-|\bar{J}|} \to R$ by

$$\hat{\psi}(\hat{p}_I) = \hat{g}_I(x)^T \hat{p}_I + \frac{1}{2}\hat{p}_I^T \hat{H}_{II}(x)\hat{p}_I,$$

and then, using this function, we define the function $\phi : R \to R$ by

$$\phi(\tau) = \hat{\psi}\left(-\tau C(x)^{-1}\frac{u(x)}{\|u(x)\|}\right),$$

where $u(x) = (C(x)^{-1})^T \hat{g}_I(x)$ and $\tau \in R$. Then

$$\begin{aligned} \phi(\tau) &= -\frac{\tau}{\|u(x)\|}\hat{g}_I(x)^T C(x)^{-1}u(x) + \frac{\tau^2}{2}\frac{1}{\|u(x)\|^2}\left(C(x)^{-1}u(x)\right)^T \hat{H}_{II}(x)C(x)^{-1}u(x) \\ &= -\tau\|u(x)\| + \frac{\tau^2}{2}\xi \\ &= \frac{\xi}{2}\left(\tau - \frac{\|u(x)\|}{\xi}\right)^2 - \frac{\|u(x)\|^2}{2\xi}, \end{aligned} \tag{3.5}$$

where $\xi = \frac{1}{\|u(x)\|^2}(C(x)^{-1}u(x))^T\hat{H}_{II}(x)C(x)^{-1}u(x)$. By assumption (2.7), we have $\xi > 0$.

Now let τ^* be the minimizer of ϕ on the interval $[0, \Delta]$ and let $\hat{p}_I^*$ denote a solution of (3.3). Then, since $\tau^* C(x)^{-1}\frac{u(x)}{\|u(x)\|}$ is feasible for (3.3), we have

$$\phi(\tau^*) = \hat{\psi}\left(-\tau^* C(x)^{-1}\frac{u(x)}{\|u(x)\|}\right) \geq \hat{\psi}(\hat{p}_I^*). \tag{3.5}$$

If $\tau^* < \Delta$, then (3.4) implies that $\tau^* = \|u(x)\|/\xi$ and

$$\phi(\tau^*) = -\frac{\|u(x)\|^2}{2\xi}. \tag{3.6}$$

On the other hand, if $\tau^* = \Delta$, then we have

$$\phi(\tau^*) = -\Delta\|u(x)\| + \frac{1}{2}\Delta^2\xi \leq -\Delta\|u(x)\| + \frac{\Delta}{2}\|u(x)\| = -\frac{\Delta}{2}\|u(x)\|, \tag{3.7}$$

since $\tau^* = \Delta$ implies $\Delta \leq \|u(x)\|/\xi$, that is, $\|u(x)\| \geq \xi\Delta$.

Consequently it follows from (3.5), (3.6) and (3.7) that

$$\begin{aligned} -\hat{\psi}(\hat{p}_I^*) &\geq \frac{1}{2}\|u(x)\| \min\left\{\Delta, \frac{\|u(x)\|}{\xi}\right\} \\ &= \frac{1}{2}\|u(x)\| \min\left\{\Delta, \frac{\|u(x)\|^3}{(C(x)^{-1}u(x))^T\hat{H}_{II}(x)C(x)^{-1}u(x)}\right\} \\ &= \frac{1}{2}\|u(x)\| \min\left\{\Delta, \frac{\|u(x)\|^3}{u(x)^T(C(x)^{-1})^T Z^T H_{II}(x) Z C(x)^{-1}u(x)}\right\}. \end{aligned} \tag{3.8}$$

From (2.5) and the definition of $D_I(x)$ and $D_J(y)$, the minimum eigenvalue of $E(x)$ is bounded away from zero for all $x \in \{x \mid f(x) \leq f(x^0)\}$, which is bounded by assumption. Thus $Z^T E(x) Z$ is uniformly positive definite, and hence by the definition of $C(x)$ in (3.2), $\|C(x)^{-1}\|$ is uniformly bounded. Moreover, Z and $H_{II}(x)$ are uniformly bounded under the given assumptions. Consequently, we have

$$u(x)^T(C(x)^{-1})^T Z^T H_{II}(x) Z C(x)^{-1}u(x) \leq \beta\|u(x)\|^2, \tag{3.9}$$

where β is some positive constant independent of x, I and J.

Next, in order to show that $u(x) = (C(x)^{-1})^T\hat{g}_I(x)$ is bounded away from zero, we first observe that

$$\begin{aligned} \|E(x)\| &\leq \max(1/x_i^2) + \max(1/y_j^2)\|A\|\|A^T\| \\ &\leq \frac{1}{\epsilon_1^2}(1 + \|A\|\|A^T\|), \end{aligned}$$

since $x_i \geq \epsilon_1$ for $i \in I$ and $y_j \geq \epsilon_1$ for $j \in J$. Thus, from (3.2), $C(x)$ is uniformly bounded. It then follows from the definition of $u(x)$ that

$$\|\hat{g}_I(x)\| \leq \|C(x)^T\|\|u(x)\| \leq \gamma\|u(x)\|, \tag{3.10}$$

where γ is a positive constant independent of x, I and J.

Under the hypothesis of the proposition, we have

$$\|\hat{p}_I^*\| \geq \epsilon_2', \tag{3.11}$$

for some constant ϵ_2'. This implies that $\hat{g}_I(x)$ must satisfy the inequality

$$\|\hat{g}_I(x)\| \geq \delta, \tag{3.12}$$

where δ is a positive constant independent of x, I and J. Because, if there is a sequence $\{x^i\}$ such that $\hat{g}_I(x^i) \to 0$, then the corresponding solutions $\hat{p}_I^{*i}$ of (3.3) have to satisfy

$$\hat{p}_I^{*i} \to 0,$$

which contradicts (3.11). Consequently it follows from (3.10) and (3.12) that

$$\|u(x)\| \geq \kappa, \tag{3.13}$$

where $\kappa = \delta/\gamma$.

Finally, using (3.9) and (3.13) to evaluate the right hand side of (3.8), we obtain the desired inequality (3.1). □

Now we establish the finite termination property of the algorithm.

Theorem 3.1 *Suppose that assumptions (2.6) and (2.7) are satisfied. For any given* $\epsilon = (\epsilon_1, \epsilon_2, \epsilon_3) > 0$, *the algorithm obtains an* ϵ*-optimal solution of (1.1) in a finite number of iterations.*

Proof. Note that the algorithm terminates only if $\|p_I^*\| < \epsilon_2$ holds and, at the same time, conditions (2.13) and (2.14) are simultaneously satisfied. Taking a closer look at the algorithm, we may therefore deduce that the algorithm fails to terminate only if one of the following two cases occurs (see Fig.1): (a) Point x is updated as $x := x + p^*$ infinitely often; and (b) Point x stays at the same place after some iteration.

First consider case (a), which implies that conditions $\|p_I^*\| \geq \epsilon_2$ and $\rho \geq \mu$ simultaneously hold infinitely often. By the definitions of $D(x)$ and $E(x)$ given in the previous section, there is a constant $\nu > 0$ independent of x and I such that

$$p_I^T E(x) p_I \geq \nu \|p_I\|^2 \qquad \text{for all } p_I \in R^{|I|}. \tag{3.14}$$

On the other hand, for the solution p_I^* of subproblem (2.4) we have

$$p_I^{*T} E(x) p_I^* \leq \Delta^2. \tag{3.15}$$

From (3.14) and (3.15), we get the inequality

$$\Delta \geq \sqrt{\nu}\, \|p_I^*\|. \tag{3.16}$$

On the other hand, if p_I^* satisfies the condition $\rho \geq \mu$, then it follows from (2.8) and (3.1) that

$$f(x + p^*) \leq f(x) - \frac{1}{2} \mu\kappa \min\{\Delta, \kappa/\beta\}. \tag{3.17}$$

Therefore, by (3.16) and (3.17), we have

$$f(x + p^*) \leq f(x) - \frac{1}{2} \mu\kappa \min\{\sqrt{\nu}\epsilon_2, \kappa/\beta\}, \tag{3.18}$$

whenever $\|p_I^*\| \geq \epsilon_2$. This inequality implies that the objective function f decreases at least by a fixed amount whenever $\|p_I^*\| \geq \epsilon_2$ and $\rho \geq \mu$. However, since f takes nonnegative values by the definition of f, it is obvious that (3.18) can hold only finitely often. Thus, case (a) does not occur.

Next, suppose that the algorithm fails to terminate because case (b) occurs. Since x remains at the same point, no elements are removed from the index sets I and J. Moreover, in this case, it is impossible that $\|p_I^*\| < \epsilon_2$ and , at the same time, either (2.13) or (2.14) is violated in an infinite number of iterations, because the number of elements in I or J increases one by one every time (2.13) or (2.14) is violated. Therefore, we only need to consider the case where conditions $\|p_I^*\| \geq \epsilon_2$ and $\rho < \mu$ simultaneously hold in an infinite number of *consecutive* iterations. Since Δ tends to zero, (3.1) implies that we eventually have

$$-\psi(x, p^*) \geq \frac{1}{2}\kappa\Delta. \tag{3.19}$$

On the other hand, since $f \in C^2$ and since x and $p^* = (p_I^*, 0)$ are bounded by the standing assumptions, there exists a constant $K > 0$, independent of x and p^*, such that

$$f(x + p^*) - f(x) - \psi(x, p^*) \leq \frac{1}{2} K \|p^*\|^2. \tag{3.20}$$

Moreover, since $\|C(x)\hat{p}_I^*\| \leq \Delta$ by the constraint of (3.3) and $\|C(x)^{-1}\|$ is uniformly bounded to the above as pointed out in the proof of Proposition 3.1, we have $\|\hat{p}_I^*\| \leq \sigma'\Delta$ for some constant $\sigma' > 0$. Thus $\|p^*\| \leq \sigma\Delta$ for some $\sigma > 0$, since $p^* = (p_I^*, 0)$ and $p_I^* = Z\hat{p}_I^*$. Hence, from (3.20), we have

$$f(x + p^*) - f(x) - \psi(x, p^*) \leq \frac{1}{2} K\sigma^2\Delta^2. \tag{3.21}$$

Consequently, if Δ tends to zero, then it follows from (3.19), (3.21) and the definition (2.8) of the ratio ρ that

$$|\rho - 1| = \left| \frac{f(x + p^*) - f(x) - \psi(x, p^*)}{\psi(x, p^*)} \right| \leq \frac{K\sigma^2\Delta}{\kappa}$$

which implies $\rho \to 1$, i.e., $\rho \geq \mu$ is eventually satisfied. This is a contradiction, and hence case (b) does not occur. This completes the proof. □

4. Numerical results

We executed the numerical experiments with the algorithm proposed in Section 2. In this algorithm, the most time consuming task is to solve subproblem (2.4) at each iteration. For solving (2.4), we transform it into the reduced subproblem (3.3) in which matrix Z is obtained from QR decomposition of A_{IJ}^T and solve subproblem (3.3) using a modification of the trust region technique [14, 15]. For the updating of Z at each iteration, we use the technique described in 12.6.2 and 12.6.3 of [7]. The program of the algorithm was coded in Fortran77. The computation was carried out using double precision arithmetic on a FACOM-M382 Computer at the Data Processing Center of Kyoto University.

To test the efficiency of the proposed method, it is compared with the successive quadratic programming (SQP) method. For the latter method, we used the program package given in Chapter 7 of [10]. This program uses direction-finding subproblems derived by modifying the second-order approximations to both objective and constraint functions of the program to avoid the Maratos effect [4].

Table 1: Comparison of the proposed method and SQP method.

		Proposed method			SQP method		
Problem	(n, m)	obj. fn	iters.	CPU	obj. fn	iters.	CPU
1	(30, 5)	1782.6	16	277	1783.3	60	1287
2	(30, 5)	791.8	19	323	791.9	62	1367
3	(30, 10)	1787.2	23	403	1787.2	68	1612
4	(30, 10)	829.6	27	454	831.1	53	1348
5	(50, 10)	3405.2	24	1906	3405.7	84	7965
6	(50, 10)	1769.9	24	1825	1775.9	73	7264
7	(50, 20)	3823.1	34	2683	3823.6	90	10451
8	(50, 20)	1945.0	32	2495	1946.1	74	8806
9	(80, 20)	5465.7	32	10350	5468.4	113	51060
10	(80, 20)	3419.1	28	9116	3421.5	109	50233
11	(80, 30)	5576.0	39	12877	5578.4	109	57521
12	(80, 30)	3495.1	43	14805	3495.7	122	63136

obj. fn = objective function value at the obtained solution
iters. = number of iterations
CPU = CPU time in msec

In order to examine performance of the proposed algorithm, we have solved the following family of test problems, of which size can be varied by choosing various values of the parameters n and m, where n is an even integer such that $n \geq 4$ and $n \geq m$:

$$\begin{aligned} &\text{minimize} \quad \frac{1}{2}\sum_{i=1}^{\ell} F_i^2(x) \\ &\text{subject to} \quad A^T x \leq b, \quad x \geq 0, \end{aligned} \tag{4.1}$$

where $\ell = 3(n-2)$, $x \in R^n$, $b \in R^m$, $A \in R^{n \times m}$ and the functions $F_j : R^n \to R$ are defined by

$$\begin{aligned} F_{6j-5}(x) &= 10\,(x_{2j} - x_{2j-1}^2), \\ F_{6j-4}(x) &= 1 - x_{2j-1}, \\ F_{6j-3}(x) &= 3\sqrt{10}\,(x_{2j+2} - x_{2j+1}^2), \\ F_{6j-2}(x) &= 1 - x_{2j+1}, \\ F_{6j-1}(x) &= \sqrt{10}\,(x_{2j} + x_{2j+2} - 2), \\ F_{6j}(x) &= \sqrt{10}\,(x_{2j} - x_{2j+2}), \end{aligned}$$

where $j = 1, 2, \cdots, \frac{1}{6}\ell$ (cf. [19]). The elements of matrix A except the last column and vector x^0 were chosen from the intervals $[-10, 10]$ and $[1, 5]$, respectively. All elements in the last column of A were set to be -1. The constant vector b in the constraints was then chosen as $b = A^T x^0 + \frac{n}{2}e$, where $e = (1, 1, \cdots, 1)^T$, thereby x^0 became an interior point of the feasible region and could be used as a starting point for the algorithm.

We have solved the above test problems for various values of n and m. In the proposed method, we set the parameter values as follows: $\epsilon_1 = 0.001, \epsilon_2 = \epsilon_3 = 0.0001$, $\mu = 0.3$,

$\gamma = 1.2$, $\eta = 0.7$ and $\Delta_{max} = 0.99$. In the SQP method, default values given in [10] were used for all parameters. Table 1 summarizes the results for the proposed method and SQP method. We may observe that the proposed method outperformed the SQP method in all runs both in terms of objective values obtained and CPU time. (Note that both methods always generate a sequence of feasible solutions for the test problem (4.1).) It should be pointed out, however, that the computational experiments assumed that the initial interior point was readily available, which would not be the case in practice. Nevertheless, the obtained results are encouraging enough to claim that the proposed method is a promising approach to linearly constrained nonlinear least squares problems.

5. Concluding Remark

In this paper we have proposed a hybrid method for solving the nonlinear least squares problem with linear inequality constraints. Because the method is of Gauss-Newton type, it only uses the first order information of the functions involved. We remark that a similar hybrid algorithm of Newton type may also be designed to solve problems with general nonlinear objective functions, if one is willing to use its second derivatives.

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