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*The Spherical Constraint in
Boolean Quadratic Programs*

Jérôme Malick

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The Spherical Constraint in Boolean Quadratic Programs

Jérôme Malick*

Thème 4 — Simulation et optimisation
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Abstract: We propose a new approach to bound Boolean quadratic optimization problems. The idea is to re-express Boolean constraints as one “spherical” constraint. Dualizing this constraint then amounts to a semidefinite least-squares problem which can be efficiently solved. Studying this dualization also provides an alternative interpretation of the SDP relaxation and reveals a new class of non-convex problems with no duality gap.

Key-words: Combinatorial optimization, SDP relaxation, Lagrangian duality, semidefinite least-squares

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La contrainte sphérique dans les problèmes quadratiques booléens

Résumé : Cet article présente une nouvelle méthode de calcul de majorants pour les problèmes d'optimisation quadratique à variables booléennes. L'idée est de ré-exprimer toutes les contraintes booléennes comme une unique contrainte que l'on appelle la contrainte sphérique. La dualisation lagrangienne de cette contrainte mène à un problème particulier de moindres carrés semi-définis qui peut donc être efficacement résolu. L'étude de cette dualisation fournit au passage une nouvelle interprétation de la relaxation SDP. Elle permet aussi de mettre en exergue une classe de problèmes d'optimisation sans saut de dualité.

Mots-clés : optimisation combinatoire, relaxation SDP, dualité lagrangienne, moindres carrés semi-défini

1 Introduction, motivations

One of the key ingredients in combinatorial optimization is bounding, which replaces the original (difficult) problem by a simpler one with larger optimal value (assuming we are maximizing). An important instance of bounding method is SDP relaxation. Its basic idea is to replace the product $x_i x_j$ by another variable X_{ij} : the space \mathbb{R}^n is thus “lifted” to the space \mathcal{S}_n of symmetric matrices. The technique is particularly relevant for Boolean quadratic problems (see [PRW95] and [LO99]). Striking examples in combinatorial optimization are max-cut and max-clique (see [Lov79] and [GW95]).

We present here a new expression of the rank one-constraint that appears in the SDP formulation of Boolean quadratic problems. We start by introducing our notation, defining Boolean quadratic problems and recalling the lifting into \mathcal{S}_n (Subsections 1.1 and 1.2). The Boolean constraints are equivalently replaced by a single quadratic constraint with respect to $X \in \mathcal{S}_n$, that we call the spherical constraint (Section 2). This re-expression allows an alternative interpretation of the SDP relaxation (Subsection 3.3) and proposes a generalization of it. Lagrangian duality then reveals the absence of duality gap when dualizing this spherical constraint (Sections 3 and 4). Dualizing the spherical constraint is the occasion to point out a class of optimization problems with no duality gap (Subsection 4.2).

1.1 Boolean quadratic problems

Let be given $m + 1$ quadratic functions defined on \mathbb{R}^n :

$$q_j(x) = x^\top Q_j x + 2b_j^\top x + c_j, \quad j = 0, \dots, m,$$

where the Q_j are symmetric matrices, the b_j lie in \mathbb{R}^n and the c_j in \mathbb{R} . To express that each variable x_i is Boolean, we also consider the quadratic functions $x \mapsto x_i^2 - 1$ for $i = 1, \dots, n$. With this data, a general Boolean quadratic problem is

$$\begin{cases} \max & q_0(x) \\ q_j(x) \geq 0, & j = 1, \dots, m \\ x_i^2 - 1 = 0, & i = 1, \dots, n, \end{cases} \quad (1)$$

(among the m inequality constraints, we might also have equalities). The maximal value of this problem is denoted by $\text{val}(1)$. In general in this paper, we denote by $\text{val}(\ast)$ the optimal value of an optimization problem (\ast) .

We can suppose that the quadratic functions q_j are homogeneous (that is $b_j = 0$ and $c_j = 0$): otherwise we homogenize the problem with the classical trick (see e.g. [NWY00]) consisting in adding one dimension as follows :

$$x^\top Q_j x + 2z b_j^\top x + c_j z^2 \quad \text{and} \quad z^2 = 1.$$

With no loss of generality, we thus consider in this paper only the simplified form of (1) (with $Q = Q_0$)

$$\begin{cases} \max & x^\top Q x \\ x^\top Q_j x \geq 0, & j = 1, \dots, m \\ x_i \in \{-1, 1\}, & i = 1, \dots, n. \end{cases} \quad (2)$$

Example 1.1 (Max-cut). *When the only constraints are $x_i \in \{-1, 1\}$, this problem is known to be an instance of the classical max-cut problem (see for instance [BTN01, Chap.4] and [GR00]).*

1.2 Lifting into \mathcal{S}_n

A convenient scalar product on the space \mathcal{S}_n of symmetric matrices is the Frobenius scalar product $\langle A, B \rangle = \text{trace}(AB) = \sum_{i=1}^n A_{ij} B_{ij}$. The reason it is so convenient for our purposes is the following relation:

$$\forall x \in \mathbb{R}^n, \quad \forall A \in \mathcal{S}_n, \quad x^\top A x = \langle A, x x^\top \rangle. \quad (3)$$

The associated norm in \mathcal{S}_n is denoted by $\|\cdot\|$. (Notice that we also denote the norm of $x \in \mathbb{R}^n$ by $\|x\|^2 = x^\top x$.) The Boolean quadratic problem (2) can be re-expressed as a linear one in \mathcal{S}_n equipped with $\langle \cdot, \cdot \rangle$: it is the classical “lifting” procedure that we quickly recall here.

We denote by diag the diagonal operator which associates to a matrix in \mathcal{S}_n its diagonal in \mathbb{R}^n . Let e_n stand for the vector of \mathbb{R}^n with all entries equal to 1 ($e_n = [1, \dots, 1]^\top$). Via (3), the objective of (2) is re-expressed as $\langle Q, X \rangle$ where we have set $X = xx^\top$. Observe that $x_i^2 = 1$ ($i = 1, \dots, n$) means $\text{diag}(X) = e_n$. Problem (2) is therefore equivalently written as

$$\begin{cases} \max & \langle Q, X \rangle \\ \langle Q_j, X \rangle \geq 0, & j = 1, \dots, m \\ \text{diag}(X) = e_n \\ X = xx^\top. \end{cases} \quad (4)$$

Example 1.2 (Max-cut). A max-cut problem is thus written

$$\begin{cases} \max & \langle W, X \rangle \\ \text{diag}(X) = e_n \\ X = xx^\top, \end{cases} \quad (5)$$

where W is the matrix of weights (W_{ij} is the weight of arc (i, j)).

The point is that the constraint $X = xx^\top$ is not convex. A classical tool to find upper bounds to (5) and more generally to (4) is the SDP relaxation (see [PRW95]). It consists in

- relaxing the non-convex constraint $X = xx^\top$ to $X \succeq xx^\top$, which is convex with respect to (x, X)
- and then realizing that the variable x is superfluous (the best to do is to take $x = 0$).

The SDP relaxation of (4) is therefore

$$\begin{cases} \max & \langle Q, X \rangle \\ \langle Q_j, X \rangle \geq 0, & j = 1, \dots, m \\ \text{diag}(X) = e_n \\ X \succeq 0. \end{cases} \quad (6)$$

We give in Proposition 3.5 an alternative interpretation to the SDP relaxation.

2 Correlation matrices and the spherical constraint

This section is devoted to studying the set of correlation matrices

$$\mathcal{C}_n = \{X \in \mathcal{S}_n : X \succeq 0, \text{diag}(X) = e_n\}. \quad (7)$$

These matrices appear in statistics to express relations between random variables. They also appear naturally in our framework when relaxing lifted Boolean programs (see (6) above).

In this paper, we often drop the dependence of notation to the dimension n if no confusion is possible. Note first that \mathcal{C} is the intersection of the closed convex cone of SDP matrices and the affine subspace $\text{diag}(X) = e$; \mathcal{C} is then a closed convex subset of \mathcal{S}_n . Furthermore it is bounded and we know a pertinent bound.

Lemma 2.1. *If $X \in \mathcal{C}$, then there holds $\|X\|^2 \leq n^2$. Therefore \mathcal{C} is compact.*

Proof. Let $X \in \mathcal{C}$. Since $X \succeq 0$, any principal minor has a nonnegative determinant. In particular we have

$$X_{ii}X_{jj} - X_{ij}^2 \geq 0.$$

With $\text{diag}(X) = e$, this yields $X_{ij}^2 \leq 1$ and therefore

$$\|X\|^2 = \sum_{i,j=1}^n X_{ij}^2 \leq n^2.$$

Being also closed, \mathcal{C} is thus a compact convex subset of \mathcal{S}_n . \square

Thus the norm of a matrix in \mathcal{C} is always lower than n . Theorem 2.3 will characterise the matrices whose norm is equal to n . Before, recall that there holds

$$\|X\|^2 = \text{trace}(X^2) = \sum_{i=1}^n [\lambda_i(X)]^2,$$

and, by analogy, we set

$$\|X\|_1 = \sum_{i=1}^n |\lambda_i(X)|.$$

Lemma 2.2. *Let $X \in \mathcal{S}_n$ be non-zero. Then we have the equivalence*

$$X \text{ is a rank-one matrix} \iff \|X\| = \|X\|_1.$$

Proof. The following result is classical and easily proved (by recurrence for instance) : for $(x_1, \dots, x_n) \in \mathbb{R}^n$, there holds

$$\sum_{i=1}^n x_i^2 \leq \left(\sum_{i=1}^n |x_i| \right)^2,$$

with equality if and only if there is at most one non-zero x_i . With this property, we can write for $X \in \mathcal{S}_n$ that

$$\sqrt{\sum_{i=1}^n \lambda_i(X)^2} \leq \sum_{i=1}^n |\lambda_i(X)|, \quad (8)$$

with equality if and only if X has rank at most 1. To conclude, just observe that equality $\|X\| = \|X\|_1$ is equivalent to the equality in (8). \square

The following characterization is then straightforward.

Theorem 2.3 (Characterization of rank-one matrices of \mathcal{C}). *Let $X \in \mathcal{C}$. The following equivalence holds:*

$$X \text{ is a rank-one matrix} \iff \|X\|^2 = n^2.$$

Proof. Let $X \in \mathcal{C}$. Since $X \succeq 0$, we have $\|X\|_1 = \text{trace}(X)$. Moreover, $\text{diag}(X) = e$ implies $\|X\|_1 = n$. Since $X \neq 0$, Lemma 2.2 gives the equivalence. \square

Since it imposes to X to lie on the Euclidian sphere of center 0 and radius n in \mathcal{S}_n , we call the constraint $\|X\|^2 = n^2$ the *spherical constraint*.

3 Introducing Lagrangian duality

We develop in this section a dual method by dualizing the spherical constraint: we define a convex function v such that

$$\forall \alpha \in \mathbb{R}, \quad \text{val}(4) \leq v(\alpha).$$

We study here the theoretical properties of this dualization. Section 4 is devoted to studying the duality gap.

3.1 Dualizing the spherical constraint

We start by reformulating Problem (4) with the help of Theorem 2.3. The constraint $X = xx^\top$ exactly expresses that the symmetric matrix X is rank-one. Then (4) can be written as

$$\begin{cases} \max & \langle Q, X \rangle \\ & \langle Q_j, X \rangle \geq 0, \quad j = 1, \dots, m \\ & X \in \mathcal{C}, \\ & \|X\|^2 = n^2. \end{cases} \quad (9)$$

Observe that we have transformed the Boolean quadratic problem (2) to Problem (9) which has only one quadratic constraint with respect of the variable $X \in \mathcal{S}_n$. To isolate this constraint, we set

$$\mathcal{C}' := \mathcal{C} \cap \{X \in \mathcal{S}_n : \langle Q_j, X \rangle \geq 0 \text{ for all } j = 1, \dots, m\}. \quad (10)$$

Obviously, \mathcal{C}' is a convex compact subset of \mathcal{S}_n (recall Lemma 2.1). Problem (9) can be rewritten

$$\begin{cases} \max & \langle Q, X \rangle \\ & X \in \mathcal{C}', \\ & \|X\|^2 = n^2. \end{cases} \quad (11)$$

Taking advantage of this new formulation, we now study the dualization of the constraint $\|X\|^2 = n^2$.

We form the Lagrangian, function of two variables, the primal $X \in \mathcal{C}'$, and the dual $\alpha \in \mathbb{R}$:

$$L(X, \alpha) = \langle Q, X \rangle - \frac{\alpha}{2}(\|X\|^2 - n^2). \quad (12)$$

We define the dual function

$$v(\alpha) = \sup_{X \in \mathcal{C}'} L(X, \alpha). \quad (13)$$

The dual problem of (11) is then

$$\begin{cases} \inf & v(\alpha) \\ & \alpha \in \mathbb{R}. \end{cases} \quad (14)$$

As usual, each value of the primal function gives a lower bound of the dual function (weak duality – see [HUL93, Chap. XII]):

$$\forall X \in \mathcal{C}', \|X\|^2 = n^2, \forall \alpha \in \mathbb{R}, \quad \langle Q, X \rangle = L(X, \alpha) \leq v(\alpha). \quad (15)$$

Therefore, we have

$$\text{val}(11) \leq \text{val}(14) \leq v(\alpha). \quad (16)$$

3.2 Properties of dual objects

Consider, for $\alpha \in \mathbb{R}$, the set of solutions of (13), that is

$$\mathcal{X}(\alpha) = \{X \in \mathcal{C}' : L(X, \alpha) = v(\alpha)\}.$$

Lemma 3.1 ($\mathcal{X}(\alpha)$ and $X(\alpha)$). *Let $\alpha \in \mathbb{R}$. Then the supremum in (13) is attained: there is a $X \in \mathcal{C}'$ such that $v(\alpha) = L(X, \alpha)$. Furthermore if $\alpha > 0$ then this X is unique; it will be denoted by $X(\alpha)$. We thus have, for $\alpha > 0$, $\mathcal{X}(\alpha) = \{X(\alpha)\}$.*

Proof. The function $L(\cdot, \alpha)$ is continuous on \mathcal{C}' which is compact. Its maximum is thus attained on \mathcal{C}' . When $\alpha > 0$, the function $L(\cdot, \alpha)$ is also strictly concave and then it reaches its maximum at a unique point. \square

When $\alpha > 0$, the matrix $X(\alpha)$ has an important geometric interpretation: it is the projection of Q/α on \mathcal{C}' . By the way, this yields an interesting feature of $X(\alpha)$: it is stable under small perturbations on Q .

Theorem 3.2 (Projection). *For $\alpha > 0$, we denote in this result by $X(\alpha, Q)$ the solution of (13). Then $X(\alpha, Q)$ is the projection of Q/α onto \mathcal{C}' . It follows that the function $X(\alpha, \cdot)$ is $1/\alpha$ -Lipschitzian on \mathcal{S}_n .*

Proof. Note that we can write, for $\alpha \neq 0$ and $X \in \mathcal{C}'$,

$$\begin{aligned} L(X, \alpha) &= \frac{\alpha}{2}n^2 - \frac{\alpha}{2}\|X\|^2 + \langle X, Q \rangle \\ &= \frac{\alpha}{2}n^2 - \frac{\alpha}{2}(\|X\|^2 - 2\langle X, Q/\alpha \rangle) \\ &= \frac{\alpha}{2}n^2 - \frac{\alpha}{2}\left(\left\|X - \frac{Q}{\alpha}\right\|^2 - \frac{\|Q\|^2}{\alpha^2}\right), \end{aligned}$$

and then there holds

$$L(X, \alpha) = \left(\frac{\alpha}{2}n^2 + \frac{1}{2\alpha}\|Q\|^2\right) - \frac{\alpha}{2}\left\|X - \frac{Q}{\alpha}\right\|^2. \quad (17)$$

For $\alpha > 0$, maximizing $L(\cdot, \alpha)$ on \mathcal{C}' thus amounts to minimizing $\| \cdot - Q/\alpha \|^2$ on \mathcal{C}' . By [HUL01, Prop.A.3.1.3], $X(\alpha, Q)$ is $1/\alpha$ -Lipschitzian with respect to Q . \square

Theorem 3.3 (Dual function). *The function v defined by (13) is closed, convex and non-decreasing on \mathbb{R} . Its subdifferential at $\alpha \in \mathbb{R}$ is*

$$\partial v(\alpha) = \text{conv} \left\{ \frac{1}{2}(n^2 - \|X\|^2) : X \in \mathcal{X}(\alpha) \right\}, \quad (18)$$

where conv denotes the convex hull. In particular, v is differentiable on $]0, +\infty[$ and, for $\alpha > 0$,

$$v'(\alpha) = \frac{1}{2}(n^2 - \|X(\alpha)\|^2).$$

Proof. Being the supremum of the family of affine functions $L(X, \cdot)$ (indexed by \mathcal{C}'), v is a closed convex function on \mathbb{R} . Since \mathcal{C}' is compact, we apply [HUL01, Th.D.4.4.2] to get (18). Lemma 2.1 then yields that

$$\partial v(\alpha) \subset [0, n^2] \subset \mathbb{R}^+$$

and then v is non-decreasing on \mathbb{R} . Whenever $\alpha > 0$, Lemma 3.1 implies that $\partial v(\alpha)$ is reduced to $\{\frac{1}{2}(n^2 - \|X(\alpha)\|^2)\}$, and [HUL01, Cor.D.2.1.4] guarantees the differentiability of v , with $v'(\alpha) = \frac{1}{2}(n^2 - \|X(\alpha)\|^2)$. \square

By (17), to compute $v(\alpha)$ when $\alpha > 0$ amounts to solving

$$m(\alpha) = \min_{X \in \mathcal{C}'} \|X - Q/\alpha\|^2 \quad (19)$$

and setting

$$v(\alpha) = \left(\frac{\alpha}{2}n^2 + \frac{1}{2\alpha}\|Q\|^2\right) - \frac{\alpha}{2}m(\alpha).$$

Example 3.4 (Max-cut). *For the particular case of Problem (5), this way to compute $v(\alpha)$ for $\alpha > 0$ amounts to compute the minimum of the following problem:*

$$\begin{cases} \min & \|X - W/\alpha\|^2 \\ \text{diag}(X) &= e_n, \\ X &\succeq 0. \end{cases} \quad (20)$$

Problem (20) and more generally (19) are actually so-called semidefinite least-squares problems (SDLS): we want to calculate $X(\alpha)$, the nearest matrix to Q/α that belongs to the intersection of the SDP cone with the half-spaces $\langle Q_j, X \rangle = 0$ and an affine subspace $\text{diag}(X) = e$ (recall Expressions (7) and (10)). Recently some algorithms have been proposed to solve SDLS problems [Hig02], [Tak03] and [Mal04]. In particular the dual algorithm proposed in [Mal04] has been shown to be efficient even to solve large SDLS problems (and then to compute $v(\alpha)$ for large n). For instance, a 3000×3000 SDLS problem is solved in about one hour on a standard computer. Remembering (16), a new way is thus open to compute upper bounds to Boolean quadratic problem via SDLS.

3.3 The instance $\alpha = 0$

It is interesting to note that the value $\alpha=0$ plays here a particular role.

Proposition 3.5 (SDP relaxation). *With notation above, Problem (13) with $\alpha=0$ is exactly the SDP relaxation of (4).*

Proof. Consider Problem (4) written in the form (9). Since the convex hull of a sphere is just the ball of same radius, we convexify the spherical constraint $\|X\|^2 = n^2$ by $\|X\|^2 \leq n^2$. By Lemma 2.1, this latter constraint is redundant with $X \in \mathcal{C}$: we obtain (6) which is the SDP relaxation of (4). To conclude, just observe from (7) and (10) that Problems (6) and (13) with $\alpha = 0$ are identical. \square

Thus replacing the rank-one constraint by the spherical constraint allows an alternative interpretation of SDP relaxation. Let us also point out the particular behavior of v when $\alpha \searrow 0$. First, because the convex function v is continuous, we have

$$\lim_{\alpha \searrow 0} v(\alpha) = v(0).$$

Also the subgradient inequality at α gives the upper bound :

$$v(\alpha) - v(0) \leq \frac{1}{2}(n^2 - \|X(\alpha)\|^2)\alpha. \quad (21)$$

Besides, the limits of $X(\alpha)$ tend to solving (6) :

Lemma 3.6. *The following limit holds:*

$$\forall Y \in \mathcal{C}', \quad \limsup_{\alpha \searrow 0} \langle Y - X(\alpha), Q \rangle \leq 0. \quad (22)$$

It follows that any cluster point of $X(\alpha)$ when $\alpha \searrow 0$ is a solution of (6).

Proof. For $\alpha > 0$, the projection $X(\alpha)$ of Q/α onto \mathcal{C}' is the unique element of \mathcal{C}' such that

$$\forall Y \in \mathcal{C}', \quad \langle Y - X(\alpha), Q/\alpha - X(\alpha) \rangle \leq 0.$$

We can write:

$$\frac{1}{\alpha} \langle Y - X(\alpha), Q \rangle \leq \langle Y - X(\alpha), X(\alpha) \rangle \leq \|Y - X(\alpha)\| \|X(\alpha)\|.$$

Multiplying by $\alpha > 0$ and bounding with Lemma 2.1, we get

$$\langle Y - X(\alpha), Q \rangle \leq 2n^2\alpha.$$

Pass to the limit to get (22). If X^* is cluster point of $X(\alpha)$ then $X^* \in \mathcal{C}'$ is feasible in (6), and (22) shows that it is optimal. \square

4 Duality gap

We show in this section that there is no duality gap between the pair of dual problems (11) and (14). We then generalize the situation to study a class of optimization problems with no duality gap.

4.1 Study of duality gap

We begin with the following observations.

Lemma 4.1. *The following properties hold:*

- (i) $\lim_{\alpha \rightarrow -\infty} v(\alpha) = \text{val}(14)$;
- (ii) *Let $(\alpha_k)_k$ a sequence tending to $-\infty$ and $s_k \in \partial v(\alpha_k)$ for all k , then $\alpha_k s_k \rightarrow 0$ when $k \rightarrow +\infty$.*

Proof. Property (i) is straightforward: v is bounded from below (see (15)) and increasing (see Theorem 3.3). We now prove (ii). In what follows, any limit is implicitly considered for $k \rightarrow +\infty$. Let (α_k) be a sequence tending to $-\infty$, and let $s_k \in \partial v(\alpha_k)$ for all k . Write the subgradient inequality at α_k :

$$\forall \beta \in \mathbb{R}, \quad v(\alpha_k) + s_k(\beta - \alpha_k) \leq v(\beta).$$

At $\beta = 2\alpha_k$, this becomes

$$v(\alpha_k) + 2s_k\alpha_k \leq v(2\alpha_k).$$

Take the limsup in both parts of the inequality to get (with (i))

$$\text{val}(14) + 2 \limsup s_k\alpha_k \leq \text{val}(14).$$

We thus have $\limsup s_k\alpha_k \leq 0$. Now take the subgradient inequality at $\beta = \alpha_k/2$

$$v(\alpha_k) - s_k \frac{\alpha_k}{2} \leq v\left(\frac{\alpha_k}{2}\right).$$

Again take the limsup and obtain (with (i))

$$\text{val}(14) + \limsup \left(-s_k \frac{\alpha_k}{2} \right) \leq \text{val}(14),$$

which becomes

$$\liminf s_k\alpha_k \geq 0.$$

Finally we have

$$\limsup s_k\alpha_k \leq 0 \leq \liminf s_k\alpha_k,$$

we can conclude that $\lim s_k\alpha_k = 0$. □

Theorem 4.2 (No duality gap). *There holds $\text{val}(11) = \text{val}(14)$. In other words, there is no duality gap between the primal problem (11) and its dual (14).*

Proof. First, observe from (15) that there holds

$$\langle Q, X \rangle \leq \text{val}(14), \quad \text{for all } X \in \mathcal{C}' \text{ such that } \|X\|^2 = n^2. \quad (23)$$

Now write for all $\alpha \in \mathbb{R}$ and all $X \in \mathcal{X}(\alpha)$,

$$\langle Q, X \rangle = L(X, \alpha) - \frac{\alpha}{2}(n^2 - \|X\|^2) = v(\alpha) - \frac{\alpha}{2}(n^2 - \|X\|^2). \quad (24)$$

Take $\alpha_k \rightarrow -\infty$ and $X_k \in \mathcal{X}(\alpha_k)$ for all k . From Theorem 3.3, $\frac{1}{2}(n^2 - \|X_k\|^2) \in \partial v(\alpha_k)$. Then with Lemma 4.1(ii), we write

$$\lim_{k \rightarrow +\infty} \langle Q, X_k \rangle = \text{val}(14).$$

Extracting a subsequence if necessary (\mathcal{C}' is compact), we may assume that $(X_k)_k$ has a limit $X \in \mathcal{C}'$. The matrix X satisfies $\|X\|^2 = n^2$, and then X achieves the equality in (23). Thus, there is no duality gap. □

Furthermore we can specify when there exists a couple (X_0, α_0) of primal-dual solutions : this is exactly when the minimum of v is attained on \mathbb{R} (see Corollary 4.5 below). The proof of this result is not difficult, but it is worth mentioning that it actually enjoys a nice generalization, presented in the next subsection.

4.2 A class of problems with no duality gap

In this subsection, we generalize the framework of the paper to reveal a class of problems with no duality gap. We end by showing that this class formalizes in particular the so-called semi-Lagrangian relaxation.

Following the notation of [HUL93, Chap.XII], we consider the primal problem

$$\begin{cases} \sup & f(u) \\ & u \in U \\ & c(u) = 0. \end{cases} \quad (25)$$

with the objective function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, the control set $U \subset \mathbb{R}^n$ and the constraint function $c : U \rightarrow \mathbb{R}^m$ that is to be dualized. The Lagrangian function related to the optimization problem (25) is, for $u \in U$ and $\lambda \in \mathbb{R}^m$,

$$\mathcal{L}(u, \lambda) = f(u) - \lambda^\top c(u).$$

The convex dual function is then

$$\theta(\lambda) = \sup\{\mathcal{L}(u, \lambda), \quad u \in U\}, \quad (26)$$

and the dual problem of (25) is

$$\inf_{\lambda \in \mathbb{R}^m} \sup_{u \in U} \mathcal{L}(u, \lambda). \quad (27)$$

For all $\lambda \in \mathbb{R}^m$ and for all $u \in U$ such that $c(u) = 0$, there holds

$$f(u) \leq \theta(\lambda). \quad (28)$$

Let us also introduce the optimal set associated to (26)

$$U(\lambda) = \{u \in U, \quad \mathcal{L}(u, \lambda) = \theta(\lambda)\}.$$

Example 4.3 (Boolean quadratic problems). *If the objective function is $f(\cdot) = \langle Q, \cdot \rangle$, the control set $U = \mathcal{C}' \subset \mathcal{S}_n$ and the dualized constraint $c(\cdot) = (\|\cdot\|^2 - n^2)/2$, we retrieve the situation of the paper. The dual function with respect to $\alpha \in \mathbb{R}$ is the function v and the optimal set is $U(\lambda) = \mathcal{X}(\alpha)$.*

It is well-known (see e.g. [ET99, Prop.VI.2.3]) that there is no duality gap if U is convex and compact and $\mathcal{L}(\cdot, \lambda)$ is concave, for all $\lambda \in \mathbb{R}^m$. However, in the situation of the paper for instance, $\mathcal{L}(\cdot, \lambda)$ is not concave, and there may be a duality gap. The following result proves that this is actually not the case if U belongs to $\{u \in \mathbb{R}^n : c(u) \leq 0\}$ (where $y \leq 0$ means the property that each entry of $y \in \mathbb{R}^m$ is non-positive).

Theorem 4.4 (No duality gap). *With the notation above, assume that there exists a solution λ^* of the dual problem (14) and that the so-called filling property holds at λ^* :*

$$\partial\theta(\lambda^*) = \text{conv}\{-c(u), \quad u \in U(\lambda^*)\}. \quad (29)$$

If for all $u \in U$ there holds $c(u) \leq 0$, then there is no duality gap : $\text{val}(25) = \text{val}(27)$. Besides, there exists a couple (u, λ^) of primal-dual solutions satisfying*

$$c(u) = 0 \quad \text{and} \quad \text{val}(25) = f(u) = \theta(\lambda^*) = \text{val}(27).$$

Proof. Since θ is convex and λ^* is a minimizer of θ on \mathbb{R}^m , we have $0 \in \partial\theta(\lambda^*)$. The filling property (29) then implies that there exist

- (i) $(\alpha_0, \dots, \alpha_m) \in [0, 1]^{m+1}$ such that $\sum_{i=0}^m \alpha_i = 1$,
- (ii) $(u_0, \dots, u_m) \in \mathbb{R}^{m+1}$ such that $u_i \in U(\lambda^*)$,

satisfying

$$0 = \sum_{i=0}^m \alpha_i c(u_i).$$

Since $c(u_i) \leq 0$ and $\alpha_i \in [0, 1]$, this equality yields $c(u_i) = 0$. The couple (u_0, λ^*) for instance reaches the equality in (28) : since $u_0 \in U(\lambda^*)$, there holds

$$f(u_0) = f(u_0) - (\lambda^*)^\top c(u_0) = \mathcal{L}(u_0, \lambda^*) = \theta(\lambda^*).$$

We can conclude that (u_0, λ^*) is a primal-dual couple of solutions and that there is no duality gap. \square

In the situation of the paper, this theorem gives the following corollary.

Corollary 4.5. *The following statements are equivalent:*

- (i) v achieves its minimum at $\alpha_0 \in \mathbb{R}$,
- (ii) there exists $(X_0, \alpha_0) \in \mathcal{X}(\alpha_0) \times \mathbb{R}$ such that $v(\alpha_0) = \langle Q, X_0 \rangle$ and $\|X_0\|^2 = n^2$,
- (iii) there exists a rank-one X_0 in $\mathcal{X}(\alpha_0)$.

Proof. (i) \Rightarrow (ii). Remembering Example 4.3, observe that the filling property (29) holds for the dual function v (Theorem 3.3). Note also that for all $X \in \mathcal{C}'$, we have $c(X) = (\|X\|^2 - n^2)/2 \leq 0$, by Lemma 2.1. The implication is thus Theorem 4.4.

(ii) \Rightarrow (iii). Straightforward with Theorem 2.3.

(iii) \Rightarrow (i). Property (ii) combined with Theorem 2.3 and (18) yields that $0 \in \partial v(\alpha_0)$ and then (i) follows. \square

Note a particular feature of this situation : if (X_0, α_0) is a primal-dual solution, any couple (X, α) such that $\alpha < \alpha_0$ and $X \in \mathcal{X}(\alpha)$ is also a primal-dual solution.

Remark 4.6 (Re-enforcing constraints and “semi-Lagrangian duality”). *A fruitful idea in combinatorial optimization is to introduce redundant constraints, providing more precise relaxations and then smaller duality gaps. In view of Theorem 4.4, it could be interesting to re-express Problem (25) into*

$$\begin{cases} \sup & f(u) \\ u \in & U', \\ c(u) = & 0. \end{cases} \quad \text{with} \quad U' = U \cap \{u \in \mathbb{R}^n : c(u) \leq 0\}. \quad (30)$$

The standard Lagrangian duality theory applied to (25) formalizes actually the semi-Lagrangian relaxation, introduced in [BTV04] in a particular case. The main result then comes from Theorem 4.4: If the filling property holds and if the dual problems of (30) has an optimal solution, the semi-Lagrangian relaxation closes the duality gap.

The situation of [BTV04] is the following: f is linear ($f(u) = c^\top u$), $U = \mathcal{X} \cap \mathbb{N}^$ where \mathcal{X} is a cone and c is affine ($c(u) = Au - b$) with A, b, c having nonnegative entries. Notice that the dual function is polyhedral and that $U \cap \{Au \leq b\}$ is finite (therefore the filling property (29) holds - see [HUL93, XII.2.3.2]). Theorem 4.4 is thus a generalization of Theorem 1 of [BTV04].*

5 Conclusion

We have proposed a new relaxation scheme in the same spirit as the SDP one and which sheds new light on it. The key property is to express the rank-one constraint as a quadratic constraint in \mathcal{S}_n , which we call the spherical constraint. Dualizing the spherical constraint is also the occasion to reveal a class of optimization problems with no duality gap.

Thus each value of the dual function v is an upper bound of the optimal value of the primal problem (11). In practice, the value $v(0)$ can be obtained by SDP interior points methods (recall Proposition 3.5). If $\alpha < 0$, the value $v(\alpha)$ is unreachable : the computation of $v(\alpha)$ amounts to minimizing a concave quadratic function which is a NP hard problem. On the other hand, by Theorem 3.2, the value $v(\alpha)$ when $\alpha > 0$ can be efficiently computed. Admittedly, this approach deteriorates the SDP bound since $v(\alpha) \geq v(0)$. However, this shortcoming is balanced by some numerical advantages:

- The solution of (19) is unique. Furthermore this solution is stable under perturbations of the matrix Q (Theorem 3.2) and tends to a solution of (6) when α tends to 0 (Lemma 3.6).
- An SDLS problem can be more efficiently solved than a SDP one of the same size. The reason is that its dual problem is more structured than the dual of (6), see [Mal04].

“Good” upper bounds are those for which a trade-off is reached between pertinence and speed of computation. For instance, SDP relaxation often gives better bounds than linear relaxation, but the technology to solve linear programs is today more efficient. Thus, in practice (inside a branch and bound method for instance), it is often more interesting to use linear relaxations schemes.

The approach of the paper is motivated, in a numerical point of view, by the performances of SDLS solver (see [Mal04] and [Rai]). This paper thus opens the way to applications of SDLS technology in combinatorics to address large quadratic Boolean problems.

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