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A deterministic annealing algorithm for approximating a solution of the linearly constrained nonconvex quadratic minimization problem[☆]

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ABSTRACT

A deterministic annealing algorithm is proposed for approximating a solution of the linearly constrained nonconvex quadratic minimization problem. The algorithm is derived from applications of a Hopfield-type barrier function in dealing with box constraints and Lagrange multipliers in handling linear equality constraints, and attempts to obtain a solution of good quality by generating a minimum point of a barrier problem for a sequence of descending values of the barrier parameter. For any given value of the barrier parameter, the algorithm searches for a minimum point of the barrier problem in a feasible descent direction, which has a desired property that the box constraints are always satisfied automatically if the step length is a number between zero and one. At each iteration, the feasible descent direction is found by updating Lagrange multipliers with a globally convergent iterative procedure. For any given value of the barrier parameter, the algorithm converges to a stationary point of the barrier problem. Preliminary numerical results show that the algorithm seems effective and efficient.

1. Introduction

The linearly constrained nonconvex quadratic minimization problem is about minimizing a nonconvex quadratic function over a polytope given by linear equality constraints and box constraints. This problem is an NP-hard problem and has many diverse applications (Horst & Pardalos, 1995). It was shown in Pardalos and Rosen (1987) that many integer and combinatorial optimization problems can be formulated as linearly constrained nonconvex quadratic minimization problems. For example, the max-bisection problem in graph theory can be formulated as a linearly constrained nonconvex quadratic minimization problem, which will be used as a testing problem. To compute a solution of the linearly constrained nonconvex quadratic minimization problem, several exact methods have been developed. They include the cutting-plane method (Tuy, 1964), the extreme point ranking method (Murty, 1968), the relaxation method (Falk & Hoffman, 1976), and the branch and bound method (Falk & Soland, 1969). Due to its computational complexity, the linearly constrained nonconvex quadratic minimization problem is difficult to solve to optimality with an exact method. Heuristics as alternatives have been developed for computing a solution of good quality to this type of problem. They include the simulated annealing procedure (Kirkpatrick, Gelatti, & Vecchi, 1983), Tabu search (Glover, 1989), and the interior-point method (Han, Pardalos, & Ye, 1992). An excellent survey of methods for solving such a problem can be found in Benson (1995), where the extensive developments of methods for solving nonconvex minimization problems are discussed.

Since Hopfield and Tank (1985), combinatorial optimization has become a popular topic in the literature of neural computation. Many neural computational models for combinatorial optimization have been developed in the literature. They include Aiyer, Niranjan, and Fallside (1990), Dang and Xu (2002), Durbin and Willshaw (1987), Gee, Aiyer, and Prager (1993), Gee and Prager (1994), Peterson and Soderberg (1989), Rangarajan, Gold, and Mjolsness (1996), Simic (1990), Urahama (1996), van den Bout and Miller III (1990), Wacholder, Han, and Mann (1989), Waugh and Westervelt (1993), Wolfe, Parry, and MacMillan (1994), Xu (1994), and Yuille and Kosowsky (1994). A systematic investigation of such neural computational models for combinatorial optimization can be found in van der Berg (1996) and Cichocki and Unbehaunen (1993). Most of these algorithms are of deterministic annealing type, which is a heuristic continuation method that attempts to find the global minimum of the effective energy at high temperature and track it as the temperature decreases. There is no guarantee that the minimum at high temperature can always be tracked to the minimum at low

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temperature, but the experimental results are encouraging (Yuille & Kosowsky, 1994).

In this paper a deterministic annealing algorithm is proposed for approximating a solution of the linearly constrained nonconvex quadratic minimization problem. The algorithm is motivated from an investigation that a continuous deformation from a convex Hopfield-type barrier function to the nonconvex quadratic function may lead to a global or near global optimal solution over a box (Dang & Xu, 2000). The main idea of the algorithm is as follows. A Hopfield-type barrier function is used as a barrier term to incorporate box constraints into the objective function. The resulting barrier function deforms from the convex Hopfield-type barrier function to the objective function as the barrier parameter decreases from one to zero. Lagrange multipliers are introduced to deal with linear equality constraints. For any given value of the barrier parameter, the algorithm searches for a minimum point of a barrier problem in a feasible descent direction, which has a desired property that the box constraints are always satisfied automatically if the step length is a number between zero and one. Preliminary numerical results show that the algorithm always yields a global or near global optimal solution, provided that the barrier parameter decreases at a slow pace.

The rest of this paper is organized as follows. We introduce the barrier problem and derive some important properties in Section 2. We describe the algorithm and prove its convergence in Section 3. We present in Section 4 some preliminary numerical results to show that the algorithm seems effective and efficient. We conclude the paper with some remarks in Section 5.

2. Hopfield-type barrier function

The problem we consider in this paper is as follows. Find a minimum point of

$$\begin{array}{ll} \min & f(x) = \frac{1}{2}x^\top Qx + c^\top x \\ \text{subject to} & Ax = b, \\ & s_j \le x_j \le t_j, \quad j = 1, 2, \dots, n, \end{array} \tag{1}$$

where Q is a symmetric indefinite or negative semidefinite matrix, $c = (c_1, c_2, \dots, c_n)^\top$ is a vector of R^n, A is an $m \times n$ matrix of full-row rank given by

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix},$$

$b = (b_1, b_2, \dots, b_m)^\top$ is a vector of R^m, and $s_j, j = 1, 2, \dots, n$, and $t_j, j = 1, 2, \dots, n$, are finite constants satisfying that $s_j < t_j, j = 1, 2, \dots, n$. Let $B = \{x \in R^n \mid s_i \le x \le t_i,\ i = 1, 2, \dots, n\}$. Clearly, B is bounded. For $j = 1, 2, \dots, n$, let a_j denote the jth column of A. Then, $a_j^\top = (a_{1j}, a_{2j}, \dots, a_{mj}), j = 1, 2, \dots, n$. Let $P = \{x \in B \mid Ax = b\}$, which is the feasible region of (1). We assume throughout this paper that P has an interior point, where an interior point of P is a point $x \in P$ with $s_i < x_i < t_i, i = 1, 2, \dots, n$.

In order to approximate a solution of (1), we introduce a Hopfield-type barrier term,

$$h_j(x_j) = (x_j - s_j)\ln(x_j - s_j) + (t_j - x_j)\ln(t_j - x_j),$$

to incorporate $s_j \le x_j \le t_j$ into the objective function, and obtain

$$\begin{array}{ll} \min & e(x; \beta) = (1-\beta)f(x) + \beta\sum_{j=1}^n h_j(x_j) \\ \text{subject to} & Ax = b, \\ & s < x < t, \end{array} \tag{2}$$

where $\beta \in [0, 1]$ is a barrier parameter. Instead of solving (1) directly, let us consider a scheme, which obtains a solution of (1) from the solution of (2) at the limit of $\beta \downarrow 0$.

Let $h(x) = \sum_{j=1}^n h_j(x_j)$. Then, $e(x; \beta) = (1-\beta)f(x) + \beta h(x)$. We define $h_j(s_j) = h_j(t_j) = (t_j - s_j)\ln(t_j - s_j), j = 1, 2, \dots, n$. Since $\lim_{x_j \to s_j^+} h_j(x_j) = \lim_{x_j \to t_j^-} h_j(x_j) = (t_j - s_j)\ln(t_j - s_j)$, hence, $h(x)$ is continuous on B. Note that

$$\frac{\partial h(x)}{\partial x_j} = \ln(x_j - s_j) - \ln(t_j - x_j) = \ln\frac{x_j - s_j}{t_j - x_j}.$$

Then,

$$\lim_{x_j \to s_j^+} \frac{\partial h(x)}{\partial x_j} \to -\infty \quad \text{and} \quad \lim_{x_j \to t_j^-} \frac{\partial h(x)}{\partial x_j} \to \infty.$$

From the compactness of P and the continuity of $\frac{\partial f(x)}{\partial x_j}$ on P, one can get that $\frac{\partial f(x)}{\partial x_j}$ is bounded on P. Thus, from

$$\frac{\partial e(x; \beta)}{\partial x_j} = (1-\beta)\frac{\partial f(x)}{\partial x_j} + \beta\frac{\partial h(x)}{\partial x_j},$$

we obtain that, for any given $\beta \in (0, 1]$,

$$\lim_{x_j \to s_j^+} \frac{\partial e(x; \beta)}{\partial x_j} \to -\infty \quad \text{and} \quad \lim_{x_j \to t_j^-} \frac{\partial e(x; \beta)}{\partial x_j} \to \infty.$$

Lemma 1. *For any given $\beta \in (0, 1]$, if x^* is a minimum point of (2), then x^* is an interior point of P, i.e. $Ax^* = b$ and $s < x^* < t$.*

Proof. Let x^0 be an interior point of P. Suppose that some component of x^*, say x_i^*, equals s_i or t_i. For any given number $\epsilon \in (0, 1]$, let $y^* = x^* + \epsilon(x^0 - x^*)$. Then, $Ay^* = b$ and $s < y^* < t$. For any given number $\delta \in (0, 1]$ satisfying $\epsilon + \delta \le 1$, let

$$z^* = y^* + \delta(x^0 - x^*) = x^* + (\epsilon + \delta)(x^0 - x^*).$$

Then, z^* is an interior point of P and can be made arbitrarily close to x^* through decreasing $\epsilon + \delta$. From the Taylor's expansion, we obtain that

$$e(z^*; \beta) = e(y^*; \beta) + \delta(x^0 - x^*)^\top \nabla_x e(y^* + \eta\delta(x^0 - x^*); \beta), \tag{3}$$

where $\eta \in [0, 1]$ and

$$\nabla_x e(x; \beta) = \left(\frac{\partial e(x; \beta)}{\partial x_1}, \frac{\partial e(x; \beta)}{\partial x_2}, \dots, \frac{\partial e(x; \beta)}{\partial x_n}\right)^\top.$$

Consider

$$\begin{aligned} &(x^0 - x^*)^\top \nabla_x e(y^* + \eta\delta(x^0 - x^*); \beta) \\ &\quad = \sum_{k=1}^n (x_k^0 - x_k^*)\frac{\partial e(y^* + \eta\delta(x^0 - x^*); \beta)}{\partial x_k}. \end{aligned}$$

Note that $y^* + \eta\delta(x^0 - x^*) = x^* + (\epsilon + \eta\delta)(x^0 - x^*)$. Let $\theta = \epsilon + \eta\delta$.

- If $x_k^* = s_k$, then $x_k^0 - x_k^* > 0$ and

$$\begin{aligned} &\lim_{\theta \to 0} \frac{\partial e(y^* + \eta\delta(x^0 - x^*); \beta)}{\partial x_k} \\ &\quad = \lim_{\theta \to 0} (1-\beta)\frac{\partial f(y^* + \eta\delta(x^0 - x^*))}{\partial x_k} \\ &\qquad + \beta\ln\frac{x_k^* + \theta(x_k^0 - x_k^*) - s_k}{t_k - x_k^* - \theta(x_k^0 - x_k^*)} \\ &\quad = \lim_{\theta \to 0} (1-\beta)\frac{\partial f(y^* + \eta\delta(x^0 - x^*))}{\partial x_k} \\ &\qquad + \beta\ln\frac{\theta(x_k^0 - x_k^*)}{t_k - s_k - \theta(x_k^0 - x_k^*)} \\ &\quad = -\infty. \end{aligned}$$