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The spherical constraint in Boolean quadratic programs

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Abstract We propose a new approach to bound Boolean quadratic optimization problems. The idea is to re-express the Boolean constraints as one "spherical" constraint, whose dualization amounts to semidefinite least-squares problems. Studying this dualization provides an alternative interpretation of the SDP relaxation. It also reveals a new class of non-convex problems with no duality gap.

Keywords SDP relaxation · Combinatorial optimization · Lagrangian duality · Convex analysis

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 a 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 [23,30]. Striking examples in combinatorial optimization are max-cut and max-clique [11,24].

This paper considers the problems of finding tight bounds for Boolean quadratic optimization problems. Using Lagrangian duality (as a mechanism to create bounds, see Ref. [22]), we consider a Boolean quadratic problem and introduce a convex function $v : \mathbb{R} \to \mathbb{R}$ where each value $v(\alpha)$ is a bound of the Boolean problem. We study the theoretical properties of this dualization, and in particular we show that $v(\alpha)$ tends to the optimal value when α tends to $-\infty$. The key is to use a new expression of the rank one-constraint that appears in the SDP formulation of Boolean quadratic problems.

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We start by introducing our notation, defining Boolean quadratic problems and recalling the lifting into $\mathcal{S}_n$ (Sects. 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 (Sect. 2.1). This re-expression allows an alternative interpretation of the SDP relaxation (Sect. 3). Lagrangian duality then reveals the absence of duality gap when dualizing this spherical constraint (Sect. 4). Unfortunately, this favorable result is theoretical only, since the dual optimal value is not computable in practice (Sect. 3). On the other hand, dualizing the spherical constraint is the occasion to point out a class of optimization problems with no duality gap (Sect. 4.1), which sheds new light on the idea of Semi-Lagrangian introduced in Ref. [7] (Sect. 4.3).

1.1 Boolean quadratic problems

Consider the $m + 1$ quadratic functions defined on $\mathbb{R}^n$:

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

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

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

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

Boolean quadratic problems appear in practice in a wide variety of applications—in financial analysis [27] or medicine [29] for example. Most of the algorithms to solve exactly the Boolean quadratic problems are of branch-and-bound type; the bounding procedure and the prunning strategy are then the two most important aspects (see Refs. [14,15] for example). We focus here only on the first aspect—bounding—and more specifically on bounding procedures based on semidefinite programming [33] after lifting in the space of symmetric matrices (as recalled in the next subsection).

In this paper, we make the following assumption: we 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., Ref. [28]) 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 the simplified form of (1) (with $Q = Q_0$)

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

Example 1 (Max-cut) Given a undirected graph with weights on the edges, the max-cut problem consists in finding a partition of the set of vertices into two parts that maximizes the sum of the weights that have one end in each part of the partition. Even if some special cases can be solved efficiently, the max-cut problem is a NP-complete problem in general [19]. This problem can be written as

$$\begin{cases} \max x^\top Qx \\ x_i \in \{-1, 1\}, \quad i = 1, \dots, n, \end{cases} \tag{3}$$

that is, as a instance of (2) with Boolean constraints only (see [6, Chap. 4, 10], among others). Note that $-Q_{ij}$ is the weight of the arc joining the vertex i and j. □

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 $\langle A, B\rangle = \operatorname{trace}(AB) = \sum_{i=1}^n A_{ij}B_{ij}$. The reason it is so convenient for our purposes is the following relation:

$$\forall x \in \mathbb{R}^n, \quad \forall A \in \mathcal{S}_n, \qquad x^\top A\, x = \langle A, xx^\top\rangle. \tag{4}$$

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 $\|x\|^2 = x^\top x$.) Thus there holds

$$\|X\|^2 = \operatorname{trace}(X^2) = \sum_{i=1}^n [\lambda_i(X)]^2 = \|\lambda(X)\|^2, \tag{5}$$

where $\lambda(X) = (\lambda_1(X), \dots, \lambda_n(X)) \in \mathbb{R}^n$ stands for the vector of eigenvalues of X. We will also consider the trace norm [13]

$$\|X\|_{\text{tr}} = \sum_{i=1}^n |\lambda_i(X)| = \|\lambda(X)\|_1, \tag{6}$$

where $\|x\|_1 = \sum |x_i|$ is the standard ℓ_1 norm on $\mathbb{R}^n$.

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 stand for the vector of $\mathbb{R}^n$ with all entries equal to 1 ($e = [1, \dots, 1]^\top$). Via (4), the quadratic functions of (2) are re-expressed as $\langle Q_j, X\rangle$ where we have set $X = xx^\top$. Observe that ${x_i}^2 = 1$ ($i = 1, \dots, n$) means $\operatorname{diag}(X) = e$. Problem (2) is therefore equivalently written as

$$\begin{cases} \max \langle Q, X\rangle \\ \langle Q_j, X\rangle \geq 0, \quad j = 1, \dots, m \\ \operatorname{diag}(X) = e, \\ X = xx^\top. \end{cases} \tag{7}$$

Example 2 (Max-cut) For instance, the max-cut problem (3) can be written

$$\begin{cases} \max \langle Q, X\rangle \\ \operatorname{diag}(X) = e, \\ X = xx^\top, \end{cases} \tag{8}$$

that is, as a semidefinite problem with the rank-one constraint. □

Remark 1 (Higher-order liftings) A family of semidefinite programming relaxations corresponding to lifting the problem into higher and higher dimensional matrix spaces was recently introduced (see [20,21]). We just consider the simple lifting in this paper to stay as simple as possible. However the material can be easily adapted to treat general liftings. □

The difficulty is now concentrated in the rank constraint $X = xx^\top$ which is not convex. A classical tool to find upper bounds to (8) and more generally to (7) is the SDP relaxation (see [30] for instance). 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 (7) is therefore

$$\begin{cases} \max \langle Q, X\rangle \\ \langle Q_j, X\rangle \geq 0, \quad j = 1, \ldots, m \\ \operatorname{diag}(X) = e \\ X \succeq 0. \end{cases} \tag{9}$$

We give in Proposition 1 an alternative interpretation to the SDP relaxation.

2 The spherical constraint and its dualization

2.1 Correlation matrices and the spherical constraint

We consider the set of so-called correlation matrices, appearing in (7)

$$\mathcal{C} = \{X \in \mathcal{S}_n : \ X \succeq 0, \ \operatorname{diag}(X) = e\}. \tag{10}$$

Correlation matrices are important objects in statistics to express relations between random variables. Note first that $\mathcal{C}$ is the intersection of the closed convex cone of SDP matrices and the affine subspace $\operatorname{diag}(X) = e$; and thus $\mathcal{C}$ is a closed convex subset of $\mathcal{S}_n$. Furthermore it is bounded and we know a tight bound, reached if and only if the matrix is rank-one. This is the content of the following easy result—which can be seen as a corollary of [1, Theorem 2.2] or a consequence of an extension of the so-called Samuelson Inequality [37, (1.4)]. We include here a simple geometric proof based on the comparison between the ℓ_1 and ℓ_2 norms.

Theorem 1 (A characterization of rank-one matrices of $\mathcal{C}$). *Let $X \in \mathcal{C}$. Then we have $\|X\| \leq n$ and the following equivalence holds:*

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

Proof For $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$, it is classical (and easily proved, by recurrence for instance) that

$$\|x\| = \sqrt{\sum {x_i}^2} \leq \sum |x_i| = \|x\|_1$$

with equality if and only if there is at most one non-zero x_i. Applying this property to $x = \lambda(X)$, we obtain for $X \in \mathcal{S}_n$ that $\|X\| \leq \|X\|_{\text{tr}}$ with equality if and only if X has rank at most 1.

Let $X \in \mathcal{C}$. Since $X \succeq 0$, we have $\|X\|_{\text{tr}} = \operatorname{trace}(X)$. Moreover, $\operatorname{diag}(X) = e$ implies $\|X\|_{\text{tr}} = n$. Since $X \neq 0$, we thus obtain the desired result. □

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 $\|X\| = n$ the *spherical constraint*. In view of the next developments, we prefer to replace it by $\|X\|^2 = n^2$.

2.2 Dualization of the spherical constraint

We can reformulate Problem (7) with the help of Theorem 1. The constraint $X = xx^\top$ exactly expresses that the symmetric matrix X is rank-one. Then (7) can be written as

$$\begin{cases} \max \langle Q, X\rangle \\ \langle Q_j, X\rangle \geq 0, \quad j = 1, \ldots, m \\ X \in \mathcal{C}, \\ \|X\|^2 = n^2. \end{cases} \tag{11}$$

Observe that we have transformed the Boolean quadratic problem (2) to Problem (11) which has only one quadratic constraint with respect to the variable $X \in \mathcal{S}_n$. To isolate this constraint, we set

$$\mathcal{C}' = \mathcal{C} \cap \{X \in \mathcal{S}_n : \langle Q_j, X\rangle \geq 0 \text{ for all } j = 1, \ldots, m\}. \tag{12}$$

Obviously, $\mathcal{C}'$ is a convex compact subset of $\mathcal{S}_n$ (recall Theorem 1). Problem (11) can be rewritten

$$\begin{cases} \max \langle Q, X\rangle \\ X \in \mathcal{C}', \\ \|X\|^2 = n^2. \end{cases} \tag{13}$$

The difficulties are now concentrated into the nonconvex constraint $\|X\|^2 = n^2$. Taking advantage of this new formulation, we now study the dualization of the constraint $\|X\|^2 = n^2$. This study will end with the property that there is no duality gap for the dualization of this nonconvex constraint (Corollaries 1 and 2); on this point, the compacity of $\mathcal{C}'$ plays an important role. So now we introduce the dual problem, and then formalize the properties of dual objects (in Sect. 2.3), discuss the computation of dual values (in Sect. 3), to take eventually a closer look to the duality gap (in Sect. 4).

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

$$L(X, \alpha) = \langle Q, X\rangle - \frac{\alpha}{2}(\|X\|^2 - n^2). \tag{14}$$

We define the dual function

$$v(\alpha) = \sup_{X \in \mathcal{C}'} L(X, \alpha). \tag{15}$$

The dual problem of (13) is then

$$\begin{cases} \inf v(\alpha) \\ \alpha \in \mathbb{R}. \end{cases} \tag{16}$$

As usual, each value of the primal function gives a lower bound of the dual function (weak duality—see [17, Chap. XII]):

$$\forall X \in \mathcal{C}', \|X\|^2 = n^2, \ \forall \alpha \in \mathbb{R}, \qquad \langle Q, X\rangle = L(X, \alpha) \leq v(\alpha). \tag{17}$$

Therefore, we have, for all $\alpha \in \mathbb{R}$

$$\text{val}(13) \leq \text{val}(16) \leq v(\alpha). \tag{18}$$

2.3 Properties of dual objects

Consider, for $\alpha \in \mathbb{R}$, the set of solutions of (15), that is

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

Lemma 1 ($\mathcal{X}(\alpha)$ and $X(\alpha)$). *Let $\alpha \in \mathbb{R}$. Then the supremum in (15) is attained: there is an $X \in \mathcal{C}'$ 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. □

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 directly an interesting feature: $X(\alpha)$ is stable under small perturbations on Q; more precisely, it is Lipschitz with respect to Q.

Theorem 2 (Projection) *For $\alpha > 0$, we denote in this result by $X(\alpha, Q)$ the solution of (15). 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

$$L(X, \alpha) = \left(\frac{\alpha}{2}n^2 + \frac{1}{2\alpha}\|Q\|^2\right) - \frac{\alpha}{2}\left\|X - \frac{Q}{\alpha}\right\|^2. \tag{19}$$

For $\alpha > 0$, maximizing $L(\cdot, \alpha)$ on $\mathcal{C}'$ thus amounts to minimizing $\|\cdot - Q/\alpha\|^2$ on $\mathcal{C}'$. By [18, Prop.A.3.1.3], $X(\alpha, Q)$ is $1/\alpha$-Lipschitzian with respect to Q. □

Theorem 3 (Dual function) *The function v defined by (15) is closed, convex and non-decreasing on $\mathbb{R}$. Its subdifferential at $\alpha \in \mathbb{R}$ is*

$$\partial v(\alpha) = \operatorname{conv}\left\{\frac{1}{2}(n^2 - \|X\|^2) : X \in \mathcal{X}(\alpha)\right\}, \tag{20}$$

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

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

Proof Being the supremum of the family of affine functions $L(X, \cdot)$ (indexed in $\mathcal{C}'$), v is a closed convex function on $\mathbb{R}$. Since $\mathcal{C}'$ is compact, we apply [18, Th.D.4.4.2] to get (20). Theorem 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 1 implies that $\partial v(\alpha)$ is reduced to $\{\frac{1}{2}(n^2 - \|X(\alpha)\|^2)\}$, and [18, Cor.D.2.1.4] guarantees the differentiability of v, with $v'(\alpha) = \frac{1}{2}(n^2 - \|X(\alpha)\|^2)$. □

3 Computation of dual function

Remembering (18), each value of the dual function gives an upper bound of val(13). According to the values of α, the computation of $v(\alpha)$ is fundamentally different whether α is null, positive or negative.

The instance $\alpha = 0$

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

Proposition 1 (SDP relaxation). *With notation above, Problem (15) with $\alpha = 0$ is exactly the* SDP *relaxation of (7).*

Proof Consider Problem (7) written in the form (11). 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 Theorem 1, this latter constraint is redundant with $X \in \mathcal{C}$: we obtain (9) which is the SDP relaxation of (7). To conclude, just observe from (10) and (12) that Problems (9) and (15) with $\alpha = 0$ are identical. □

Thus replacing the rank-one constraint by the spherical constraint allows an alternative interpretation of the SDP relaxation. In a way, (15) generalizes the SDP relaxation. Besides, the value $v(0)$ can be obtained by any SDP solver, in particular SDP interior points methods (see the reference book [33]), as well as spectral bundle methods [16] or low rank methods [3].

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:

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

Besides, the limits of $X(\alpha)$ tend to solving (9).

Lemma 2 *The following limit holds:*

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

It follows that any cluster point of $X(\alpha)$ when $\alpha \searrow 0$ is a solution of (9).

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

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

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 Theorem 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 (9), and (22) shows that it is optimal. □

Thus a solution of the linear SDP problem (9) could be approached by some $X(\alpha)$ which are ad hoc projections. This can be related to the idea of changing a linear program by parametric quadratic programs, which has appeared in the literature in [26,34] for instance.

The case $\alpha > 0$

By Theorem 2 and (19), computing $v(\alpha)$ when $\alpha > 0$ amounts to solving

$$m(\alpha) = \min_{X\in\mathcal{C}'} \|X - Q/\alpha\|^2 \tag{23}$$

and setting

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

Example 3 (Max-cut) For the particular case of Problem (8), the computation of the minimum value of

$$\begin{cases} \min \|X - Q/\alpha\|^2 \\ \operatorname{diag}(X) = e, \\ X \succeq 0 \end{cases} \tag{24}$$

gives the value $v(\alpha)$ for $\alpha > 0$. □

Problem (24) and more generally (23) are actually so-called semidefinite (constrained) 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 $\langle Q_j, X\rangle \geq 0$ and an affine subspace $\operatorname{diag}(X) = e$ (recall Expressions (10) and (12)).

Recently several algorithms have been proposed to solve SDLS problems [12,25,31,35,36]. In particular, the dual algorithm proposed in [25] has been shown to be efficient, even to solve large SDLS problems (and then to compute $v(\alpha)$ for large n). For instance, 100×100 SDLS problems (with data entries randomly generated in $[-1, 1]$) are solved instantly at the precision 10^{-7}. Similar 3000×3000 SDLS problems are solved in about one hour (on a standard computer). Regarding numerical results, we refer to [25, Sect. 5]. (The recent work [31] shows even better numerical resuls for a particular class of SDLS problems.) This seems to open a new way to compute upper bounds to large Boolean quadratic problems via SDLS. In view of the growing performances of SDLS solvers, this approach might be interesting to replace SDP solvers for some particular Boolean problems. However, a complete comparison between the SDLS bounds and the SDP bounds still has to be conducted. This comparison should involve accuracy and speed of computation between the different algorithms for SDLS and for SDP (see references above) on this particular problem of bounding Boolean quadratic problems. This is beyond the scope of this paper and we differ this for future research.

Note an important feature however: because v is non-decreasing (Theorem 3), we have $v(\alpha) \geq v(0)$ for $\alpha > 0$. In other words, the SDP relaxation always gives more accurate bounds than the ones computed by SDLS.

We present below a preliminary experiment to give a rough comparison between SDLS and SDP bounds. We consider a max-cut problem (24) with randomly generated 0-1 weights matrix (with 70% of 1) of size 500×500. We compute $v(\alpha)$ via solving (23) for different

Table 1 Computation of bounds $v(\alpha)$ for random max-cut of size 500×500

α	`Error`	`Iters`	`Time`
1	94%	9	28
0.1	52%	16	53
0.01	10%	33	106
0.001	1%	89	275

values of α using a primitive implementation of the algorithm of Ref. [25] and with the stopping test $\|\mathrm{diag}(X) - e\| \leq 10^{-6}$. Simulations were run on an Intel P4 3.2 Ghz processor machine using the MATLAB-like free software SCILAB [32]. The results are collected in Table 1 which shows:

- `iters`, the number of iterations of the prototype of the algorithm of Ref. [25];
- `time`, the cputime (in seconds);
- `error`, the "a posteriori" majoration (21) of the relative difference between the bound $v(\alpha)$ and the SDP bound $v(0)$:

$$0 \leq \frac{v(\alpha) - v(0)}{|v(\alpha)|} \leq \frac{(n^2 - \|X(\alpha)\|^2)\alpha}{2|v(\alpha)|} = \mathtt{error}.$$

We observe that the relative difference between $v(\alpha)$ and the SDP bound is less than 1% when taking $\alpha = 0.001$. Note also that when α tends to 0, the SDLS problem becomes more difficult. This is an expected phenomenon in view of the numerical simulations of Ref. [25, 5.3.2].

The case $\alpha < 0$

If $\alpha < 0$, the value $v(\alpha)$ is unreachable: the computation of $v(\alpha)$ amounts to minimizing a concave quadratic function (see (14) and (15)), which is a NP hard problem in general. Despite this negative observation, the present approach has some theoretical value, as shown in the next section.

4 Duality gap

We show in this section that there is no duality gap between the pair of dual problems (13) and (16) (see Sect. 4.2). We begin with generalizing the framework of the paper to reveal an interesting class of problems with no duality gap (Sect. 4.1). We end by showing that this class formalizes in particular the so-called semi-Lagrangian relaxation of [7] (Sect. 4.3).

4.1 A class of problems with no duality gap

In this subsection, we go up to a more general context to study a class of problems with no duality gap. Following the notation of [19, Chap.XII], we consider the primal problem

$$\begin{cases} \sup f(u) \\ u \in U, \\ c(u) = 0 \end{cases} \tag{25}$$

with the objective function f: $\mathbb{R}^n \to \mathbb{R}$, the control set $U \subset \mathbb{R}^n$ and the constraint function c: $U \to \mathbb{R}^m$ that is to be dualized. We denote the m components of c by c_i: $U \to \mathbb{R}$ (for

$i = 1, \dots, m$). To emphasize the key arguments, we stick to the general framework of [19, Chap.XII], making as few assumptions as possible: we just assume for the sequel that f and c are continuous and that the feasible set $U \cap c^{-1}(\{0\})$ is non-empty.

The Lagrangian function related to the optimization problem (25) is, for the primal variable $u \in U$ and the dual variable $\lambda \in \mathbb{R}^m$,

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

The convex dual function is then

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

and the dual problem of (25) is

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

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

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

Example 4 (Boolean quadratic problems) If the objective is $f(\cdot) = \langle Q, \cdot \rangle$, as a function of the primal variable $u = X \in \mathcal{S}_n$, if the control set is $U = \mathcal{C}' \subset \mathcal{S}_n$ and if the dualized constraint is $c(\cdot) = (\|\cdot\|^2 - n^2)/2$, we retrieve the situation of the paper. The lagrangian with respect to $\lambda = \alpha \in \mathbb{R}$ is

$$\mathscr{L}(u, \lambda) = L(X, \alpha) = \langle Q, X \rangle - \frac{\alpha}{2}(\|X\|^2 - n^2),$$

the dual function is v and the optimal set is $U(\lambda) = \mathcal{X}(\alpha) \neq \varnothing$. □

It is well-known (see [8, Prop.VI.2.3] for instance) that there is no duality gap between (25) and (27) if U is convex and compact and $\mathscr{L}(\cdot, \lambda)$ is concave, for all $\lambda \in \mathbb{R}^m$. Otherwise non-convexities usually introduce a duality gap. In the situation of Example 4 for instance, $\mathscr{L}(\cdot, \lambda)$ is not concave, and there may be a duality gap.

However, the folowing "unilateral property"

$$c(u) \leq 0, \quad \text{for all } u \in U \tag{28}$$

(where $y \leq 0$ means that each entry of $y \in \mathbb{R}^m$ is non-positive) is able to cancel the duality gap even in the non-convex case.

Theorem 4 (No gap under dual assumption) *With the notation above, we assume that there exists a dual solution $\lambda^\star \in \mathbb{R}^m$, that $U(\lambda^\star) \neq \varnothing$, and that the so-called filling property holds [17, Chap. XII]:*

$$\partial\theta(\lambda^\star) = \operatorname{conv}\left\{-c(u), \quad u \in U(\lambda^\star)\right\}.$$

If (28) holds, then there is no duality gap and, in addition, there exists a couple $(u^\star, \lambda^\star)$ of primal-dual solutions satisfying

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

Proof Convexity yields $0 \in \partial\theta(\lambda^\star)$. By Carateodory's Theorem (see [18, Theorem 1.3.6] for instance), the filling property then implies that there exist

(i) $\alpha_0, \dots, \alpha_m \geq 0$ such that $\sum_{i=0}^m \alpha_i = 1$,

(ii) $u_0, \dots, u_m \in U(\lambda^\star)$,

satisfying

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

Since $c(u_i) \leq 0$ and $\alpha_i \geq 0$, this equality guarantees that $\alpha_i\, c(u_i) = 0$ for $i = 0, \dots, m$. There is (at least) one nonzero α_i, call it α_0. Therefore we have $c(u_0) = 0$, and this yields

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

The result follows from weak duality: $(u^\star = u_0, \lambda^\star)$ is a primal-dual couple of solutions and there is no duality gap. □

The proof of this result, though simple, calls for rather advanced concepts of convex analysis. It also requires the existence of a dual solution, which we cannot gaurantee without further assumptions. It is thus interesting to look at this no-duality-gap result from another point of view. Since, the $c_i(u)$ are non-positive, observe that for any $\lambda \in \mathbb{R}^m$

$$\theta(\lambda) = \max_{u \in U}\; f(u) - \sum_{i=1}^{n} \lambda_i c_i(u) = \max_{u \in U} f(u) - \sum_{i=1}^{n} (-\lambda_i) \max\{-c_i(u), 0\}.$$

Evaluated at $\lambda_\mu = (-\mu, \dots, -\mu)$ (with $\mu \in \mathbb{R}_+$), this becomes

$$\theta(\lambda_\mu) = \max_{u \in U} f(u) - \mu \sum_{i=1}^{n} \max\{-c_i(u), 0\}.$$

which clearly reveals a penalty function. From the standard penalty point of view, it turns out that the same tightness property also holds under a primal assumption.

Theorem 5 (No gap under primal assumption) *Assume that there exists for all $\mu > 0$ a solution $u_\mu \in U$ to the problem to maximize the function $f(u) - \mu \sum_{i=1}^{n} \max\{-c_i(u), 0\}$ subject to $u \in U$, and that $\{u_\mu\}$ is contained in a compact subset of U. If (28) holds, then there is no duality gap:* val(25) = val(27).

Proof Note that weak duality yields

$$\text{val}(25) \leq \text{val}(27) = \inf_{\lambda \in \mathbb{R}^m} \theta(\lambda) \leq \inf_{\mu \geq 0} \theta(\lambda_\mu). \tag{29}$$

The assumption of the theorem is meant to apply [5, Theorem 9.2.2], which gives

$$\inf_{\mu \geq 0} \theta(\lambda_\mu) = \lim_{\mu \to +\infty} \theta(\lambda_\mu) = \max_{c(u) \geq 0, u \in U} f(u).$$

From the unilaterality property (28), the last term is exactly val(25). Combining with (29), the result follows. □

From the penalisation point of view, this no-gap result for our nonconvex problem is less surprising. Note also that the assumptions of these two theorems, though different in nature, are quasi equivalent and correspond essentially to a sort of compactness, sufficient to get the filling property [17, XII.2.3.2] or to ensure the tightness of penalisation [5, 9.2.2].

The main difference in these two theorems is the existence of a dual solution which ensures in Theorem 4 the existence of primal solution as well. There is no corresponding assumption in Theorem 5; by contrast, the compactness assumption, ensuring the tightness of the penalization, is not sufficient to ensure the existence of a dual solution. We would need furthermore a Slater constraint qualification in Theorem 5 to get the existence of a dual solution [2, 4.3.7] together with the exactness of the penalisation [9, 14.3].

4.2 Case of spherical constraint

The situation studied in this paper follows the same pattern (recall Example 4). Thus Theorem 5 gives the abscence of gap when dualizing the spherical constraint.

Corollary 1 (No duality gap) *There holds* $\mathrm{val}(13) = \mathrm{val}(16)$. *In other words, there is no duality gap between the primal problem (13) and its dual (16). In fact,*

$$\lim_{\alpha\to-\infty} v(\alpha) = \mathrm{val}(13).$$

Proof Theorem 1 yields that the closed set $\mathcal{C}'$ is bounded and more precisely that $c(X) = \frac{1}{2}(\|X\|^2 - n^2) \le 0$ for all $X \in \mathcal{C}'$. Theorem 5 yields that there is no duality gap. Since v is bounded from below (see (17)) and increasing (see Theorem 3), we obtain that v tends to $\mathrm{val}(16) = \mathrm{val}(13)$ when $\alpha \to -\infty$. This also comes from the proof of Theorem 5. □

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 $\mathbb{R}$.

Corollary 2 (Primal-dual solution) *The three 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, observe that the filling property holds for the dual function v (Theorem 3). Note also that for all $X \in \mathcal{C}'$, we have $c(X) = (\|X\|^2 - n^2)/2 \le 0$, by Theorem 1. This implication is thus Theorem 4.
$(ii) \Rightarrow (iii)$. Straightforward with Theorem 1.
$(iii) \Rightarrow (i)$. Property (iii) combined with Theorem 1 and (20) yields that $0 \in \partial v(\alpha_0)$ and then (i) follows. □

4.3 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. We consider in this section the re-enforcement of the general problem (25) consisting in adding the contraint $c(u) \le 0$. In others words, we replace (25) by the equivalent problem

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

Dualizing (30) amounts to minimizing the re-enforced dual function

$$\theta'(\lambda) = \sup_{u\in U'} \mathscr{L}(u, \lambda). \tag{31}$$

Clearly enough, Theorem 4 guarantees that

$$\min \theta'(\lambda) = \mathrm{val}(30),$$

if θ' attains its minimum at some $\lambda^\star$ satisfying the filling property.

Minimizing (31) instead of (26) is precisely the approach of [7] (see also the recent [4]) in the following situation: 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 non-negative entries. Notice that the dual function is polyhedral and that $U \cap \{Au \leq b\}$ is finite (therefore the filling property holds—see [17, XII.2.3.2]). Theorem 4 is thus a generalization of Theorem 1 of [7]. Thus the standard Lagrangian duality theory applied to (30) formalizes the semi-Lagrangian approach.

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.

"Good" upper bounds are those for which a trade-off is reached between accuracy 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 sometimes more interesting to use linear relaxation schemes.

Similarly, our proposal deteriorates the SDP bound, while it might take advantage of the performances of SDLS solvers. Besides, the solution of (23) is unique, stable under perturbations of the matrix Q (Theorem 2), and approaches a solution of (9) (Lemma 2).

The main contribution of the paper is perhaps theoretical: we concentrate the whole difficulty of Boolean quadratic problems into the single "nice-looking" spherical constraint, establishing one more link between combinatorial and non-linear optimization.

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