10 COMBINING TRUST REGION AND AFFINE SCALING FOR LINEARLY CONSTRAINED NONCONVEX MINIMIZATION

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Abstract: An interior point method is proposed for a general nonlinear (nonconvex) minimization with linear inequality constraints. This method is a combination of the trust region idea for nonlinearity and affine scaling technique for constraints. Using this method, the original objective function is monotonically decreased.

In the proposed approach, a Newton step is derived directly from the complementarity conditions. A trust region subproblem is formed which yields an approximate Newton step as its solution asymptotically. The objective function of the trust region subproblem is the quadratic approximation to the original objective function plus an augmented quadratic convex term. Similar to an augmented Lagrangian function, this augmentation adds positive curvature in the range space of the constraint normals.

The global convergence is achieved by possibly using trust regions with different shapes. A reflection technique, which accelerates convergence, is described. Explicit sufficient decrease conditions are proposed.

Computational results of a two-dimensional trust region implementation are reported for large-scale problems. Preliminary experiments suggest that this method can be effective; a relatively small number of function evaluations are required for some medium and large test problems.

Keywords: trust region, Dikin-affine scaling, an interior point method, Newton, reflection

1 INTRODUCTION

Interior point methods have proven to be an efficient approach for solving large scale linear and convex programming problems: see [24] for a comprehensive bibliography. An appealing property of these methods is that a small number of iterations is typically required to obtain an accurate solution for a large problem. This property, if achievable, is even more attractive for a *nonlinear* programming problem since function evaluation can be a dominant and costly computation.

Interior point methods share a common characteristic: they avoid approaching the boundary prematurely. The majority of interior point methods can be interpreted as following the central path to optimality, e.g., [21; 31]. The exception is the classical affine scaling algorithm [15; 33]. An affine scaling method uses a diagonal scaling technique to compute a damped step which ultimately leads to convergence to a solution. Despite the absence of a polynomial convergence property, an affine scaling method is the only type of interior point method which monotonically decreases the original objective function; it stands out for its simplicity and typically good computational performance, e.g., [1; 5; 33].

There has been great interest in generalizing interior point methods to nonlinear (nonconvex) programming problems, e.g., [16; 36; 9; 12; 14; 35; 25; 19; 4]. However, this has proven to be a difficult and challenging task.

For a nonconvex problem, a minimization method is typically able to compute a local minimizer at best. This does not prevent its usefulness since an initial point is often provided in applications and the local minimizer in the neighborhood of this initial point can be sufficient. The majority of interior point methods are based on the view that it is worthwhile to sacrifice decrease of the original objective function in order to gain centrality, e.g., [21; 31]. This view may not be reasonable for nonconvex problems; achieving centrality can cause loss of information provided by the initial point and possibly cause convergence to a local minimizer with a higher objective function value than that of the initial point. FIG. 1.1 illustrates this effect: x_1 is the minimizer of the

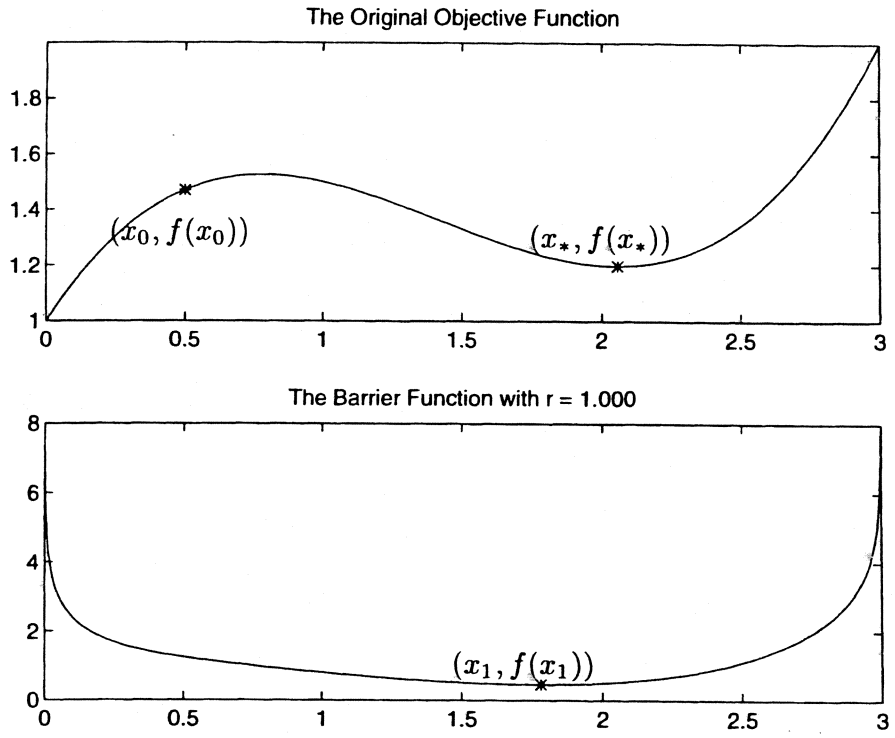

Figure 1.1 Loss of the Information from the Starting Point: $\min_{0 \le x \le 3} f(x)$

barrier function for the original bound constrained problem with the barrier parameter $r = 1$. Using a barrier function method with the initial x_0 and $r = 1$, the iterates will converge to the local minimizer x_*. Using an algorithm which monotonically decreases the objective function with the same initial x_0, the iterates will converge to the local minimizer $x = 0$.

Monotonicity offers a natural connection to the original problem. Monotonicity and the simplicity of an affine scaling method makes it particularly appealing and suitable for constrained nonconvex minimization. Based on this philosophy, Newton type affine scaling algorithms have been considered for various structured linear and nonlinear programming problems [8; 7; 26; 9; 27; 25; 2; 14]. These methods represent a generalization of the affine scaling methods to piecewise linear and nonlinear minimization. Such algorithms have fast local convergence and typically solve a large problem in a small number of iterations. For minimization with simple bounds, Newton steps are derived from the first order necessary conditions directly and globalization is successfully achieved us-

ing a trust region approach [9]. For l_p problems and minimization of the sums of Euclidean distances, the resulting algorithms become a natural enhancement of the classical IRLS and Weiszfeld algorithms [26; 25].

We consider the problem of minimizing a general nonlinear (nonconvex) function subject to linear inequality constraints,

$$\begin{aligned} & min_{x \in \Re^n} f(x) \\ & \text{subject to} \quad Ax \geq b, \end{aligned} \tag{1.1}$$

where $A^T = [a_1, \cdots, a_m] \in \Re^{n \times m}$. Let $\mathcal{F} \stackrel{\text{def}}{=} \{x : Ax \geq b\}$. The strictly feasible region $int(\mathcal{F}) \stackrel{\text{def}}{=} \{x : Ax > b\}$ is assumed to be non-empty and a strictly feasible initial point $x_0 \in int(\mathcal{F})$ is given. Moreover, $f(x)$ is twice continuously differentiable in $\mathcal{F}$.

In this article, a trust region and affine scaling interior point method (TRAM) is proposed for a general nonlinear minimization problem (1.1) with linear inequality constraints. Specifically, TRAM exhibits the following characteristics:

- the iterates $\{x_k\}$ are in the interior of the feasible region and the dual multiplier approximations are only feasible in the limit;
- the Newton steps are derived from the complementarity conditions;
- the original objective function $f(x)$ is decreased monotonically;
- the trust region subproblems yield approximate Newton steps asymptotically; these trust region subproblems can be solved using existing trust region techniques;
- a reflection technique is used to accelerate convergence.

The presentation of the paper is organized as follows. In §2, an affine scaling Newton process is firstly derived from the complementarity conditions of the problem (1.1). Section §3 includes globalization of this Newton process within a trust region context. A trust region subproblem which yields approximate Newton steps asymptotically is motivated in §3. The shapes of the trust regions necessary for convergence are analyzed in §3. The proposed TRAM algorithm is outlined §3.1. A two-dimensional trust region generalization is included in §3.2. Explicit decrease conditions for convergence to a local minimizer are described in §3.3. A useful reflection technique is described in §3.2. Preliminary computational results are presented in §4. Concluding remarks and possible future research are included in §5.

In a separate paper [11], convergence properties of the proposed method are presented.

2 AN AFFINE SCALING NEWTON APPROACH

The first order optimality conditions of a constrained minimization problem consist of the complementarity conditions, primal feasibility, and dual feasibility. The following is a classical characterization of a local minimizer of the linearly constrained problem (1.1), e.g., see Fletcher [18].

First Order Necessary Conditions

If x_* is a local minimizer of (1.1), then there exist Lagrangian multipliers λ_* such that x_*, λ_* satisfy:

$$\nabla f_* - A^T\lambda_* = 0, \tag{2.1}$$

$$Ax_* - b \geq 0, \tag{2.2}$$

$$\lambda_* \geq 0, \tag{2.3}$$

$$(\lambda_*)_i(a_i^T x_* - b_i) = 0, \qquad 1 \leq i \leq m. \tag{2.4}$$

Second Order Sufficiency Conditions

If at x_* there exist λ_* which satisfy (2.1)-(2.4), $d^T\nabla^2 f_* d > 0$ for all $d \neq 0$, $a_i^T d \geq 0$ for all $a_i^T x_* - b_i = 0$, and $a_i^T d = 0$ for all $(\lambda_*)_i > 0$, then x_* is a strict local minimizer of (1.1).

Condition (2.2) is referred to as primal feasibility, (2.3) is dual feasibility. Conditions (2.1) and (2.4) are called the complementarity conditions and can be equivalently expressed as an $(m+n)$-by-$(m+n)$ nonlinear system of equations

$$\text{diag}(Ax - b)\lambda = 0 \qquad \text{and} \qquad A^T\lambda - \nabla f = 0. \tag{2.5}$$

If there is no index i such that $(\lambda_*)_i = a_i^T x_* - b_i = 0$, then *strict complementarity* is said to hold.

Complementarity has played a central role in the successful primal-dual interior point methods for linear and convex programming problems. The primal dual interior point method [23], proposed by Kojima, Mizuno and Yoshise in 1987, maintains both the primal-dual strict feasibility and can be considered as a damped Newton process on the perturbed complementarity conditions. For (1.1), this perturbed complementarity conditions correspond to

$$\text{diag}(Ax - b)\lambda = \rho e \qquad \text{and} \qquad A^T\lambda - \nabla f(x) = 0.$$

The parameter $\rho > 0$ is decreased to zero as a solution is approached.

Fiacco and McCormick [17] first considered this perturbed KKT condition for an inequality constrained nonlinear programming problem. If $f(x)$ is convex, the solution to this nonlinear system, as the parameter $\rho > 0$ varies,

defines a central path in the strictly feasible region. For a convex programming problem, primal and dual feasibility together with complementarity sufficiently characterize a solution.

Extension of a primal and dual method to a general nonconvex problem has proven to be difficult and challenging [16; 14; 19; 4]. The first order necessary conditions is no longer sufficient in characterizing a local minimizer for a *nonconvex* minimization problem. For example, a 2-norm penalty function has been used to measure satisfaction of the first order necessary conditions for a nonconvex problem in [16]. This method does not necessarily converge to a local minimizer of the original minimization problem since the second order necessary conditions may fail to hold.

We believe that monotonic decrease of the original objective function, if achievable, is an important property of a minimization algorithm for nonconvex problems. This property enables a direct connection to the original minimization problem. It can make use of information such as an available starting point. We demonstrate that a Newton process based on the complementarity conditions (2.5) can be used in combination with the trust region idea to achieve convergence by monotonically decreasing the original objective function.

Let $F(x, \lambda) = 0$ denote the complementarity conditions (2.5), i.e.,

$$F(x, \lambda) \stackrel{\text{def}}{=} \begin{bmatrix} \text{diag}(Ax - b)\lambda \\ \nabla f(x) - A^T\lambda \end{bmatrix}.$$

The Newton step for $F(x, \lambda) = 0$ at (x_k, λ_k) is

$$\begin{bmatrix} \text{diag}(\lambda_k)A & \text{diag}(Ax_k - b) \\ \nabla^2 f_k & -A^T \end{bmatrix} \begin{bmatrix} d_k^N \\ d_k^\lambda \end{bmatrix} = - \begin{bmatrix} \text{diag}(Ax_k - b)\lambda_k \\ \nabla f_k - A^T\lambda_k \end{bmatrix}. \tag{2.6}$$

If x_k is strictly feasible, then $\text{diag}(Ax_k - b)$ is positive definite. An alternative way of computing the Newton step (2.6) is to solve a n-by-n symmetric linear system,

$$(A^T(\text{diag}(\lambda_k)\text{diag}(Ax_k - b)^{-1})A + \nabla^2 f_k)d_k^N = -\nabla f_k, \tag{2.7}$$

with the dual multipliers $\lambda_{k+1}^N = \lambda_k^N + d_k^\lambda$ updated as

$$\lambda_{k+1}^N = -\text{diag}(\lambda_k)\text{diag}(Ax_k - b)^{-1}Ad_k^N.$$

The Newton system (2.6) has appealing properties in a neighborhood of a local minimizer x_* satisfying the second order sufficiency conditions. This is described in Theorem 2.1. Its proof is straightforward and can be found in [11]. Let $(v; w)$ denote the column vector in $\Re^{n+m}$ formed from the vectors $v \in \Re^n$ and $w \in \Re^m$.

Theorem 2.1 *Assume that $f(x) : \mathcal{F} \to \Re$ is twice continuously differentiable and the second order sufficiency conditions of (1.1) are satisfied at $(x_*; \lambda_*)$. Assume further that strict complementarity holds at x_* and $\{a_i : (\lambda_*)_i > 0\}$ are linearly independent. Then*

(a) The Jacobian matrix $\nabla F(x_*, \lambda_*)$ is nonsingular;

(b) The symmetric matrix $(A^T(diag(\lambda)diag(Ax-b)^{-1})A+\nabla^2 f(x))$ is positive definite when $x \in int(\mathcal{F})$ and $(x; \lambda)$ is sufficiently close to $(x_*; \lambda_*)$.

3 A TRUST REGION GLOBALIZATION

An immediate consequence of Theorem 2.1 is that, if $x_k \in int(\mathcal{F})$ is in a sufficiently small neighborhood of a solution, the Newton step d_k^N of (2.5) is descent for the objective function $f(x)$. This suggests that, using this Newton process, local convergence can be achieved from the interior of the feasible region with a monotonic decrease of the objective function.

Maintaining strict feasibility can be done with a simple backtracking technique. This technique can be used to avoid approaching a boundary prematurely, which is important for the success of an interior point method.

Assume that $x_k + d_k$ brings a sufficient decrease of the objective function but possibly violates strict feasibility. Then a damped step $\alpha_k d_k$ can be taken where

$$\alpha_k \stackrel{\text{def}}{=} \theta_k \alpha_k^*, \quad 0 < \theta_0 \leq \theta_k < 1, \quad \alpha_k^* \stackrel{\text{def}}{=} \min(1, \beta_k) \tag{3.1}$$

and

$$\beta_k \stackrel{\text{def}}{=} \min\{-\frac{a_i^T x_k - b_i}{a_i^T d_k}, \quad -\frac{a_i^T x_k - b_i}{a_i^T d_k} > 0\}.$$

The parameter θ_k determines the damped step $\alpha_k d_k$. Its choice is important for the convergence properties of an affine scaling method for linear programming [28; 32].

It is also possible to maintain strict dual feasibility, $\lambda > 0$. However, since global convergence is achieved by monotonic decrease of $f(x)$, and maintaining dual feasibility can lead to a smaller stepsize, we allow violation of dual feasibility. Hence only primal strict feasibility, $Ax > b$, is maintained in the proposed method; however, the dual multipliers play an important role in determining the next step, particularly asymptotically.

The local Newton process needs to be globalized. Next we show that a Newton step can be globalized using a trust region approach. The main trust region subproblem is motivated in §3. A trust region subproblem, which is useful occasionally for quickly departing from a nearly binding constraint, is described

in §3. The model algorithm is summarized in §3.1. A two dimensional trust region subproblem is considered in §3.2. A reflection line search is proposed in §3.2 to accelerate convergence.

A Trust Region Subproblem

Assume that x_k is strictly feasible. Let $\psi_k(d)$ denote the quadratic approximation for $f(x)$ at x_k, i.e.,

$$\psi_k(d) \stackrel{\text{def}}{=} \nabla f_k^T d + \frac{1}{2} d^T \nabla^2 f_k d. \tag{3.2}$$

Further, assume that the quadratic approximation $\psi_k(d)$ is a "good" approximation to $f(x_k + d) - f(x_k)$ within the trust region $\|d\|_2 \leq \Delta_k$. The goal is to produce a step s_k, $x_k + s_k \in int(\mathcal{F})$, such that the quadratic approximation $\psi_k(d)$ (and hence $f(x)$) achieves a good decrease. The Newton step (2.6) locally produces a good decrease for $f(x)$ but it may not be descent globally. Furthermore, a damped step of the trust region solution $\min_{\|d\|_2 \leq \Delta_k} \psi_k(d)$ may fail to produce a sufficient decrease due to feasibility restriction. We want to formulate a trust region subproblem with the following properties:

- it is closely connected to the Newton step d_k^N for fast local convergence;
- it produces a strictly feasible step which yields a sufficient decrease.

Let C_k and D_k denote diagonal matrices:

$$C_k \stackrel{\text{def}}{=} \text{diag}(|\lambda_k|), \qquad D_k \stackrel{\text{def}}{=} \text{diag}(Ax_k - b).$$

Replacing $\text{diag}(\lambda_k)$ by C_k in (2.6), the *modified* Newton step d_k,

$$\begin{bmatrix} C_k A & D_k \\ \nabla^2 f_k & -A^T \end{bmatrix} \begin{bmatrix} d_k \\ \lambda_{k+1} \end{bmatrix} = - \begin{bmatrix} 0 \\ \nabla f_k \end{bmatrix}, \tag{3.3}$$

approximates the Newton step sufficiently accurately, hence retains fast convergence. Moreover, this modified Newton step d_k is a minimizer of the augmented quadratic $\psi_k(d) + \frac{1}{2} d^T A^T D_k^{-1} C_k A d$, which can be considered a quadratic convex regularization of the constrained problem (1.1) at x_k. The quadratic approximation $\psi_k(d)$ is sufficiently decreased if its convex regularization $\psi_k(d) + \frac{1}{2} d^T A^T D_k^{-1} C_k A d$ is sufficiently decreased. Using the augmented quadratic as the objective function, a trust region subproblem consistent with the approximate Newton step d_k is

$$\begin{aligned} &\min_{d \in \Re^n} \psi_k(d) + \frac{1}{2} d^T A^T D_k^{-1} C_k A d \\ \text{subject to} \quad &\|(d; D_k^{-\frac{1}{2}} A d)\|_2 \leq \Delta_k. \end{aligned} \tag{3.4}$$

The affine scaling $D_k^{-\frac{1}{2}}$ controls the shape of the trust region so that a posterior damping for strict feasibility can retain a large portion of the trust region solution. Letting $\hat{d} \stackrel{\text{def}}{=} D_k^{-\frac{1}{2}} Ad$, the trust region subproblem (3.4) is equivalent to

$$\begin{aligned} \min_{d\in\Re^n,\hat{d}\in\Re^m} \quad & \psi_k(d) + \frac{1}{2}\hat{d}^T C_k \hat{d} \\ \text{subject to} \quad & Ad - D_k^{\frac{1}{2}}\hat{d} = 0 \\ & \|(d;\hat{d})\|_2 \le \Delta_k. \end{aligned} \tag{3.5}$$

Since (3.4) and (3.5) are equivalent, we subsequently use these two formulations interchangeably depending on the context. Since problem (3.5) is a 2-norm trust region subproblem with consistent equality constraints, existing techniques for computing a solution can be applied to (3.5).

The augmented term $\frac{1}{2}d^T A^T D_k^{-1} C_k Ad$ in the objective function of the subproblem (3.4) serves a similar purpose to the augmented Lagrangian function for a constrained minimization problem [20]: it adds positive curvature in the space spanned by the constraint normals. In addition, the curvature augmentation is such that the minimizer of this augmented quadratic $\psi_k(d) + \frac{1}{2}d^T A^T D_k^{-1} C_k Ad$ lies in the null space of the binding constraint normals asymptotically. Together with the affine scaling $D_k^{-\frac{1}{2}}$ in the trust region bound, the augmentation implies that a damped step of the solution p_k of the subproblem yields a sufficient decrease, if p_k yields a sufficient decrease.

Consider the Newton step $(p_k^N; \hat{p}_k^N)$ of the trust region subproblem (3.5), i.e.,

$$\hat{H}_k(p_k^N; \hat{p}_k^N) = -\begin{bmatrix} \nabla f_k \\ 0 \end{bmatrix} + \begin{bmatrix} A^T \\ -D_k^{\frac{1}{2}} \end{bmatrix} \lambda_{k+1}^p, \tag{3.6}$$

where $\hat{H}_k \stackrel{\text{def}}{=} \hat{H}(x_k \lambda_k)$ and

$$\hat{H}(x,\lambda) \stackrel{\text{def}}{=} \begin{bmatrix} \nabla^2 f(x) & 0 \\ 0 & C \end{bmatrix}, \quad C = \text{diag}(|\lambda|).$$

The matrix $\hat{H}_k$ is the Hessian of the augmented quadratic in (3.5).

A Newton step p_k^N, with respect to (2.5), is the approximate Newton step d_k (3.3) since

$$\begin{bmatrix} C_k A & D_k \\ \nabla^2 f_k & -A^T \end{bmatrix} \begin{bmatrix} p_k^N \\ \lambda_{k+1}^p \end{bmatrix} = -\begin{bmatrix} 0 \\ \nabla f_k \end{bmatrix}. \tag{3.7}$$

Theorem 3.1 and 3.2 indicate that the trust region subproblem is consistent with the original nonlinear minimization (1.1) with respect to the second order optimality. Proofs for these theorems can be found in [11].

Theorem 3.1 *Assume that* $[A, D_*]$ *has full row rank at* $x_* \in \mathcal{F}$ *and the complementarity conditions are satisfied at* $(x_*; \lambda_*)$. *Let the columns of* Z_* *denote an orthonormal basis for the null space of* $[A, D_*]$. *If* $Z_*^T \hat{H}_* Z_*$ *is positive semidefinite, then* $d^T \nabla^2 f_* d \geq 0$ *for any* d *satisfying* $a_i^T d = 0$ *for all* i *with* $a_i^T x_* - b_i = 0$.

Assume that the pair $(x_*; \lambda_*)$ satisfies the first order necessary conditions with strict complementarity, then the *second* order necessary conditions are satisfied at x_* if $Z_*^T \hat{H}_* Z_*$ is positive semidefinite. Theorem 3.2 indicates that quadratic convergence ensues if a damped Newton step p_k^N is taken locally.

Theorem 3.2 *Assume* $0 < \mu < 1$ *and* $f(x) : \mathcal{F} \to \Re$ *is twice continuously differentiable. Assume that* $\{x_k\}$ *converges to* x_*, *a point satisfying the second order sufficiency conditions with strict complementarity, and* $\{a_i : a_i^T x_* - b_i = 0\}$ *are linearly independent. Then, for sufficiently large* k, $Z_k^T \hat{H}_k Z_k$ *is positive definite and*

$$f(x_k + s_k) - f(x_k) < \mu \psi_k(s_k), \qquad \text{where } s_k = \theta_k \alpha_k^* p_k^N \text{ and } \theta_0 \leq \theta_k < 1,$$

and α_k^* *is defined in (3.1). In addition, if* $x_{k+1} = x_k + s_k$ *for sufficiently large* k *and* $|\theta_k - 1| = O(\|(x_k; \lambda_k) - (x_*; \lambda_*)\|_2)$, *then* $\{(x_k; \lambda_k^p)\}$ *converges quadratically to* $(x_*; \lambda_*)$.

Moving Away from a Nearly Binding Constraint

The trust region subproblem (3.4) addresses complementarity, second order necessary requirement and fast local convergence. The only condition yet to be considered is dual feasibility. The trust region subproblem (3.4) is not effective near a non-optimal point satisfying all the necessary optimality conditions except dual feasibility, since both the solution of the trust region subproblem (3.4) and the Newton step p_k^N are zero at such a point. This situation can occur in a strictly linear problem; however, the nonlinearity of a problem (1.1) can either alleviate or exacerbate this problem. On the one hand, the iterates may approach a boundary more slowly due to nonlinearity of $f(x)$. On the other hand, once close to a boundary, the nonlinearity of $f(x)$ may make it harder to move away.

Starting from a relatively centered initial point, the above situation may be rare or may not occur at all. However, when encountered, it is necessary to move away from some nearly binding hyperplane $a_i^T x - b_i = 0$. This situation can be identified by a measurement for satisfaction of complementarity conditions and dual feasibility.

Let j_0 identify a hyperplane from which departure is desired, e.g.,

$$(\lambda_k)_{j_0} \stackrel{\text{def}}{=} \min\{(\lambda_k)_i \ : \ |a_i^T x - b_i| < \sigma \text{ and } (\lambda_k)_i < 0\}, \tag{3.8}$$

where $\sigma > 0$ is a small constant. Let $\tilde{D}_k$ be the modified affine scaling matrix of D_k:

$$(\tilde{D}_k)_{ii} \stackrel{\text{def}}{=} \begin{cases} (D_k)_{ii} & \text{if } i \neq j_0 \\ 1 & \text{otherwise.} \end{cases} \tag{3.9}$$

When there is no i with $|a_i^T x_k - b_i| < \sigma$ and $(\lambda_k)_i < 0$, it is assumed that $j_0 = 0$ and thus $D_k = \tilde{D}_k$. The trust region $\|(d; \tilde{D}_k^{-\frac{1}{2}} Ad)\|_2 \leq \Delta_k$ is elongated along the normal a_{j_0} of the hyperplane identified, see FIG. 3.1. The following subproblem is more appropriate near a non-optimal complementarity point:

$$\begin{aligned} \min_{d \in \Re^n} \quad & \psi_k(d) + \frac{1}{2} d^T A^T \tilde{D}_k^{-1} C_k A d \\ \text{subject to} \quad & \|(d; \tilde{D}_k^{-\frac{1}{2}} Ad)\|_2 \leq \Delta_k. \end{aligned} \tag{3.10}$$

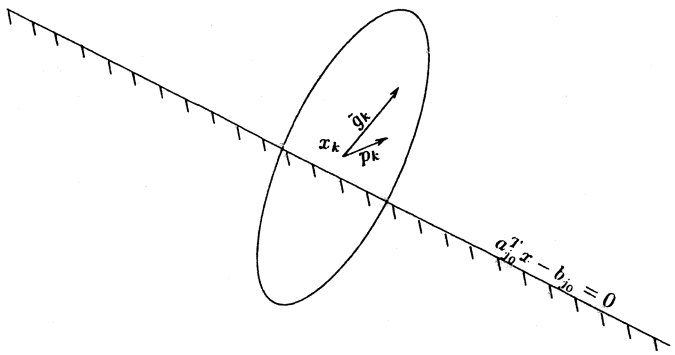

Figure 3.1 Leaving the Hyperplane $a_{j_0}^T x - b_{j_0} = 0$

The Proposed Trust Region Algorithm

Using the trust region subproblems derived in §3 and §3, the general framework of the proposed trust region and affine scaling interior point method is described

in FIG. 3.2. Assume that a strictly feasible initial point $x_0 \in int(\mathcal{F})$ is given. The proposed algorithm generates a sequence $\{x_k\}$ in the interior of the feasible region $\mathcal{F}$ which converge to a solution.

TRAM Let $0 < \mu < \eta < 1$ and $x_0 \in int(\mathcal{F})$.

Step 1 Evaluate f_k, ∇f_k and $B_k \approx \nabla^2 f_k$; compute an approximate Lagrangian multiplier λ_k and let $C_k = \text{diag}(|\lambda_k|)$.

Step 2 Compute a step s_k, $x_k + s_k \in int(\mathcal{F})$, based on the trust region subproblem

$$\begin{aligned} \min_{d \in \Re^n} \quad & \psi_k(d) + \frac{1}{2} d^T A^T S_k^{-1} C_k A d \\ \text{subject to} \quad & \|[d; S_k^{-\frac{1}{2}} d]\|_2 \leq \Delta_k. \end{aligned}$$

Step 3 Compute $\rho_k = [f(x_k + s_k) - f(x_k)]/\psi(s_k)$.

Step 4 If $\rho_k > \mu$ then set $x_{k+1} = x_k + s_k$. Otherwise set $x_{k+1} = x_k$. Update Δ_k as specified.

Updating Trust Region Size Δ_k
Let $0 < \gamma_1 < 1 < \gamma_2$ be given.

1. If $\rho_k \leq \mu$ then set $\Delta_{k+1} \in (0, \gamma_1 \Delta_k]$.
2. If $\rho_k \in (\mu, \eta)$ then set $\Delta_{k+1} \in [\gamma_1 \Delta_k, \Delta_k]$.
3. If $\rho_k \geq \eta$ then set $\Delta_{k+1} \in [\Delta_k, \gamma_2 \Delta_k]$.

Figure 3.2 A Trust Region and Affine Scaling Interior Point Method

Consider the k-th iteration and let $x_k \in int(\mathcal{F})$. Assume further that $\psi_k(d)$ approximates $f(x_k + d) - f(x_k)$ sufficiently accurately; otherwise, the usual trust region size adjustment mechanism can be used to ensure this. The goal of the computation at the k-th iteration is to produce a step s_k such that $x_k + s_k \in int(\mathcal{F})$ and $\psi_k(s_k)$ is sufficiently decreased. This task is accomplished in **Step 2**. A step s_k is computed via solving a trust region subproblem which minimizes a quadratic objective function subject to a trust region bound constraint in the 2-norm measure,

$$\min_{d \in \Re^n} \quad \psi_k(d) + \frac{1}{2} d^T A^T S_k^{-1} C_k A d$$

$$\text{subject to} \qquad \|(d; S_k^{-\frac{1}{2}} d)\|_2 \leq \Delta_k, \tag{3.11}$$

where S_k equals either $D_k^{\frac{1}{2}}$ or $\tilde{D}_k^{\frac{1}{2}}$. The presence of the affine scaling S_k is crucial: it allows for a sufficiently large step. The affine scaling matrix S_k typically equals D_k equals $\text{diag}(Ax_k - b)$. Occasionally S_k equals $\tilde{D}_k$ to facilitate staying away from the boundary. Asymptotically, however, S_k equals D_k and the trust region solution is an approximate Newton step for the complementarity conditions (2.5). Therefore fast local convergence can be achieved.

The affine scaling matrix $S_k \in \{D_k, \tilde{D}_k\}$ can be specified to satisfy the sufficient decrease conditions for optimality, see §3.3. Next we illustrate how a two-dimensional subspace trust region approach can replace the full space trust region subproblem (3.11).

A Two-dimensional Trust Region Algorithm

Computing a solution to the full-space trust region subproblem (3.11) can be too costly for a large scale problem (1.1). Similar to a subspace approach for unconstrained minimization [3], an appropriate small-dimensional trust region subproblem can be used to approximate the full space trust region subproblem, e.g.,

$$\begin{aligned} \min_{d\in\Re^n, \hat{d}\in\Re^m} \quad & \psi_k(d) + \frac{1}{2}\hat{d}^T C_k \hat{d} \\ \text{subject to} \quad & Ad - S_k^{\frac{1}{2}}\hat{d} = 0, \quad (d;\hat{d}) \in \mathcal{S}_k \\ & \|(d;\hat{d})\|_2 \leq \Delta_k. \end{aligned} \tag{3.12}$$

Here $\mathcal{S}_k$ denotes a small-dimensional subspace in $\Re^{n+m}$, e.g., $|\mathcal{S}_k| = 2$. Performance of a subspace algorithm depends on the choice of the subspace $\mathcal{S}_k$. In order to set up $\mathcal{S}_k$ effectively, we analyze a few important approximate solutions to the trust region subproblem.

Let us first consider the typical choice of $S_k = D_k$. If the second order information is absent, i.e., $\nabla^2 f_k = 0$ and $C_k = 0$ in (3.5), the solution of the trust region solution (3.5) is in the projected gradient direction $(g_k; \hat{g}_k)$,

$$\begin{aligned} g_k &\stackrel{\text{def}}{=} -(\nabla f_k - A^T\lambda_k), \\ \hat{g}_k &\stackrel{\text{def}}{=} D_k^{-\frac{1}{2}} A g_k, \end{aligned} \tag{3.13}$$

where λ_k is the least squares solution to

$$\begin{bmatrix} A^T \\ -D_k^l \end{bmatrix} \lambda \stackrel{\text{LS}}{=} \begin{bmatrix} \nabla f_k \\ 0 \end{bmatrix}, \tag{3.14}$$

with $l = \frac{1}{2}$; more generally, $l \geq \frac{1}{2}$ can be used. Moving along the projected gradient direction $(g_k; \hat{g}_k)$ is an attempt to satisfy the complementarity conditions (2.5) via a least squares approach.

Asymptotically, the Newton step p_k^N is a solution to the trust region subproblem. However, globally p_k^N may not always be a good approximate solution, e.g., p_k^N may not exist or it may be a poor approximate solution when the Hessian of the augmented quadratic is indefinite.

In order to yield a good decrease for $\psi_k(d) + \frac{1}{2} d^T A^T D_k^{-1} C_k A d$ when its Hessian is indefinite, a negative curvature direction is important. Since a Newton step p_k^N is a Newton step for the augmented quadratic objective, i.e.,

$$(A^T(C_k D_k^{-1})A + \nabla^2 f_k) p_k^N = -\nabla f_k, \tag{3.15}$$

negative curvature can be detected, then computed in the process of computing the desired approximate Newton step. A negative curvature direction of (3.15) can be computed by either a partial Cholesky factorization [20] or using a conjugate gradient process with an incomplete Cholesky factorization as a preconditioner.

An effective subspace S_k can be formed from the first and second order approximate solutions to the trust region subproblem (3.5). Let d_k^c denote the solution of (3.15) if its coefficient matrix is positive definite and the computed negative curvature direction of (3.15) otherwise. We propose to choose S_k to be spanned by the projected gradient g_k and the second order direction d_k^c. The projected gradient is especially important when a problem is nearly degenerate. The addition of the Newton or the negative curvature directions are important for fast global and local convergence. The two dimensional subspace trust region subproblem is

$$\begin{aligned} \min_{d \in \Re^n, \hat{d} \in \Re^m} \quad & \psi_k(d) + \frac{1}{2} d^T A^T D_k^{-1} C_k A d \\ \text{subject to} \quad & d \in \text{span}\{g_k, d_k^c\} \\ & \|(d; D_k^{-\frac{1}{2}} A d)\|_2 \leq \Delta_k. \end{aligned} \tag{3.16}$$

Since $[g_k, \hat{g}_k]$ and $[d_k^c, \hat{d}_k^c]$ both satisfy $Ad - D_k^{\frac{1}{2}} \hat{d} = 0$, the 2-dimensional trust region subproblem (3.16) can be solved by first computing an orthonormal basis for S_k in $O(n+m)$ flops and then solving a trust region problem in $\Re^2$ with a constant cost. Computation of g_k and d_k^c is the main cost for a 2-dimensional subspace trust region algorithm.

With respect to the choice $S_k = \tilde{D}_k$, a Newton direction or a negative curvature direction can be computed from

$$(A^T(C_k \tilde{D}_k^{-1})A + \nabla^2 f_k)\tilde{d}_k = -\nabla f_k. \tag{3.17}$$

A first order approximate solution for (3.10) is a projected gradient direction $\tilde{g}_k$,

$$\tilde{g}_k \stackrel{\text{def}}{=} -(\nabla f_k - A^T \tilde{\lambda}_k), \tag{3.18}$$

where $\tilde{\lambda}_k$ solves

$$\begin{bmatrix} A^T \\ -\tilde{D}_k^l \end{bmatrix} \lambda \stackrel{\text{LS}}{=} \begin{bmatrix} \nabla f_k \\ 0 \end{bmatrix}, \qquad l \geq \frac{1}{2}. \tag{3.19}$$

The projected direction $\tilde{g}_k$ is descent for $\psi_k(d)$ and leads to departure from the hyperplane $a_{j_0}^T x - b_{j_0} = 0$.

Let $\tilde{d}_k^c$ denote the Newton step (3.17) when it exists and a negative curvature direction of (3.17) otherwise. Using the projected gradient direction $\tilde{g}_k$ and the second-order direction $\tilde{d}_k^c$, the two-dimensional trust region subproblem is

$$\begin{aligned} \min_{d \in \Re^n} \quad & \psi_k(d) + \frac{1}{2} d^T A^T S_k^{-1} C_k A d \\ \text{subject to} \quad & d \in \text{span}\{\tilde{g}_k, \tilde{d}_k^c\} \\ & \|(d; S_k^{-\frac{1}{2}} A d)\|_2 \leq \Delta_k, \qquad S_k = \tilde{D}_k. \end{aligned}$$

Compared to the unsymmetric linear system (3.3), the n-by-n symmetric Newton system (3.15) is preferable since it leads to a negative curvature direction when the Hessian of $\psi_k(d) + \frac{1}{2} d^T A^T D_k^{-1} C_k A d$ is indefinite. The disadvantage of using the symmetric n-by-n linear system (3.15) rather than the unsymmetric $(m+n)$-by-$(m+n)$ linear system (3.3) is the increasing ill-condition of (3.15) as a solution is approached. The stability of the related linear system for linear programming has been studied [37; 34]. Similar issues are yet to be investigated for the linear system (3.15) for a nonlinear programming problem (1.1).

A Reflection Line Search

The effectiveness of an interior point method depends, in part, on the ability to avoid getting close to the boundary prematurely. A trust region algorithm using the subproblem (3.4) is similar to a Dikin affine scaling algorithm in that no explicit effort is made to stay central when computing a descent direction. For a Dikin affine scaling method, it is desirable that an initial point x_0 is approximately centered and damping is used to avoid getting close to a boundary prematurely.

Explicit effort can be made to facilitate staying away from boundary and achieve further decrease. A special line search has been used in [8] for linear l_1 problems. For a nonlinear minimization with bound constraints, a reflection line

search and its effectiveness is illustrated in [9; 10; 2]. We now examine a similar reflection technique for the problem (1.1) with linear inequality constraints.

Assume that x_k is the current strictly feasible point and d_k is an approximate solution to the trust region subproblem (3.11). If $S_k = D_k$ and x_k is close to a hyperplane $a_i^T x = b_i$, then a solution p_k to the trust region subproblem (3.11) will be nearly tangential to the hyperplane. However, the trust region may be outside of the feasible region, see FIG. 3.3. To maintain strict feasibility, it is possible to simply take a damped step by backtracking. Let us consider the reflection direction p_k^R of p_k against the hyperplane $a_i^T x - b_i = 0$, i.e.,

$$p_k^R = p_k - \frac{2a_i^T p_k}{a_i^T a_i} a_i.$$

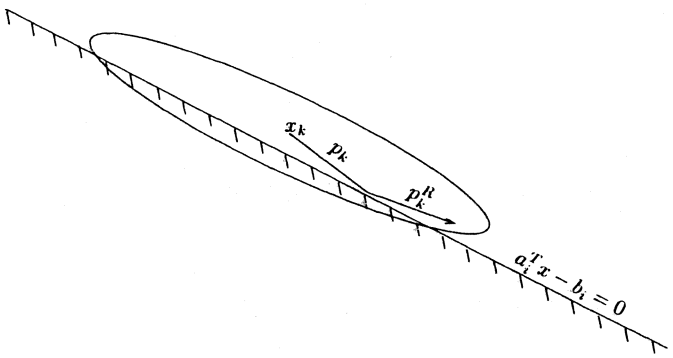

Figure 3.3 Trust Region and Reflection

Use of the reflection direction p_k^R has several benefits:

1. p_k^R points away from the hyperplane $a_i^T x = b_i$;
2. moving along p_k^R is likely to yield continual decrease of the objective $\psi_k(d)$;
3. p_k^R can be computed with little cost.

This reflection process can be repeated for each p_k^R. The effectiveness of the reflection search is demonstrated with computational examples, see Table 4.7 in §4.

Sufficient Decrease Conditions

Consider the current strictly feasible point x_k. A step s_k, with $\|s_k\|_2 \leq \Delta_k$ and $x_k + s_k \in int(\mathcal{F})$, needs to be computed to generate a sufficient decrease of the quadratic approximation $\psi_k(d)$. Typically, the trust region subproblem (3.11) with S_k equal to D_k leads to such a step. However, occasionally, the subproblem with S_k equal to $\tilde{D}_k$, forcing departure from a constraint, is more appropriate. To decide on the scaling S_k, we examine sufficient decrease conditions for optimality.

The sufficient decrease conditions emerge naturally in the two dimensional subspace trust region context. From inspection of (3.13) it follows that, the complementarity conditions are satisfied at x_k if and only if $(g_k; \hat{g}_k) = 0$, where

$$g_k = -(\nabla f_k - A^T \lambda_k),$$
$$\hat{g}_k = -D_k^{\frac{3}{2}} \lambda_k,$$

and λ_k solves

$$\begin{bmatrix} A^T \\ -D_k \end{bmatrix} \lambda \overset{\text{LS}}{=} \begin{bmatrix} \nabla f_k \\ 0 \end{bmatrix}.$$

Let $\theta_k \in [\theta_0, 1)$, $0 < \theta_0 < 1$, be a damping parameter for strict feasibility, as in (3.1). Let $g_k^* \overset{\text{def}}{=} \alpha_k g_k$, $\alpha_k = \theta_k \alpha_k^*$, denote a damped minimizer of the augmented quadratic objective along g_k within the feasible trust region, i.e., α_k^* solves

$$\min_{0 \leq \alpha \leq \Delta_k / \|(g_k; D_k^{-\frac{1}{2}} A g_k)\|_2} \{\psi_k(\alpha g_k) + \frac{\alpha^2}{2} g_k^T A^T D_k^{-1} C_k A g_k,\ x_k + \alpha g_k \in \mathcal{F}\}. \quad (3.20)$$

This suggests that a sufficient decrease of $\psi_k(d)$ measured against $\psi_k(g_k^*)$ leads to satisfaction of complementarity. This is expressed in condition (AS.1) in FIG. 3.4.

The projected gradient $\tilde{g}_k$ attempts to satisfy (3.18),

$$\begin{bmatrix} A^T \\ -\tilde{D}_k \end{bmatrix} \tilde{\lambda} = \begin{bmatrix} \nabla f_k \\ 0 \end{bmatrix}.$$

Assume that strict complementarity is satisfied at x_k. Then dual feasibility is satisfied when $\tilde{g}_k = 0$ and $\tilde{D}_k \tilde{\lambda}_k = 0$. The damped minimizer $\tilde{g}_k^* \overset{\text{def}}{=} \alpha_k \tilde{g}_k$, $\alpha_k = \theta_k \alpha_k^*$, is along the projected gradient $\tilde{g}_k$ where α_k^* solves

$$\min_{0 \leq \alpha \leq \Delta_k / \|(\tilde{g}_k; \tilde{D}_k^{-\frac{1}{2}} A \tilde{g}_k)\|_2} \{\psi_k(\alpha \tilde{g}_k) + \frac{\alpha^2}{2} \tilde{g}_k^T A^T \tilde{D}_k^{-1} C_k A \tilde{g}_k,\ x_k + \alpha \tilde{g}_k \in \mathcal{F}\}. \quad (3.21)$$

This leads to condition (AS.2) in FIG. 3.4 for dual feasibility.

Finally condition (AS.3) is sufficient for second order optimality and fast local convergence when p_k^* is defined as a damped minimizer, e.g.,

$$p_k^* \stackrel{\text{def}}{=} \alpha_k p_k, \quad \alpha_k = \theta_k \alpha_k^*, \quad \alpha_k = \min(1, \beta_k), \tag{3.22}$$

and β_k is the stepsize to the boundary along p_k and $(p_k; \hat{p}_k)$ is a solution to the trust region subproblem (3.5).

Sufficient Decrease Conditions. Let $0 < \beta_{cs}, \beta_{df}, \beta_q < 1$ and $\beta_s > 0$. Let g_k be defined by (3.13), $\tilde{g}_k$ be defined by (3.18) and p_k be a solution to (3.5). Let g_k^*, $\tilde{g}_k^*$ and p_k^* be as defined as in (3.20), (3.21) and (3.22) respectively. Let $\|s_k\|_2 \leq \beta_s \Delta_k$. The sufficient decrease conditions are:
(AS.1) $\psi_k(s_k) < \beta_{cs}(\psi_k(g_k^*) + \frac{1}{2} {g_k^*}^T A^T D_k^{-1} C_k A g_k^*)$;
(AS.2) $\psi_k(s_k) < \beta_{df}(\psi_k(\tilde{g}_k^*) + \frac{1}{2} {\tilde{g}_k^*}^T A^T \tilde{D}_k^{-1} C_k A \tilde{g}_k^*)$;
(AS.3) $(\psi_k(s_k) + \frac{1}{2} s_k^T A^T D_k^{-1} C_k A s_k) < \beta_q(\psi_k(p_k^*) + \frac{1}{2} {p_k^*}^T A^T D_k^{-1} C_k A p_k^*)$.

Figure 3.4 Sufficient Decrease Conditions for the First and Second Order Optimality

Conditions (AS.1), (AS.2) and (AS.3) are closely related to the sufficient decrease conditions proposed for the bound constrained minimization problem [9] and the nonlinear l_1 problem [25]. In [11], these conditions will be rigorously analyzed to establish convergence properties for the linearly constrained minimization (1.1). Essentially, under reasonable assumptions, if (AS.1) is satisfied at each iteration, then any limit point of $\{x_k\}$ will satisfy the complementarity conditions. If, in addition, (AS.2) is satisfied *asymptotically*, then any limit point with strict complementarity also satisfies the first order necessary conditions. Furthermore, if (AS.3) is satisfied *asymptotically*, then the second order necessary condition is satisfied at a limit point with strict complementarity. Finally, with the additional assumption the second order sufficiency conditions at a limit point, convergence is locally quadratic.

Clearly, a step s_k can be determined to satisfy (AS.1), (AS.2) and (AS.3) at every iteration if g_k, $\tilde{g}_k$ and p_k are computed. However since (AS.2) and (AS.3) only need to be satisfied *asymptotically*, less costly alternatives exist. In particular, the reflection search discussed in §3.2 can be combined with a dogleg line search to satisfy these conditions.

4 COMPUTATIONAL EXPERIENCE

To illustrate its potential, preliminary computational experience is reported for our TRAM implementation. A trust region subproblem is solved via a two dimensional approximation as described in §3.2. The projected gradient

g_k is computed using a sparse least squares solver, e.g., [30]. A reflection technique described in §3.2 is incorporated. The details of the implemented two-dimensional subspace algorithm are described in FIG. 4.1.

A large scale nonlinear minimization test problem (1.1) is generated in a similar fashion to the test problems for a nonlinear minimization subject to simple bounds [9; 13]. Nonlinear objective functions $f(x)$ are chosen from two classes: the nonlinear test problem collection for unconstrained minimization [29], and the molecule minimization problem. In the latter, the objective function $f(x)$ has the following formulation [22; 6],

$$f(x) = \sum_{(i,j)\in\mathcal{S}} (\|x_i - x_j\|_2^2 - d_{ij}^2)^2,$$

where x_i denotes the position of the atom and d_{ij} is the known distance between a pair of atoms (i, j).

The inequality constraints $Ax \geq b$ consist of lower bounds, upper bounds and inequality constraints obtained from a random sparse matrix $C^T = [c_1, c_2, \cdots, c_{m_0}] \in \Re^{n\times m_0}$ with the 5-point difference pattern. Solving an unconstrained minimization problem first, the constraints $Ax \geq b$ are formulated in a fashion similar to the bound constraints in the test problems used in [9; 13].

For the results reported subsequently, computation is terminated when

$$\text{either} \quad \theta_k \leq \text{tol} \quad \text{or} \quad \frac{f(x_k) - f(x_{k+1})}{\max(1, |f(x_k)|)} \leq \text{tol},$$

where tol equals 10^{-8}.

Table 4.1 lists the number of function evaluations required for each testing problem using standard nonlinear test functions. The number of iterations required is typically small, e.g., less than 20. In addition, computation of the projected gradient $\tilde{g}_k$ is infrequent for the generated test problems in Table 4.1; $\tilde{g}_k$ is computed 42 times for the 64 tests.

Table 4.2 tabulates the statistics of the computed solutions. The numbers under the column *opt* are the optimality measurement θ_k at termination and the values under *deg* are the strict complementarity measurement $\min(Ax_k - b + |\lambda_k|)$ at termination. It is evident that there are many constraints active (typically far more than the number of iterations required to solve a problem). A substantial portion of the active constraints at the computed solution are not simple bounds. Fairly good accuracy is obtained, even in the presence of near degeneracy. Note that column "deg" measures only one type of degeneracy. Ill conditioning can also come from near singularity of the projected Hessian (which seems to occur for problems GENSING, CHAINGENSING and DEGENSING). In Table 4.2, for problems GENWOOD, CHAINWOOD and

A 2-dimensional TRAM Algorithm. Assume that $x_0 \in \Re^n$ with $Ax_0 > b$ is given. Let $\mu = 0.05$ and $\eta = 0.75$.

Step 1 Evaluate f_k, ∇f_k, $\nabla^2 f_k$; Compute the projected gradient g_k, Lagrangian multiplier λ_k and C_k; Compute a complementarity measure $\theta_k^{\mathrm{c}} = \|D_k \lambda_k\|_\infty$, dual feasibility measure $\theta_k^{\mathrm{d}} = \min_{(\lambda_k)_i<0}(|(\lambda_k)_i|)$ and a first order optimality measure $\theta_k = (\theta_k^{\mathrm{c}} + \theta_k^{\mathrm{d}})/(1 + \theta_k^{\mathrm{c}} + \theta_k^{\mathrm{d}})$;

Step 2 **if** $\theta_k^{\mathrm{c}} < 10^{-2}\min(1, \theta_k^{\mathrm{d}})$, compute $\tilde{g}_k$; **end**;
if $\theta_k^{\mathrm{c}} > 10^{-2}\min(1, \theta_k^{\mathrm{d}})$ **or**
$\psi_k(g_k^*) + \frac{1}{2} g_k^{*T} A^T D_k^{-1} C_k A g_k^* < \psi_k(\tilde{g}_k^*) + \frac{1}{2}\tilde{g}_k^{*T} A^T \tilde{D}_k^{-1} C_k A \tilde{g}_k^*$
$S_k = D_k$;
else
$S_k = \tilde{D}_k$; $g_k^* = \tilde{g}_k^*$; $g_k = \tilde{g}_k$;
end
Compute d_k^c by (3.15) and let p_k solve a 2-dimensional suproblem

$$\begin{aligned} \min_{d \in \Re^n} \quad & \psi_k(d) + \frac{1}{2} d^T A^T S_k^{-1} C_k A d \\ \text{subject to} \quad & d \in \operatorname{span}\{g_k, d_k^c\} \\ & \|[d; S_k^{-\frac{1}{2}} A d]\|_2 \le \Delta_k. \end{aligned}$$

if $(\psi_k(p_k^*) + \frac{1}{2} p_k^{*T} A^T D_k^{-1} C_k A p_k^*) \le 0.99(\psi_k(g_k^*) + \frac{1}{2} g_k^{*T} A^T D_k^{-1} C_k A g_k^*)$
$s_k = p_k^*$;
else
let p_k^R be the damped minimizer of $\psi_k(d)$ along the reflection path of p_k;
$s_k = \operatorname{argmin}\{\psi_k(d) : d = \alpha g_k^* + (1-\alpha) p_k^R,\ 0 \le \alpha \le 1\}$;
end

Step 3 Compute $\rho_k = [f(x_k + s_k) - f(x_k)]/\psi_k(s_k)$;

Step 4 If $\rho_k > \mu$ then set $x_{k+1} = x_k + s_k$. Otherwise set $x_{k+1} = x_k$.
Update Δ_k as specified in FIG. 3.2.

Figure 4.1 A 2-dimensional Trust Region Affine Scaling Method for Minimization Subject to Linear Inequality Constraints

Number of Function Evaluations				
(m, n)	(350, 100)	(875, 250)	(1750, 500)	(3500, 1000)
GENROSE	14	13	20	14
GENSING	21	34	43	43
CHAINSING	17	22	35	26
DEGENSING	23	28	25	31
GENWOOD	13	17	16	20
CHAINWOOD	16	12	15	16
BROYDEN1A	12	13	23	26
BROYDEN1B	12	14	18	28
BROYDEN2A	16	22	27	22
BROYDEN2B	17	21	17	22
TOINTBROY	19	14	43	34
CRAGGLEVY	19	21	28	29
AUGMLAGN	77	78	52	141
BROWN3	12	15	18	17
BVP	53	6	11	5
VAR	16	13	15	17

Table 4.1 Number of Function Evaluations

Statistics at Termination				
problems	#fevals	activities	opt	deg
GENROSE	14	504	10^{-10}	10^{-3}
GENSING	43	646	10^{-4}	10^{-3}
CHAINSING	26	677	10^{-3}	10^{-3}
DEGENSING	31	671	10^{-7}	10^{-5}
GENWOOD	20	798	10^{-5}	10^{-5*}
CHAINWOOD	16	807	10^{-6}	10^{-3*}
BROYDEN1A	26	693	10^{-9}	10^{-4}
BROYDEN1B	28	695	10^{-9}	10^{-4}
BROYDEN2A	22	483	10^{-7}	10^{-4*}
BROYDEN2B	22	511	10^{-8}	10^{-4}
TOINTBROY	34	709	10^{-7}	10^{-4}
CRAGGLEVY	29	377	10^{-8}	10^{-4}
AUGMLAGN	141	442	10^{-8}	10^{-3}
BROWN3	17	686	10^{-8}	10^{-4}
BVP	5	1	10^{-5}	10^{-7}
VAR	17	646	10^{-9}	10^{-4}

Table 4.2 Characteristics of the Computed Solutions $(m, n) = (3500, 1000)$

Number of Function Evaluations				
(250,100)	(500,200)	(750,300)	(1000,400)	(1250,500)
48	54	64	65	65
41	53	42	53	53
36	46	67	97	97
36	42	44	65	65
31	40	69	65	65
32	66	67	73	73
30	50	76	95	95
44	55	55	65	65
33	47	65	52	52
46	39	56	63	63
37.7	49.2	60.5	69.3	82.7

Table 4.3 Number of Function Evaluations for Molecule Problems with Constraints

Number of Function Evaluations				
(350,100)	(700,200)	(1050,300)	(1400,400)	(1750,500)
36	46	72	64	70
49	31	34	56	101
28	31	113	77	67
30	46	52	127	63
35	24	72	94	62
19	28	49	35	69
20	36	55	46	41
27	35	37	87	52
26	28	38	46	65
38	40	55	49	49
30.7	34.5	57.7	68.1	63.9

Table 4.4 Number of Function Evaluations for Molecule Problems with Constraints

#fevals	activities	opt	deg
64	208	10^{-6}	10^{-5}
56	79	10^{-6}	10^{-6}
77	171	10^{-9}	10^{-5}
127	103	10^{-9}	10^{-4}
94	122	10^{-7}	10^{-5}
35	260	10^{-9}	10^{-4}
46	262	10^{-7}	10^{-6}
87	219	10^{-9}	10^{-5}
46	165	10^{-6}	10^{-5}
49	155	10^{-8}	10^{-5}

Table 4.5 Characteristics of the Computed Solutions for Molecule Problems $(m, n) = (1750, 500)$

Number of Function Evaluations				
100	200	300	400	500
55	94	108	152	119
39	72	103	132	138
46	128	75	124	138
53	84	98	114	101
57	84	120	99	167
48	78	112	127	187
71	76	98	138	116
41	95	89	120	124
66	64	100	206	171
66	103	90	125	120

Table 4.6 Number of Function Evaluations for Unconstrained Molecule Problems

BROYDEN2A, the gradients of the active constraints are structurely rank deficient, e.g., GENWOOD and BROYDEN2A are deficient by 1, CHAINWOOD by 2.

Tables 4.3-4.5 illustrate performance of our 2-dimensional TRAM implementation when the objective function is a molecule minimization. Here the objective function is a quartic; this class of problems is difficult to solve due to the presence of negative curvature. Again $\tilde{g}_k$ is computed infrequently: 6 times for the 50 problem instances in Table 4.4. As indicated by Table 4.3 and 4.4, the number of iterations grows with the problem size, although the number of function evaluations are still significantly less than the number of active constraints at the solution, see Table 4.5. The growth of the number of iterations, as the problem dimension is increased, is probably due to the severe nonlinear and nonconvex nature of the molecule minimization problem rather than the technique of handling constraints. This is certainly supported by the computational results in Table 4.6 in which each molecule testing problem is unconstrained. We observe a similar growth in the number of function evaluations as the problem size is increased. This suggests that, for these problems, the approximation of the full space trust region subproblem by a two-dimensional trust region subproblem becomes increasingly less accurate as the problem size is increased.

In Table 4.7 the effectiveness of reflection is illustrated: the first column under each problem size entry list the number of function evaluations with a reflection and the second column without a reflection. The maximum number of reflections allowed is 20 at each iteration and the cost of reflection is insignificant. It is evident that the reflection technique significantly improved the efficiency of the algorithm.

5 CONCLUDING REMARKS

The main objective of this article is to motivate a trust region and affine scaling interior point method (TRAM) for general nonlinear (nonconvex) minimization with linear inequality constraints.

Based on the belief that a monotonic decrease of the original objective function is important for general nonlinear minimization, a Newton step based on the nonlinear system of equations expressing the complementarity conditions is considered. A trust region subproblem is formed consistent with the Newton step. This trust region subproblem yields an approximate Newton step for the complementarity conditions asymptotically. The quadratic objective function of the trust region subproblem is the quadratic Taylor approximation $\psi_k(d)$ to the original objective function $f(x)$ plus a convex quadratic term determined by affine scaling and the Lagrangian multiplier approximation. Affine scaling in

Number of Function Evaluations									
(250,100)		(500,200)		(750,300)		(1000,400)		(1250,500)	
46	51	83	85	65	94	86	108	77	124
33	58	58	58	53	87	80	155	120	196
33	44	69	71	73	177	97	229	81	122
42	70	39	63	42	99	83	101	69	81
44	84	40	66	109	121	86	91	81	139
28	40	77	101	90	117	75	134	130	141
26	32	51	59	78	134	76	148	83	161
37	46	82	127	93	161	77	93	94	130
41	58	48	56	51	71	75	258	71	138
30	52	30	62	54	95	69	92	79	106
36	53.5	57.7	74.8	70.8	115.6	80.4	140.9	88.5	133.8

Table 4.7 With and Without Reflection for Constrained Random Molecule Problem s

both the quadratic objective function and the trust region bound constraint allows the fast convergence of the iterates from the strictly feasible region. Since the effectiveness of an interior point method depends, in parts, on avoiding approaching the boundary of the feasible region prematurely, a reflection line search is proposed to facilitate this.

The proposed algorithm TRAM is related to a Dikin-affine scaling algorithm. However, our typical affine scaling is $D_k^{-\frac{1}{2}}$ rather than D_k^{-1} and there is an augmented term in the objective function contributes additional scaling. In addition, the proposed algorithm is a Newton-type algorithm for a nonlinear minimization and has fast local convergence.

Explicit decrease conditions are proposed for complementarity, dual feasibility and second order optimality. Global and local convergence analysis of the TRAM algorithm is presented in [11].

A two-dimensional subspace trust region framework is analyzed and implemented for large scale problems. Within this subspace framework, the main computation of each iteration can be done using (partial) Cholesky factorization and least squares solve. Preliminary computational results suggest that the proposed method can be effective.

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