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An active set truncated Newton method for large-scale bound constrained optimization[☆]

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ABSTRACT

An active set truncated Newton method for large-scale bound constrained optimization is proposed. The active sets are guessed by an identification technique. The search direction consists of two parts: some of the components are simply defined; the other components are determined by the truncated Newton method. The method based on a nonmonotone line search technique is shown to be globally convergent. Numerical experiments are presented using bound constrained problems in the CUTEr test problem library. The numerical performance reveals that our method is effective and competitive with the famous algorithm TRON.

1. Introduction

Consider the solution of the bound constrained nonlinear programming problem

$$\min f(x), \quad x \in \Omega := \{x \in \mathcal{R}^n : l \le x \le u\}, \tag{1.1}$$

where f is a real-valued, continuously differentiable function in an open set containing Ω. Here $l < u$ and possibly, $l_i = -\infty$ or $u_i = \infty$.

The optimization problem (1.1) has received much attention in recent decades and a number of different methods for its solution have been developed [1–11]. Among the methods, active set methods are widely used in solving the bound constrained optimization problem. Early active set methods [12] are quite efficient for small dimensional problems, but are unattractive for large-scale problems [1,5]. The main reason is that typically at each step of the algorithm, at most one constraint can be added to or dropped from the active set. The potential worst-case may appear, where each of the possible 3^n active sets is visited before discovering the optimal one [13]. Recently, there has been a growing interest in the design of active set methods, that are capable of making rapid changes to incorrect predictions [14,6–8,10]. We refer to papers [13,8] for a review on recent advances in this area.

Recently, based on the identification technique [6], Xiao and Hu [10] proposed an active set subspace Barzilai–Borwein gradient method (SBB). Preliminary numerical results show that the identification technique works well and the SBB method is competitive with the well-known SPG2 method [2]. Although the SBB method has an attractive global convergence theory and is computationally effective, the convergence rate can be slow in a neighborhood of a local minimizer. To accelerate the

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convergence, we propose an active set truncated Newton method in the paper. Specifically, at each iteration, the active variables and free variables are defined by the identification technique [6]; we use the method in [6] to update the active variables and use the truncated Newton method to update the free variables. An advantage of the truncated Newton method to solve the subproblem is that the method can be used to solve large-scale problems. In addition, the method has the following advantages: (a) all iterates are feasible and rapid changes in the active set are allowed; (b) the main computational burden is given by the approximate solution of a square line system whose dimension is equal to the number of free variables; (c) the method based on a nonmonotone line search technique is shown to be globally convergent; (d) preliminary numerical experiments show that the method is effective and competitive with the famous software TRON [9].

The paper is organized as follows. We propose the algorithm in Section 2. In Section 3, we show that the proposed algorithm is globally convergent. In Section 4, we test the performance of the proposed algorithm and compare it with the TRON method [9].

Throughout the paper, $\|\cdot\|$ denotes the Euclidean norm of vectors. Let $P_\Omega(x)$ denote the projection of x on the set Ω. If $w = (w_1, w_2, \dots, w_n)^T$ is a n dimension vector and I is an index set such that $I \subset \{1, 2, \dots, n\}$, we denote by w_I the subvector with components $w_i,\ i \in I$, and denote by $w_I \geq 0$ the subvector with components $w_i \geq 0,\ i \in I$.

2. Motivation and properties

In this section, by the use of the identification technique in [6], we propose an active set truncated Newton method for (1.1). We begin with some notation. Let $\bar{x}$ be a stationary point of (1.1), and consider the associated active sets

$$\bar{L} = \{i : \bar{x}_i = l_i\}, \qquad \bar{U} = \{i : \bar{x}_i = u_i\}.$$

Furthermore, let

$$\bar{F} = \{1, \dots, n\} \setminus (\bar{L} \cup \bar{U})$$

be the set of the free variables. By using this notation, a vector $\bar{x}$ is said to be a stationary point for (1.1) if and only if it satisfies:

$$\begin{cases} i \in \bar{L} \Rightarrow g_i(\bar{x}) \geq 0 \\ i \in \bar{F} \Rightarrow g_i(\bar{x}) = 0 \\ i \in \bar{U} \Rightarrow g_i(\bar{x}) \leq 0 \end{cases} \tag{2.1}$$

where $g_i(x)$ is the ith component of the gradient vector of f at x. Facchinei, Júdice and Soares [6] gave the following approximations $L(x)$, $F(x)$ and $U(x)$ to $\bar{L}$, $\bar{F}$, $\bar{U}$, respectively,

$$\begin{aligned} &L(x) = \{i : x_i \leq l_i + a_i(x) g_i(x)\}, \\ &U(x) = \{i : x_i \geq u_i + b_i(x) g_i(x)\}, \\ &F(x) = \{1, \dots, n\} \setminus (L(x) \cup U(x)), \end{aligned} \tag{2.2}$$

where $a_i(x)$ and $b_i(x),\ i = 1, \dots, n$ are nonnegative, continuous, bounded function defined on Ω, such that if $x_i = l_i$ or $x_i = u_i$ then $a_i(x) > 0$ or $b_i(x) > 0$, respectively. The following theorem shows that $L(x)$, $F(x)$ and $U(x)$ are indeed good estimates of $\bar{L}$, $\bar{F}$ and $\bar{U}$. For the proof, see Theorem 3.1 in [6].

Theorem 2.1. *For any $x \in \Omega$, $L(x) \cap U(x) = \emptyset$. Furthermore, if $\bar{x}$ is a stationary point of problem (1.1) at which the strict complementarity holds, then there exists a neighborhood $N(\bar{x})$ of $\bar{x}$ such that*

$$L(x) = \bar{L}, \qquad F(x) = \bar{F}, \qquad U(x) = \bar{U}, \quad \forall\, x \in N(\bar{x}).$$

Following the idea of [6], we are going to develop an active set truncated Newton method as follows. We firstly define the search direction. Let $x^k = (x_1^k, x_2^k, \dots, x_n^k)^T \in \Omega$ be the current point at iteration k. For simplicity, we let $L^k = L(x^k)$, $U^k = U(x^k)$ and $F^k = F(x^k)$. Define the direction $d^k = (d^k_{L^k}, d^k_{F^k}, d^k_{U^k})^T$ by

$$d_i^k = l_i - x_i^k, \quad i \in L^k \tag{2.3}$$

and

$$d_i^k = u_i - x_i^k, \quad i \in U^k. \tag{2.4}$$

In what follows, we are going to define $d^k_{F^k}$. For this, we define the active set indices of f at x^k as follows:

$$A(x^k) = \{i : x_i^k = l_i \text{ or } x_i^k = u_i\}.$$

The active set indices are further subdivided into those indices:

$$A_1(x^k) = \{i : x_i^k = l_i,\ g_i(x^k) \geq 0\}, \qquad A_2(x^k) = \{i : x_i^k = l_i,\ g_i(x^k) < 0\}$$

and

$$A_3(x^k) = \{i : x_i^k = u_i,\ g_i(x^k) \leq 0\}, \qquad A_4(x^k) = \{i : x_i^k = u_i,\ g_i(x^k) > 0\}.$$