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## TECHNICAL NOTE

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### Sufficient Global Optimality Conditions for Bivalent Quadratic Optimization

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

12 **Key Words.** Quadratic optimization with binary variables, global  
13 optimality, sufficient optimality condition, quadratic assignment prob-  
14 lem.

#### 15 1. Introduction

16 We consider the bivalent quadratic optimization problem

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

17  
18 where  $Q \in \mathcal{S}^n$  and where  $E_i \in \mathcal{S}^n, \forall i = 1, \dots, m, c, d_i \in \mathbb{R}^n$ , and  $f_i \in \mathbb{R}$   
19 for all  $i = 1, \dots, m$ ; here,  $\mathcal{S}^n$  denotes the space of  $n \times n$  symmetric real  
20 matrices. These problems are known to be NP hard even when the qua-  
21 dratic constraints are absent; see Ref. 1.

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

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

$$\begin{aligned} & \min \quad (1/2)x^T Qx + c^T x, \\ 27 \quad & \text{s.t.} \quad x \in \{-1, 1\}^n. \end{aligned}$$

## 28 2. Results

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

$$32 \quad x = Xe,$$

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

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

$$\begin{aligned} 37 \quad & Q + \text{Diag} \left( -XQx - X \left( \sum_{i=1}^m z_i E_i \right) x - Xc - (1/2)XD^T z \right) \\ & + \sum_{i=1}^m z_i E_i \geq 0, \end{aligned}$$

39 then  $x$  is a global optimal solution for QP.

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

$$46 \quad \nabla L(x^*, \lambda^*) = 0$$

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

$$48 \quad \nabla^2 L(x, \lambda^*) \succeq 0, \quad \forall x.$$

49 The proof below verifies that the Hessian of the Lagrangian is posi-  
 50 tive semidefinite (i.e., the Lagrangian is convex); stationarity holds by

51 substituting for the vector of Lagrange multipliers corresponding to the  
 52 bivalency constraints.

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

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

56 Now, consider the Lagrangian function associated with QP,

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

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

$$64 \quad \inf_x L(x, y, z) > -\infty$$

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

$$66 \quad Q + Y + \sum_{i=1}^m z_i E_i \geq 0 \tag{1}$$

67 and

$$68 \quad \left( Q + Y + \sum_{i=1}^m z_i E_i \right) x + c + (1/2)D^T z = 0 \tag{2}$$

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

$$70 \quad y := -XQx - X \left( \sum_{i=1}^m z_i E_i \right) x - Xc - (1/2)XD^T z,$$

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

$$72 \quad XX = I,$$

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

74 Consider now the dual problem

$$75 \quad \sup_{y,z} h(y, z),$$

76 where

$$77 \quad h(y, z) = \inf_x L(x, y, z).$$

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

$$79 \quad h(y, z) = -(1/2)x^T \left( Q + Y + \sum_{i=1}^m z_i E_i \right) x - (1/2)y^T e - (1/2)z^T f.$$

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

$$82 \quad h(y, z) = (1/2)x^T Qx + (1/2)x^T \left( \sum_{i=1}^m z_i E_i \right) x + c^T x$$

$$83 \quad + (1/2)x^T D^T z - (1/2)z^T f.$$

84 But, since  $x$  is feasible, the second, fourth, and fifth terms sum up to zero.  
85 Therefore, we see that the value of the dual function equals the value of  
86 the primal objective function, which is sufficient to ensure global optimal-  
87 ity of  $x$  from basic duality theory [c.f. Rockafellar (Ref. 5)].  $\square$

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

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

$$98 \quad (\text{LCQP}) \quad \min \quad (1/2)x^T Qx + c^T x,$$

$$99 \quad \text{s.t.} \quad Ax = b,$$

$$100 \quad x \in \{-1, 1\}^n,$$

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

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

$$104 \quad \lambda_{\min}(Q)e \geq XQx + Xc + XA^T z,$$

105 then  $x$  is a global optimal solution for LCQP.

106 **Proof.** The sufficient condition reduces to

$$107 \quad Q + \text{Diag}(-XQx - Xc - XA^T z) \succeq 0.$$

108 Since we have always

$$109 \quad \lambda_{\min}(Q + Y) \geq \lambda_{\min}(Q) + \lambda_{\min}(Y),$$

110 the above condition is satisfied if

$$111 \quad \lambda_{\min}(Q) \geq -\lambda_{\min} \text{Diag}(-XQx - Xc - XA^T z).$$

112 But since the right-hand matrix is diagonal, the result follows.  $\square$

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

116 The main result of the paper is related also to the work of  
 117 Hiriart-Urruty on global optimality conditions for nonconvex optimization  
 118 problems developed in a series of papers; see e.g. Refs. 7–9. Hiriart-Urruty  
 119 develops a general global optimality condition, based on a generalized  
 120 subdifferential concept, and specializes the condition to several problems  
 121 of nonconvex optimization, including maximization of a convex quadratic  
 122 function subject to strictly convex quadratic inequalities, minimization of  
 123 a quadratic function subject to a single quadratic inequality (trust-region  
 124 problem) and subject to two quadratic inequalities (two-trust-region prob-  
 125 lem). While the sufficient condition obtained in Theorem 4.6 of Ref. 8 fol-  
 126 lows essentially from the result that we used in our Theorem 2.1 (see also  
 127 Remark 2.1), our result further develops that of Hiriart-Urruty by exploit-  
 128 ing the special bivalency structure and yields more compact sufficiency con-  
 129 dition. Hiriart-Urruty obtains also conditions that are both necessary and  
 130 sufficient in Refs. 7–9 for nonconvex quadratic programs. However, these  
 131 results involve a condition stating that some homogeneous function mixing  
 132 first-order and second-order information about the problem data should  
 133 have a constant sign on a convex cone, in addition to the first-order stati-  
 134 onarity condition. It is not clear at present whether these conditions could  
 135 be simplified further, in the presence of bivalency constraints in addition

136 to the quadratic equality constraints, and lead to implementable criteria.  
 137 An effort in this direction is reported in Ref. 10, where the Hiriart-Urruty  
 138 global optimality conditions have been implemented and tested with some  
 139 success on unconstrained quadratic 0–1 optimization problems.

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

142 **Corollary 2.2.** Let  $x$  be a feasible point. If there exists  $z \in \mathbb{R}^m$  satis-  
 143 fying

$$144 \quad Xc + XA^T z \leq 0,$$

145 then  $x$  is a global optimal solution.

146 Note that it is equally easy to treat inequality constraints by restrict-  
 147 ing the sign of the multiplier; see Theorem 2.2 below.

148 The above results admit natural extensions to nonconvex quadratic  
 149 programs with matrix variables and orthonormality constraints. In partic-  
 150 ular, consider the following quadratic assignment problem:

$$\begin{aligned} 151 \quad (\text{QAP}) \quad & \min \quad \text{Tr}(AXBX^T) + \text{Tr}(CX^T), \\ & \text{s.t.} \quad XX^T = I, \\ & \quad \quad Xe = e, \\ & \quad \quad X^T e = e, \\ & \quad \quad X \geq 0, \end{aligned}$$

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

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

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

$$157 \quad B \otimes A - I \otimes (AXBX^T + CX^T - (ue^T + ew^T + T)X^T) \geq 0,$$

158 then  $X$  is global optimal in QAP.

159 **Proof.** The proof is essentially identical to the proof of Theorem 2.1,  
 160 with the necessary modifications.  $\square$

161 The sufficient condition remains an LMI with some linear side con-  
 162 ditions.

163 A well-known relaxation of the QAP is the following nonconvex  
 164 quadratic program defined over orthonormal matrices (Stiefel manifold)

165 known as the eigenvalue bounds program for  $C \equiv 0$  (see Refs. 11–12 and  
166 results and references therein):

$$\begin{aligned} 167 \quad & \min \quad \text{Tr}(AXBX^T) + \text{Tr}(CX^T), \\ 168 \quad & \text{s.t.} \quad XX^T = I. \end{aligned}$$

169 The sufficient condition for optimality is simplified in this case.

170 **Corollary 2.3.** Let  $X$  be an orthonormal matrix. If

$$171 \quad \lambda_{\min}(B \otimes A) \geq \lambda_{\max}(AXBX^T + CX^T),$$

172 then  $X$  is global optimal.

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

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

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Uncorrected Proof