JOURNAL OF OPTIMIZATION THEORY AND APPLICATIONS: Vol. 122, No. 2, pp. 433–440, August 2004 (© 2004)

TECHNICAL NOTE

Sufficient Global Optimality Conditions for Bivalent Quadratic Optimization

M. Ç. PINAR[1]

Communicated by P. Tseng

Abstract. We prove a sufficient global optimality condition for the problem of minimizing a quadratic function subject to quadratic equality constraints where the variables are allowed to take values -1 and 1. We extend the condition to quadratic problems with matrix variables and orthonormality constraints, and in particular to the quadratic assignment problem.

Key Words. Quadratic optimization with binary variables, global optimality, sufficient optimality conditions, quadratic assignment problem.

1. Introduction

We consider the bivalent quadratic optimization problem

$$\begin{aligned}
\text{(QP)} \quad & \min \quad (1/2)x^T Qx + c^T x, \\
& \text{s.t.} \quad x^T E_i x + d_i^T x = f_i, \quad \forall i = 1, \ldots, m, \\
& \qquad\quad x \in \{-1, 1\}^n,
\end{aligned}$$

where $Q \in \mathcal{S}^n$ and where $E_i \in \mathcal{S}^n, \forall i = 1, \ldots, m, c, d_i \in \mathbb{R}^n$, and $f_i \in \mathbb{R}$ for all $i = 1, \ldots, m$; here, $\mathcal{S}^n$ denotes the space of $n \times n$ symmetric real matrices. These problems are known to be NP hard even when the quadratic constraints are absent; see Ref. 1.

The purpose of this note is to present a sufficient condition for global optimality in QP and to give a natural extension to nonconvex quadratic

[1]Associate Professor, Department of Industrial Engineering, Bilkent University, Bilkent, Ankara, Turkey.

programs in matrix variables, and in particular to the quadratic assignment problem. The result is inspired by the work of Beck and Teboulle (Ref. 2), which gave a sufficient condition for optimality in the problem

$$\begin{aligned} \min \quad & (1/2)x^T Qx + c^T x, \\ \text{s.t.} \quad & x \in \{-1, 1\}^n. \end{aligned}$$

2. Results

Let D^T denote the $n \times m$ matrix with columns d_i, $i = 1, \ldots, m$. We define $X = \text{Diag}(x)$ to be the $n \times n$ diagonal matrix with diagonal equal to the vector x. Naturally,

$$x = Xe,$$

where e represents the n-dimensional vector of ones. We use $\otimes$ to denote Kronecker product. Our main result is the following.

Theorem 2.1. Let x be a feasible point for QP. If there exists $z \in \mathbb{R}^m$ which solves

$$Q + \text{Diag}\left(-XQx - X\left(\sum_{i=1}^m z_i E_i\right)x - Xc - (1/2)XD^T z\right) + \sum_{i=1}^m z_i E_i \succeq 0,$$

then x is a global optimal solution for QP.

Remark 2.1. The proof of this theorem follows from the following well-known fact; see e.g. Refs. 3–4. The Karush–Kuhn–Tucker (KKT) conditions are sufficient for optimality if the Lagrangian function is convex in the unknown x for the optimal Lagrange multiplier. More precisely, let λ^* denote the optimal Lagrange multiplier. The KKT conditions for the equality constrained problem at x^* are stationarity and feasibility, i.e.,

$$\nabla L(x^*, \lambda^*) = 0$$

for x^* feasible. The convexity of $L(., \lambda^*)$ is equivalent to

$$\nabla^2 L(x, \lambda^*) \succeq 0, \quad \forall x.$$

The proof below verifies that the Hessian of the Lagrangian is positive semidefinite (i.e., the Lagrangian is convex); stationarity holds by substituting for the vector of Lagrange multipliers corresponding to the bivalency constraints.

Proof. The proof is essentially identical to the proof of Theorem 2.3 of Ref. 2 with the necessary modifications. We write QP as

$$\begin{array}{lll} \text{(QP)} & \min & (1/2)x^T Qx + c^T x, \\ & \text{s.t.} & x^T E_i x + d_i^T x = f_i, \quad \forall i = 1, \ldots, m, \\ & & x_j^2 = 1, \qquad\qquad\quad\; \forall j = 1, \ldots, n. \end{array}$$

Now, consider the Lagrangian function associated with QP,

$$L(x, y, z) = (1/2)x^T \left(Q + Y + \sum_{i=1}^{m} z_i E_i \right) x - (1/2)y^T e + c^T x \\ -(1/2)z^T f + (1/2)x^T D^T z,$$

where we have introduced multipliers $y \in \mathbb{R}^n$, $Y = \mathrm{Diag}(y)$, for the bivalency constraints, and multipliers $z \in \mathbb{R}^m$ for the first set of quadratic constraints after multiplying all constraints by one half, and have rearranged the expression of the function L to regroup quadratic and linear terms together. It is well known that we have

$$\inf_x L(x, y, z) > -\infty$$

if and only if there exist multipliers y and z such that

$$Q + Y + \sum_{i=1}^{m} z_i E_i \succeq 0 \tag{1}$$

and

$$\left(Q + Y + \sum_{i=1}^{m} z_i E_i \right) x + c + (1/2)D^T z = 0 \tag{2}$$

is consistent for some x. For a feasible x, define

$$y := -XQx - X \left(\sum_{i=1}^{m} z_i E_i \right) x - Xc - (1/2)XD^T z,$$

for some $z \in \mathbb{R}^m$. It is verified easily, using the fact that

$$XX = I,$$

that the vector y so defined satisfies (2) along with x and z.

Consider now the dual problem

$$\sup_{y,z} h(y, z),$$

where

$$h(y, z) = \inf_{x} L(x, y, z).$$

Using (2), we write immediately $h(y, z)$ as

$$h(y, z) = -(1/2)\, x^T \left(Q + Y + \sum_{i=1}^{m} z_i E_i \right) x - (1/2)\, y^T e - (1/2)\, z^T f.$$

Now, evaluate h at the point (x, y, z) defined above. Using the fact that $XX = I$, a simple calculation shows that this yields

$$h(y, z) = (1/2)\, x^T Qx + (1/2)\, x^T \left(\sum_{i=1}^{m} z_i E_i \right) x + c^T x$$
$$+ (1/2)\, x^T D^T z - (1/2)\, z^T f.$$

But, since x is feasible, the second, fourth, and fifth terms sum up to zero. Therefore, we see that the value of the dual function equals the value of the primal objective function, which is sufficient to ensure global optimality of x from basic duality theory [c.f. Rockafellar (Ref. 5)]. □

Notice that the sufficient condition involves the solution of a linear matrix inequality (LMI) and as such can be checked using polynomial-time interior-point methods; see Ref. 6. However, it is difficult admittedly to find a feasible point for problem QP; in fact this is as difficult as the minimization problem itself. Furthermore, the original Beck–Teboulle conditions are simpler as they do not involve dual variables. The increased complexity of the sufficient conditions is the price to be paid for dealing with a harder problem.

When one has only linear constraints, the sufficient condition becomes simpler. Consider the following linearly constrained problem:

$$\begin{array}{lll} \text{(LCQP)} & \min & (1/2)\, x^T Qx + c^T x, \\ & \text{s.t.} & Ax = b, \\ & & x \in \{-1, 1\}^n, \end{array}$$

where $Q \in \mathcal{S}^n$, $A \in \mathbb{R}^{m \times n}$, and $b \in \mathbb{R}^m$.

Corollary 2.1. Let x be a feasible point for LCQP. If there exists $z \in \mathbb{R}^m$ which solves

$$\lambda_{\min}(Q)e \geq XQx + Xc + XA^T z,$$

then x is a global optimal solution for LCQP.

Proof. The sufficient condition reduces to

$$Q + \mathrm{Diag}(-XQx - Xc - XA^T z) \succeq 0.$$

Since we have always

$$\lambda_{\min}(Q + Y) \geq \lambda_{\min}(Q) + \lambda_{\min}(Y),$$

the above condition is satisfied if

$$\lambda_{\min}(Q) \geq -\lambda_{\min}\mathrm{Diag}(-XQx - Xc - XA^T z).$$

But since the right-hand matrix is diagonal, the result follows. □

Notice that the condition in Corollary 2.1 is closer to the original result of Beck and Teboulle (i.e., Theorem 2.3 of Ref. 2), which did not involve an LMI condition.

The main result of the paper is related also to the work of Hiriart-Urruty on global optimality conditions for nonconvex optimization problems developed in a series of papers; see e.g. Refs. 7–9. Hiriart-Urruty develops a general global optimality condition, based on a generalized subdifferential concept, and specializes the condition to several problems of nonconvex optimization, including maximization of a convex quadratic function subject to strictly convex quadratic inequalities, minimization of a quadratic function subject to a single quadratic inequality (trust-region problem) and subject to two quadratic inequalities (two-trust-region problem). While the sufficient condition obtained in Theorem 4.6 of Ref. 8 follows essentially from the result that we used in our Theorem 2.1 (see also Remark 2.1), our result further develops that of Hiriart-Urruty by exploiting the special bivalency structure and yields more compact sufficiency condition. Hiriart-Urruty obtains also conditions that are both necessary and sufficient in Refs. 7–9 for nonconvex quadratic programs. However, these results involve a condition stating that some homogeneous function mixing first-order and second-order information about the problem data should have a constant sign on a convex cone, in addition to the first-order stationarity condition. It is not clear at present whether these conditions could be simplified further, in the presence of bivalency constraints in addition to the quadratic equality constraints, and lead to implementable criteria. An effort in this direction is reported in Ref. 10, where the Hiriart-Urruty global optimality conditions have been implemented and tested with some success on unconstrainted quadratic 0–1 optimization problems.

When one deals with a linear bivalent program ($Q \equiv 0$), we have the following corollary.

Corollary 2.2. Let x be a feasible point. If there exists $z \in \mathbb{R}^m$ satisfying

$$Xc + XA^T z \leq 0,$$

then x is a global optimal solution.

Note that it is equally easy to treat inequality constraints by restricting the sign of the multiplier; see Theorem 2.2 below.

The above results admit natural extensions to nonconvex quadratic programs with matrix variables and orthonormality constraints. In particular, consider the following quadratic assignment problem:

$$\begin{array}{lll} \text{(QAP)} & \min & \mathrm{Tr}(AXBX^T) + \mathrm{Tr}(CX^T), \\ & \text{s.t.} & XX^T = I, \\ & & Xe = e, \\ & & X^T e = e, \\ & & X \geq 0, \end{array}$$

where A, B are symmetric $n \times n$ matrices and C, X are an $n \times n$ matrices.

We use $\mathbb{R}_+^{n \times n}$ to denote the space of $n \times n$ real nonnegative matrices.

Theorem 2.2. Let X be a feasible point for QAP. If there exists $u \in \mathbb{R}^n$, $w \in \mathbb{R}^n$, and $T \in \mathbb{R}_+^{n \times n}$, with $T_{ij} = 0$ for all (i, j), such that $X_{ij} > 0$ satisfy the LMI

$$B \otimes A - I \otimes \left(AXBX^T + CX^T - (ue^T + ew^T + T)X^T \right) \succeq 0,$$

then X is global optimal in QAP.

Proof. The proof is essentially identical to the proof of Theorem 2.1, with the necessary modifications. □

The sufficient condition remains an LMI with some linear side conditions.

A well-known relaxation of the QAP is the following nonconvex quadratic program defined over orthonormal matrices (Stiefel manifold) known as the eigenvalue bounds program for $C \equiv 0$ (see Refs. 11–12 and results and references therein):

$$\begin{aligned} \min \quad & \mathrm{Tr}(AXBX^T) + \mathrm{Tr}(CX^T), \\ \text{s.t.} \quad & XX^T = I. \end{aligned}$$

The sufficient condition for optimality is simplified in this case.

Corollary 2.3. Let X be an orthonormal matrix. If

$$\lambda_{\min}(B \otimes A) \geq \lambda_{\max}(AXBX^T + CX^T),$$

then X is global optimal.

Note that the conditions obtained in Refs. 11–12 have proved important in relaxations for QAP. They have been used by Anstreicher and coauthors in Refs. 13–14 and follow-up numerical work, to solve many previously unsolved hard instances of QAP.

As future work, it would be interesting to look for necessary conditions for QP and related problems and test the usefulness of the conditions of the present paper in algorithms for QAP among others.

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