Low-rank optimization for semidefinite convex problems*

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Abstract

We propose an algorithm for solving nonlinear convex programs defined in terms of a symmetric positive semidefinite matrix variable X. This algorithm rests on the factorization $X = YY^T$, where the number of columns of Y fixes the rank of X. It is thus very effective for solving programs that have a low rank solution. The factorization $X = YY^T$ evokes a reformulation of the original problem as an optimization on a particular quotient manifold. The present paper discusses the geometry of that manifold and derives a second order optimization method. It furthermore provides some conditions on the rank of the factorization to ensure equivalence with the original problem. The efficiency of the proposed algorithm is illustrated on two applications: the maximal cut of a graph and the sparse principal component analysis problem.

1 Introduction

Many combinatorial optimization problems can be relaxed into a convex program. These relaxations are mainly introduced as a tool to obtain lower and upper bounds on the problem of interest. The relaxed solutions provide approximate solutions to the original program. Even when the relaxation is convex, computing its solution might be a demanding task in the case of large-scale problems. In fact, most convex relaxations of combinatorial problems consist in expanding the dimension of the search space by optimizing over a symmetric positive semidefinite matrix variable of the size of the original problem. Fortunately, in many cases, the relaxation is tight once its solution is rank one, and it is expected that the convex

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relaxation, defined in terms of a matrix variable that is likely to be very large, presents a low-rank solution. This property can be exploited to make a direct solution of the convex problem feasible in large-scale problems.

The present paper focuses on the convex optimization problem,

$$\min_{X \in \mathbb{S}^n} f(X)$$
s.t.
$$\operatorname{Tr}(A_i X) = b_i, \ A_i \in \mathbb{S}^n, b_i \in \mathbb{R}, \ i = 1, \dots, m,$$

$$X \succ 0, \tag{1}$$

where the function f is convex and $\mathbb{S}^n = \{X \in \mathbb{R}^{n \times n} | X^T = X\}$ denotes the set of the symmetric matrices of $\mathbb{R}^{n \times n}$. In general, the solution of this convex program has to be searched in a space of dimension $\frac{n(n+1)}{2}$. An approach is proposed for solving (1) that is able to deal with a large dimension n once the following assumptions hold.

Assumption 1 The program (1) presents a low-rank solution X^* , i.e.,

$$rank(X^*) = r \ll n.$$

Assumption 2 The symmetric matrices A_i satisfy

$$A_i A_j = 0,$$

for any $i, j \in \{1, ..., m\}$ such that $i \neq j$.

Assumption 2 is fulfilled, e.g., by the spectahedron,

$$\mathcal{S} = \{ X \in \mathbb{S}^n | X \succeq 0, \text{Tr}(X) = 1 \},$$

and the elliptope,¹

$$\mathcal{E} = \{ X \in \mathbb{S}^n | X \succeq 0, \operatorname{diag}(X) = \mathbf{1} \}. \tag{2}$$

Assumption 1 suggests to factorize the optimization variable X as

$$X = YY^T \tag{3}$$

with $Y \in \mathbb{R}^{n \times p}$. This leads to a nonlinear optimization program in terms of the matrix Y,

$$\min_{Y \in \mathbb{R}^{n \times p}} f(YY^T)
\text{s.t.} \quad \text{Tr}(Y^T A_i Y) = b_i, \ A_i \in \mathbb{S}^n, b_i \in \mathbb{R}, \ i = 1, \dots, m.$$
(4)

Program (4) searches a space of dimension np, which is much lower than the dimension of the symmetric positive semidefinite matrices X. However, this program is no longer convex.

A further potential difficulty of the program (4) is that the solutions are not isolated. For any solution \tilde{Y} and any orthogonal matrix Q of $\mathbb{R}^{p \times p}$, i.e., $Q^T Q = I$, the matrix $\tilde{Y}Q$ is also a

¹The elliptope is also known as the set of correlation matrices.

solution. In other words, the program (4) is invariant by right multiplication of the unknown with an orthogonal matrix. This issue is not harmful for simple gradient schemes but it greatly affects the convergence of second order methods (see e.g., [AMS08] and [AIDV08]). In order to take into account the inherent symmetry of the solution, the algorithm developed in this paper does not optimize on the Euclidean space $\mathbb{R}^{n\times p}$. Instead, one considers a search space, whose points are the equivalence classes $\{YQ|Q\in\mathbb{R}^{p\times p},Q^TQ=I\}$. The minimizers of (4) are isolated in that quotient space.

It is important to mention that the rank r of the solution X^* is usually unknown. The algorithm we propose for solving (1) thus provides a method that finds a local minimizer Y_* of (4) with an approach that increments p until a sufficient condition is satisfied for Y_* to provide the solution $Y_*Y_*^T$ of (1). The proposed algorithm converges monotonically towards the solution of (1), is based on superlinear second order methods, and is provided with an indicator of convergence able to control the accuracy of the results.

The idea of reformulating a convex program into a nonconvex one by factorization of the matrix unknown is not new and was investigated in [BM03] for solving semidefinite programs (SDP). While the setup considered in [BM03] is general but restricted to gradient methods, the present paper further exploits the particular structure of the equality constraints (Assumption 2) and proposes second-order methods that lead to a descent algorithm with guaranteed superlinear convergence. The authors of [GP07] also exploit the factorization (3) to efficiently solve optimization problems that are defined on the elliptope (2). Whereas the algorithms in [GP07] evolve on the *Cholesky manifold*—a submanifold of $\mathbb{R}^{n\times p}$ whose intersection with almost all equivalence classes is a singleton—, the methods proposed here work conceptually on the entire quotient space and numerically in $\mathbb{R}^{n\times p}$, using the machinery of Riemannian submersions.

The paper is organized as follows. Section 3 derives conditions for an optimizer of (4) to represent a solution of the original problem (1). A meta-algorithm for solving (1) based on the factorization (3) is built upon these theoretical results. Section 4 describes the geometry of the underlying quotient manifold and proposes an algorithm for solving (4) based on second order derivative information. Sections 5 and 6 illustrate the new approach on two applications: the maximal cut of a graph and the sparse principal component analysis problem.

2 Notations

Given a function $f: \mathbb{S}^n \to \mathbb{R}: X \mapsto f(X)$, we define the function

$$\tilde{f}: \mathbb{R}^{n \times p} \to \mathbb{R}: Y \mapsto \tilde{f}(Y) = f(YY^T).$$

The operator $\nabla \cdot$ stands for the first order derivative, i.e., the matrix $B = \nabla_X f(X_0)$ represents the gradient of f with respect to the variable X evaluated at the point X_0 . f is assumed to

be differentiable and B is defined element wise by

$$B_{i,j} = \frac{\partial f}{\partial X_{i,j}}(X_0).$$

Finally,

$$D_X f(X_0)[Z] = \lim_{t \to 0} \frac{f(X_0 + tZ) - f(X_0)}{t},$$

denotes the derivative with respect to X of the function f at the point X_0 in the direction Z. It holds that

$$D_X f(X_0)[Z] = \langle \nabla_X f(X_0), Z \rangle,$$

where $\langle \cdot, \cdot \rangle$ denotes the Frobenius inner product $\langle Z_1, Z_2 \rangle = \text{Tr}(Z_1^T Z_2)$.

3 Optimality conditions

This section derives and analyzes the optimality conditions of both programs (1) and (4). These provide theoretical insight about the rank p at which (4) should be solved as well as conditions for an optimizer of (4) to represent a solution of the original problem (1). A meta-algorithm for solving (1) is then derived from these results.

3.1 First-order optimality conditions

Lemma 1 A symmetric matrix $X \in \mathbb{S}^n$ solves (1) if and only if there exist a vector $\sigma \in \mathbb{R}^m$ and a symmetric matrix $S \in \mathbb{S}^n$ such that the following holds,

$$\operatorname{Tr}(A_{i}X) = b_{i},$$

$$X \succeq 0,$$

$$S \succeq 0,$$

$$SX = 0,$$

$$S = \nabla_{X}f(X) - \sum_{i=1}^{m} \sigma_{i}A_{i}.$$

$$(5)$$

Proof. These are the first order KKT-conditions, which are necessary and sufficient in case of convex programs [BV04].

Lemma 2 If Y is a local optimum of (4), then there exists a vector $\lambda \in \mathbb{R}^m$ such that

$$\operatorname{Tr}(Y^T A_i Y) = b_i,$$

$$(\nabla_X f(Y Y^T) - \sum_{i=1}^m \lambda_i A_i) Y = 0.$$
(6)

If the $\{A_iY\}_{i=1,...,m}$ are linearly independent, the vector λ is unique.

Proof. These are the first order KKT-conditions for the program (4).

Given a local minimizer Y of (4), one readily notices that all but one condition of Lemma 1 hold for the symmetric positive semidefinite matrix YY^T . Comparison of Lemma 1 and Lemma 2 therefore provides the following relationship between the nonconvex program (4) and the convex program (1).

Theorem 3 A local minimizer Y of the nonconvex program (4) provides the solution YY^T of the convex program (1) if and only if the matrix

$$S_Y = \nabla_X f(YY^T) - \sum_{i=1}^m \lambda_i A_i \tag{7}$$

is positive semidefinite for the Lagrangian multipliers λ_i that satisfy (6).

Proof. Check the conditions of Lemma 1 for the tuple
$$\{X, S, \sigma\} = \{YY^T, S_Y, \lambda\}.$$

It is important to note that, under Assumption 2, the Lagrangian multipliers in (6) have the closed-form expression,

$$\lambda_i = \frac{\text{Tr}(Y^T A_i \nabla_X f(YY^T) Y)}{\text{Tr}(Y^T A_i^2 Y)}.$$
(8)

Hence, the dual matrix S_Y in (7) can be explicitly evaluated at an optimizer Y of (4).

3.2 Second-order optimality conditions

Let $\mathcal{L}(Y,\lambda)$ denote the Lagrangian of the nonconvex program (4), i.e.,

$$\mathcal{L}(Y,\lambda) = f(YY^T) - \sum_{i=1}^{m} \lambda_i (\text{Tr}(Y^T A_i Y) - b_i).$$

In the following, the Lagrangian multipliers λ are assumed to satisfy (6). A necessary condition for $Y \in \mathbb{R}^{n \times p}$ to be optimal is that it is a critical point, i.e., $\nabla_Y \mathcal{L}(Y, \lambda) = 0$.

Lemma 4 For a minimizer $Y \in \mathbb{R}^{n \times p}$ of (4), one has

$$\operatorname{Tr}(Z^T D_Y \nabla_Y \mathcal{L}(Y, \lambda)[Z]) \ge 0$$
 (9)

for any matrix $Z \in \mathbb{R}^{n \times p}$ that satisfies,

$$Tr(Z^T A_i Y) = 0, \ i = 1, \dots, m. \tag{10}$$

Proof. These are the second order KKT-conditions of the program (4).

Lemma 5 Because of the convexity of f(X), one always has

$$\frac{1}{2}\operatorname{Tr}(Z^T D_Y \nabla_Y \mathcal{L}(Y, \lambda)[Z]) = \operatorname{Tr}(Z^T S_Y Z) + \alpha$$
(11)

with $\alpha \geq 0$ and for any matrix Z that satisfies (10). The term α cancels out once $YZ^T = 0$.

Proof. By noting that $\nabla_Y \mathcal{L}(Y,\lambda) = 2S_Y Y$, one has

$$\frac{1}{2} \text{Tr}(Z^T D_Y \nabla_Y \mathcal{L}(Y, \lambda)[Z]) =$$

$$\operatorname{Tr}(Z^T S_Y Z) + \operatorname{Tr}(Z^T D_Y (\nabla_X f(YY^T))[Z]Y) - \sum_{i=1}^m D_Y \lambda_i[Z] \operatorname{Tr}(Z^T A_i Y). \quad (12)$$

The last term of (12) cancels out by virtue of (10) and the convexity of the function f(X) ensures the second term of (12) to be nonnegative, i.e.,

$$\operatorname{Tr}(Z^T D_Y(\nabla_X f(YY^T))[Z]Y) = \frac{1}{2} \operatorname{Tr}((YZ^T + ZY^T) D_Y(\nabla_X f(YY^T))[Z])$$
$$= \frac{1}{2} \operatorname{Tr}(W^T D_X(\nabla_X f)[W])$$
$$\geq 0,$$

where $X = YY^T$ and $W = YZ^T + ZY^T \in S_n$.

Theorem 6 A local minimizer Y of the program (4) provides the solution $X = YY^T$ of the program (1) if it is rank deficient.

Proof. For the matrix $Y \in \mathbb{R}^{n \times p}$ to span a r-dimensional subspace, the following factorization has to hold,

$$Y = \tilde{Y}M^T, \tag{13}$$

with $\tilde{Y} \in \mathbb{R}^{n \times r}$ and M a full rank matrix of $\mathbb{R}^{p \times r}$. Let $M_{\perp} \in \mathbb{R}^{p \times (p-r)}$ be an orthogonal basis for the orthogonal complement of the column space of M, i.e., $M^T M_{\perp} = 0$ and $M_{\perp}^T M_{\perp} = I$. For any matrix $\tilde{Z} \in \mathbb{R}^{n \times (p-r)}$, the matrix $Z = \tilde{Z} M_{\perp}^T$ satisfies

$$YZ^T = 0$$

such that the conditions (10) hold and α cancels out in (11). Thus, by virtue of Lemmas 4 and 5,

$$\operatorname{Tr}(Z^T S_Y Z) \ge 0,$$

for matrices $Z = \tilde{Z}M_{\perp}^T$, i.e., the matrix S_Y is positive semidefinite and $X = YY^T$ is a solution of the problem (1).

Corollary 7 In the case p = n, any local minimizer $Y \in \mathbb{R}^{n \times n}$ of the program (4) provides the solution $X = YY^T$ of the program (1).

Proof. If Y is rank deficient, the matrix $X = YY^T$ is optimal for (1) by virtue of Theorem 6. Otherwise, the matrix S_Y is zero because of the second condition in (6) and X is optimal for (1).

3.3 An algorithm to solve the convex problem

The proposed algorithm consists in solving a sequence of nonconvex problems (4) of increasing dimension until the resulting local minimizer Y represents a solution of the convex program (1). Both Theorems 3 and 6 provide conditions to check this fact. When the program (4) is solved in a dimension p smaller than the unknown rank r, none of these conditions can be

fulfilled. The dimension p is thus incremented after each resolution of (4). In order to ensure a monotone decrease of the cost function through the iterations, the optimization algorithm that solves (4) is initialized with a matrix corresponding to Y with an additional zero column appended, i.e., $Y_0 = [Y|0]$. Since this initialization occurs when the local minimizer $Y \in \mathbb{R}^{n \times p}$ of (4) does not represent the solution of (1), Y_0 is a saddle point of the nonconvex problem for the dimension p + 1. This can be a critical issue for many optimization algorithms. Fortunately, in the present case, a descent direction from Y_0 can be explicitly evaluated. For Lemma 5, the matrix Z = [0|v], for instance, where 0 is a zero matrix of the size of Y and v is the eigenvector of S_Y related to the smallest algebraic eigenvalue verifies,

$$\frac{1}{2}\text{Tr}(Z^T D_Y \nabla_Y \mathcal{L}(Y_0, \lambda)[Z]) = v^T S_Y v \le 0,$$

since $Y_0Z^T=0$ for the Lagrangian multipliers λ given in (8). All these elements lead to the meta-algorithm displayed in Algorithm 1. The parameter ε fixes a threshold on the eigenvalues of S_Y to decide about the nonnegativity of this matrix. ε is chosen to 10^{-12} in our implementation.

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Algorithm 1: Meta-algorithm for solving the convex program (1) ^2
input : Initial rank p_0, initial iterate Y^{(0)} \in \mathbb{R}^{n \times p_0} and parameter \varepsilon.

output: The solution X of the convex program (1).

begin p \leftarrow p_0
Y_p \leftarrow Y^{(0)}
stop \leftarrow 0
while stop \neq 1 do
Initialize an optimization scheme with Y_p to find a local minimum Y_p^* of (4) by exploiting a descent direction Z_p if available.

if p = p_0 and rank(Y_p^*) < p then
| \text{ stop } = 1 
else
| Find the smallest eigenvalue <math>\lambda_{\min} and the related eigenvector V_{\min} of the matrix S_Y (7).

if \lambda_{\min} \geq -\varepsilon then
| \text{ stop } = 1 
else
| P \leftarrow p + 1 
| S \leftarrow p \leftarrow p + 1 
| Y_p \leftarrow [Y_p^*] 0]
| A \text{ descent direction from the saddle point } Y_p \text{ is given by } Z_p = [0|V_{\min}].
| X \leftarrow Y_p^* Y_p^{*T} 
end
```

²A Matlab implementation of Algorithm 1 with the manifold-based optimization method of Section 4 can be downloaded from http://www.montefiore.ulg.ac.be/~journee.

It should be mentioned that, to check the optimality for the convex program (1) of a local minimizer Y_p^* , the rank condition of Theorem 6 is computationally cheaper to evaluate than the nonnegativity condition of Theorem 3. Nevertheless, the rank condition does not provide a descent direction to escape saddle points. It furthermore requires to solve the program (4) at a dimension that is strictly greater than r, the rank of the solution of (1). Hence, this condition is only used at the initial rank p_0 and holds if p_0 is chosen larger than the unknown r. Numerically, the rank of $Y_{p_0}^*$ is computed as the number of singular values that are greater than a threshold fixed at 10^{-6} . The algorithm proposed in [BM03] exploits exclusively the rank condition of Theorem 6. For this reason, each optimization of (4) has to be randomly initialized and the algorithm in [BM03] is not a descent algorithm.

By virtue of Corollary 7, Algorithm 1 stops at the latest once p=n. The applications proposed in Sections 5 and 6 indicate that in practice, however, the algorithm stops at a rank p that is much lower than the dimension n. If $p_0 < r$, then the algorithm stops once p equals the rank r of the solution of (1). These applications also illustrate that the magnitude of smallest eigenvalue λ_{\min} of the matrix S_Y can be used to monitor the convergence. The value $|\lambda_{\min}|$ indicates whether the current iterate is close to satisfy the KKT conditions (5). This feature is of great interest once an approximate solution to (1) is sufficient. The threshold ε set on λ_{\min} controls then the accuracy of the result.

A trust-region scheme based on second-order derivative information is proposed in the next section for computing a local minimum of (4). This method is provided with a convergence theory that ensures the iterates to converge towards a local minimizer.

Hence, the proposed algorithm presents the following notable features. First, it converges toward the solution of the convex program (1) by ensuring a monotone decrease of the cost function. Then, the magnitude of the smallest eigenvalue of S_Y provides a mean to monitor the convergence. Finally, the inner problem (4) is solved by second-order methods featuring superlinear local convergence.

4 Manifold-based optimization

We now derive an optimization scheme that solves the nonconvex and nonlinear program,

$$\min_{\substack{Y \in \mathbb{R}^{n \times p} \\ \text{s.t.}}} \tilde{f}(Y)
\text{s.t.} \quad \text{Tr}(Y^T A_i Y) = b_i, \ A_i \in \mathbb{S}^n, b_i \in \mathbb{R}, \ i = 1, \dots, m,$$
(14)

where $\tilde{f}(Y) = f(YY^T)$ for some $f: \mathbb{S}^n \to \mathbb{R}$.

As previously mentioned, Program (14) is invariant by right-multiplication of the variable Y by orthogonal matrices. The critical points of (14) are thus non isolated. The proposed

algorithm exploits this symmetry by optimizing the cost $\tilde{f}(\cdot)$ on the quotient

$$\mathcal{M} = \bar{\mathcal{M}}/\mathcal{O}_p$$

where $\mathcal{O}_p = \{Q \in \mathbb{R}^{p \times p} | Q^T Q = I\}$ is the orthogonal group and $\bar{\mathcal{M}} = \{Y \in \mathbb{R}^{n \times p} : \text{Tr}(Y^T A_i Y) = b_i, i = 1, ..., m\}$ is the feasible set.³ Each point of the quotient \mathcal{M} is an equivalence class

$$[Y] = \{YQ|Q \in \mathcal{O}_n\}. \tag{15}$$

It can be proven that the quotient \mathcal{M} presents a manifold structure [AMS08]. Program (14) is thus strictly equivalent to the optimization problem,

$$\min_{[Y]\in\mathcal{M}} \bar{f}([Y]),$$

for the function $\bar{f}: \mathcal{M} \to \mathbb{R}: [Y] \mapsto \bar{f}([Y]) = \tilde{f}(Y)$.

Several unconstrained optimization methods have been generalized to search spaces that are differentiable manifolds. This is, e.g., the case of the trust-region approach. Details on this algorithm can be found in [ABG07, AMS08]. It is important to mention that this algorithm is provided with a convergence theory whose results are similar to the ones related to classical unconstrained optimization. In particular, trust-region methods on manifolds converge globally to stationary points of the cost function if the inner iteration produces a model decrease that is better than a fixed fraction of the Cauchy decrease; such a property is achieved, e.g., by the Steihaug-Toint inner iteration. Since the iteration is moreover a descent method, convergence to saddle points or local maximizers is not observed in practice. It is possible to obtain guaranteed convergence to a point where the second-order necessary conditions of optimality hold, by using inner iterations that exploit the model more fully (e.g., the inner iteration of Moré and Sorensen), but these inner iterations tend to be prohibitively expensive for large-scale problems. For appropriate choices of the inner iteration stopping criterion, trust-region methods converge locally superlinearly towards the nondegenerate local minimizers of the cost function. The parameter θ in Equation (10) of [ABG07] has been set to one, which guarantees a quadratic convergence.

A few important objects have to be specified to exploit the trust-region algorithm of [ABG07] in the present context. First, the tangent space at a point Y of the manifold $\bar{\mathcal{M}}$,

$$T_Y \bar{\mathcal{M}} = \{ Z \in \mathbb{R}^{n \times p} : \operatorname{Tr}(Y^T A_i Z) = 0, \ i = 1, \dots, m \},$$

has to be decomposed in two orthogonal subspaces, the *vertical space* $\mathcal{V}_Y \mathcal{M}$ and the *horizontal space* $\mathcal{H}_Y \mathcal{M}$. The vertical space $\mathcal{V}_Y \mathcal{M}$ corresponds to the tangent space to the equivalence classes,

$$\mathcal{V}_Y \mathcal{M} = \{ Y \Omega : \Omega \in \mathbb{R}^{p \times p}, \ \Omega^T = -\Omega \}.$$

 $^{{}^3\}mathbb{R}^{n\times p}_*$ is the noncompact Stiefel manifold of full-rank $n\times p$ matrices. The nondegeneracy condition is required to deal with differentiable manifolds.

The horizontal space $\mathcal{H}_Y \mathcal{M}$ is the orthogonal complement of $\mathcal{V}_Y \mathcal{M}$ in $T_Y \overline{\mathcal{M}}$, i.e.,

$$\mathcal{H}_Y \mathcal{M} = \{ Z \in T_Y \bar{\mathcal{M}} : Z^T Y = Y^T Z \}, \tag{16}$$

for the Euclidean metric $\langle Z_1, Z_2 \rangle = \text{Tr}(Z_1^T Z_2)$ for all $Z_1, Z_2 \in T_Y \bar{\mathcal{M}}$. Expression (16) results from the equality $\text{Tr}(S\Omega) = 0$ that holds for any symmetric matrix S and skew-symmetric matrix Ω of compatible dimension.

Let $N_Y \bar{\mathcal{M}}$, the normal space to $\bar{\mathcal{M}}$ at Y, denote the orthogonal complement of $T_Y \bar{\mathcal{M}}$ in $\mathbb{R}^{n \times p}$, i.e., $N_Y \bar{\mathcal{M}} = \{\sum_{i=1}^m \alpha_i A_i Y, \ \alpha \in \mathbb{R}^m\}$. Hence, the Euclidean space $\mathbb{R}^{n \times p}$ can be divided into three mutually orthogonal subspaces,

$$\mathbb{R}^{n\times p}=\mathcal{H}_Y\mathcal{M}\oplus\mathcal{V}_Y\mathcal{M}\oplus\mathcal{N}_Y\bar{\mathcal{M}}.$$

The trust-region algorithm proposed in [ABG07] requires a projection $P_Y(\cdot)$ from $\mathbb{R}^{n\times p}$ to $\mathcal{H}_Y\mathcal{M}$ along $\mathcal{V}_Y\mathcal{M}\oplus N_Y\bar{\mathcal{M}}$. The following theorem provides a closed-form expression.

Theorem 8 Let Y be a point on $\overline{\mathcal{M}}$. For a matrix $Z \in \mathbb{R}^{n \times p}$, the projection $P_Y(\cdot) : \mathbb{R}^{n \times p} \to \mathcal{H}_Y \mathcal{M}$ is given by

$$P_Y(Z) = Z - Y\Omega - \sum_{i=1}^{m} \alpha_i A_i Y,$$

where Ω is the skew symmetric matrix that solves the Sylvester equation

$$\Omega Y^T Y + Y^T Y \Omega = Y^T Z - Z^T Y,$$

and with the coefficients

$$\alpha_i = \frac{\operatorname{Tr}(Z^T A_i Y)}{\operatorname{Tr}(Y^T A_i^2 Y)}.$$

Proof. Any vector $Z \in \mathbb{R}^{n \times p}$ presents a unique decomposition

$$Z = Z_{\mathcal{V}_Y \mathcal{M}} + Z_{\mathcal{H}_Y \mathcal{M}} + Z_{N_Y \bar{\mathcal{M}}},$$

where each element $Z_{\mathcal{X}}$ belongs to the Euclidean space \mathcal{X} . The orthogonal projection $\mathcal{P}_{Y}(\cdot)$ extracts the component that lies in the horizontal space, i.e.,

$$P_Y(Z) = Z - Y\Omega - \sum_{i=1}^{m} \alpha_i A_i Y,$$

with Ω a skew symmetric matrix. The parameters Ω and α are determined from the linear equations

$$Y^T P_Y(Z) = P_Y(Z)^T Y,$$

$$Tr(Y^T A_i P_Y(Z)) = 0, \quad i = 1 \dots m,$$

which are satisfied by any element of the horizontal space.

The projection $P_Y(\cdot)$ provides simple formulas to compute derivatives of the function \bar{f} (defined on the quotient manifold) from derivatives of the function \tilde{f} (defined in the Euclidean space). The gradient corresponds to the projection on the horizontal space of the gradient of the function $\tilde{f}(Y)$, i.e.,

$$\operatorname{grad} \bar{f}(Y) = P_Y(\nabla_Y \tilde{f}(Y)).$$

The Hessian applied on a direction $Z \in \mathcal{H}_Y \mathcal{M}$ is given by

$$\operatorname{Hess}\bar{f}(Y)[Z] = P_Y(D_Y(P_Y(\nabla_Y \tilde{f}(Y)))[Z]),$$

where the directional derivative $D_Y(\cdot)[\cdot]$ is performed in the Euclidean space $\mathbb{R}^{n\times p}$.

Finally, a last ingredient needed by the trust-regions algorithm in [ABG07] is a retraction $\mathcal{R}_Y(\cdot)$ that maps a search direction Z (an element of the horizontal space at Y) to a matrix representing a new point on the manifold \mathcal{M} . Such a mapping is for example given by the projection of the matrix $\tilde{Y} = Y + Z$ along the Euclidean space $N_Y \bar{\mathcal{M}}$, i.e.,

$$\mathcal{R}_Y(Z) = [\tilde{Y} + \sum_{i=1}^m \alpha_i A_i \tilde{Y}], \tag{17}$$

where $[\cdot]$ denotes the equivalence class (15) and the coefficients α_i are chosen such that

$$Tr(\bar{Y}^T A_i \bar{Y}) = b_i,$$

with $\bar{Y} = \tilde{Y} + \sum_{i=1}^{m} \alpha_i A_i \tilde{Y}$. Under Assumption 2, the coefficients α_i are easily computed as the solution of the quadratic polynomial,

$$\alpha_i^2 \text{Tr}(\tilde{Y}^T A_i^3 \tilde{Y}) + 2\alpha_i \text{Tr}(\tilde{Y}^T A_i^2 \tilde{Y}) + \text{Tr}(\tilde{Y}^T A_i \tilde{Y}) = b_i.$$

In case of the elliptope \mathcal{E} , Equation (17) becomes,

$$\mathcal{R}_Y(Z) = [\text{Diag}((Y+Z)(Y+Z)^T)^{-\frac{1}{2}}(Y+Z)],$$

where Diag(X) denotes the diagonal matrix whose diagonal elements are those of X and the brackets refer to the equivalence class (15). For the spectahedron \mathcal{S} , the retraction (17) is given by

$$\mathcal{R}_Y(Z) = \left[\frac{Y + Z}{\sqrt{\text{Tr}((Y + Z)^T (Y + Z))}} \right].$$

The complexity of the manifold-based trust-region algorithm in the context of program (14) is dominated by the computational cost required to evaluate the objective $\tilde{f}(Y)$, the gradient $\nabla_Y \tilde{f}(Y)$ and the directional derivative $D_Y(\nabla_Y \tilde{f}(Y))[Z]$. Hence, the costly operations are performed in the Euclidean space $R^{n \times p}$, whereas all manifold-related operations, such as evaluating a metric, a projection and a retraction, are of linear complexity with the dimension

5 Optimization on the elliptope: the max-cut SDP relaxation

A first application of the proposed optimization method concerns the maximal cut of a graph.

The maximal cut of an undirected and weighted graph corresponds to the partition of the vertices in two sets such that the sum of the weights associated to the edges crossing between these two sets is the largest. Computing the maximal cut of a graph is a NP-complete problem. Several relaxations to that problem have been proposed. The most studied one is the 0.878-approximation algorithm [GW95] that solves the following semidefinite program (SDP),

$$\begin{aligned} & \min_{X \in \mathbb{S}^n} & \operatorname{Tr}(AX) \\ & \text{s.t.} & \operatorname{diag}(X) = \mathbf{1}, \\ & & X \succeq 0, \end{aligned}$$

where $A = -\frac{1}{4}L$ with L the Laplacian matrix of the graph and 1 is a vector of all ones. This relaxation is tight in case of a rank-one solution.

As previously mentioned, the elliptope,

$$\mathcal{E} = \{ X \in \mathbb{S}^n | X \succeq 0, \operatorname{diag}(X) = \mathbf{1} \},\$$

satisfies Assumption 2. Hence, Program (18) is a good candidate for the proposed framework. Using the factorization $X = YY^T$, the optimization problem is defined on the quotient manifold $\mathcal{M}_{\mathcal{E}} = \bar{\mathcal{M}}_{\mathcal{E}}/\mathcal{O}_p$, where

$$\bar{\mathcal{M}}_{\mathcal{E}} = \{ Y \in \mathbb{R}_*^{n \times p} : \operatorname{diag}(YY^T) = \mathbf{1} \}.$$

The complexity of Algorithm 1 in the present context is of order $O(n^2p)$. This complexity is dominated by both the manifold-based optimization and the eigenvalue decomposition of the dual variable S_Y , that are $O(n^2p)$. The computational cost related to the manifold-based optimization is however reduced in case of matrices A that are sparse.

Table 1 presents computational results obtained with Algorithm 1 for computing the maximal cut of a set of graphs. The parameter n denotes the number of vertices of these graphs and corresponds thus to the size of the variable X in (18). More details on these graphs can be found in [BM03] and references therein. The low-rank method is compared with the SD-PLR algorithm proposed in [BM03], that also exploits the low rank factorization $X = YY^T$ in the case of semidefinite programs (SDP). The rank of the optimizer Y^* indicates that the factorization $X = YY^T$ reduces significantly the size of the search space. Concerning the computational time, it is important to mention that Algorithm 1 has been implemented in Matlab, whereas a C implementation of the SDPLR algorithm has been provided by the authors of [BM03]. Although this renders a rigorous comparison of the computational load difficult, Table 1 suggests that both methods perform similarly.

			Objective values		CPU ti	CPU time (sec)	
Graph	n	$\operatorname{Rank}(Y^*)$	Algo. 1	SDPLR	Algo. 1	SDPLR	
toruspm3-8-50	512	8	-527.81	-527.81	17	3	
toruspm 3-15-50	3375	15	-3474.79	-3474.76	1051	181	
torusg3-8	3375	7	-3187.61	-3188.09	375	228	
G1	800	13	-12083.2	-12083.1	57	35	
G11	800	5	-629.16	-629.15	53	15	
G14	800	13	-3191.57	-3191.53	82	13	
G22	2000	18	-14136.0	-14135.9	358	101	
G32	2000	5	-1567.58	-1567.57	158	69	
G35	2000	14	-8014.57	-8014.33	525	68	
G36	2000	13	-8005.60	-8005.80	459	115	
G58	5000	8	-20111.3	-20135.4	1881	1119	

Table 1: Computational results of Algorithm 1 (implemented in Matlab) and the SDPLR algorithm (implemented in C) on various graphs.

Figure 1 depicts the monotone convergence of the Algorithm 1 for the graph toruspm3-15-50. The number of iterations is displayed on the bottom abscissa, whereas the top abscissa stands for the rank p. Figure 2 indicates that the smallest eigenvalue λ_{\min} of the dual matrix S_Y monotonically increases to zero. One notices that the magnitude of λ_{\min} gives some insight on the current accuracy.

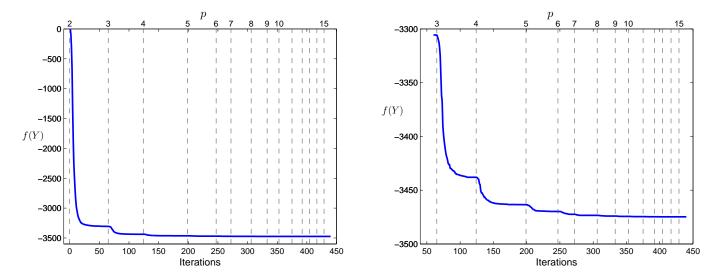


Figure 1: Monotone decrease of the cost function $f(Y) = \text{Tr}(Y^T A Y)$ through the iterations (bottom abscissa) and with the rank p (top abscissa) in the case of the graph toruspm3-15-50.

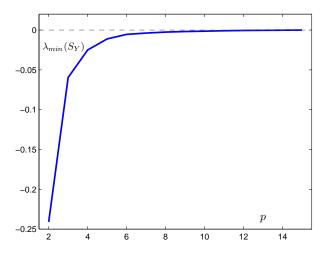


Figure 2: Evolution of the smallest eigenvalue of the matrix S_Y (case of the graph toruspm3-15-50).

6 Optimization on the spectahedron: the sparse PCA problem

This section presents three nonlinear programs that concern the sparse principal component analysis problem and that can be efficiently solved with the proposed low-rank optimization approach.

Principal component analysis (PCA) is a tool that reduces multidimensional data to lower dimension. Given a data matrix $A \in \mathbb{R}^{m \times n}$, the first principal component consists in the best rank-one approximation of the matrix A in the least square sense. This decomposition is performed via estimation of the dominant eigenvector of the empirical covariance matrix $\Sigma = A^T A$. In many applications, it is of great interest to get sparse principal components, i.e., components that yield a good low-rank approximation of A while involving a limited number of nonzero elements. In case of gene expression data where the matrix A represents the expression of n genes through m experiments, getting factors that involve just a few genes, but still explain a great part of the variability in the data, appears to be a modelling assumption closer to the biology than the regular PCA [TJA⁺07]. This tradeoff between variance and sparsity is the central motivation of sparse PCA methods. More details on the sparse PCA approach can be found in [ZHT06, dEJL07] and references therein.

Sparse PCA is the problem of finding the unit-norm vector $x \in \mathbb{R}^n$ that maximizes the Rayleigh quotient of the matrix $\Sigma = A^T A$ but contains a fixed number of zeros, i.e.,

$$\max_{x \in \mathbb{R}^n} x^T \Sigma x$$
s.t. $x^T x = 1$, (19)
$$\operatorname{Card}(x) \leq k$$
,

where k is an integer with $1 \le k \le n$ and Card(x) is the cardinality of x, i.e., the number of

non zero components. Finding the optimal sparsity pattern of the vector x is of combinatorial complexity. Several algorithms have been proposed in the literature that find an approximate solution to (19). We refer to [dEJL07] for references on these methods. Let us finally mention that the data matrix A does not necessarily have to present a sparse pattern. In the context of compressed sensing, for example, one needs to compute the sparse principal component of a matrix A that is full and sampled from a gaussian distribution [dBE07].

Recently, two convex relaxations have been derived that require to minimize some nonlinear convex functions on the spectahedron $\mathcal{S} = \{X \in \mathbb{S}^m | X \succeq 0, \operatorname{Tr}(X) = 1\}$. Both of these relaxations consider a variation of (19), in which the cardinality appears as a penalty instead of a constraint, i.e.,

$$\max_{x \in \mathbb{R}^n} \quad x^T \Sigma x - \rho \operatorname{Card}(x)$$
s.t.
$$x^T x = 1,$$
(20)

with the parameter $\rho \geq 0$.

6.1 A first convex relaxation to the sparse PCA problem

In [dEJL07], Problem (20) is relaxed to a convex program in two steps. First, a convex feasible set is obtained by lifting the unit norm vector variable x into a matrix variable X that belongs to the spectahedron, i.e.,

$$\max_{X \in \mathbb{S}^n} \operatorname{Tr}(\Sigma X) - \rho \operatorname{Card}(X)$$
s.t.
$$\operatorname{Tr}(X) = 1,$$

$$X \succeq 0.$$
(21)

The relaxation (21) is tight for rank-one matrices. In such cases, the vector variable x in (20) is related to the matrix variable X according to $X = xx^T$. Then, for (21) to be convex, the cardinality penalty is replaced by a convex l_1 penalty, i.e.,

$$\max_{X \in \mathbb{S}^n} \operatorname{Tr}(\Sigma X) - \rho \sum_{i,j} |X_{ij}|$$
s.t.
$$\operatorname{Tr}(X) = 1,$$

$$X \succeq 0.$$
(22)

Finally, a smooth approximation to (22) is obtained by replacing the absolute value by the differentiable function $h_{\kappa}(x) = \sqrt{x^2 + \kappa^2}$ with the parameter κ that is very small. A too small κ might, however, lead to ill-conditioned Hessians and thus to numerical problems.

The convex program,

$$\max_{X \in \mathbb{S}^n} \operatorname{Tr}(\Sigma X) - \rho \sum_{i,j} h_{\kappa}(X_{ij})$$
s.t.
$$\operatorname{Tr}(X) = 1,$$

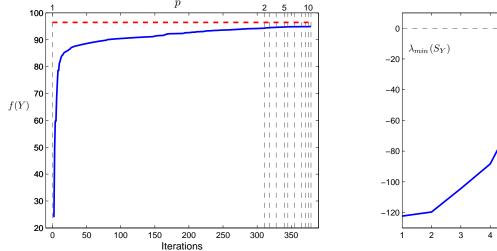
$$X \succeq 0,$$
(23)

fits within the framework (1). The variable X is thus factorized in the product YY^T and the optimization is performed on the quotient manifold $\mathcal{M}_{\mathcal{S}} = \bar{\mathcal{M}}_{\mathcal{S}}/\mathcal{O}_p$ where

$$\bar{\mathcal{M}}_{\mathcal{S}} = \{ Y \in \mathbb{R}_*^{n \times p} : \text{Tr}(Y^T Y) = 1 \}.$$

The computational complexity of Algorithm 1 in the context of program (23) is of order $O(n^2p)$. It should be mentioned that the DSPCA algorithm derived in [dEJL07] and that has been tuned to solve program (22) features a complexity of order $O(n^3)$.

Figure 3 illustrates the monotone convergence of Algorithm 1 on a random gaussian matrix A of size 50×50 . The sparsity weight factor ρ has been chosen to 5 and the smoothing parameter κ equals 10^{-4} . The maximum of the nonsmooth cost function in (22) has been computed with the DSPCA algorithm [dEJL07]. One first notices that the smooth approximation in (23) slightly underestimates the nonsmooth cost function (22). The maximizers of both (22) and (23) are, however, almost identical. Then, we should mention that all numerical experiments performed with the DSPCA algorithm for solving (22) resulted in a rank one matrix. So, the solution of (23) is expected to be close to rank one. This explains why the improvement in terms of objective value is very small for ranks larger than one. A heuristic to speed up the computations would thus consist in computing an approximate rank one solution of (23), i.e., Algorithm 1 is stopped after the iteration p = 1. Finally, on the right hand plot, Figure 3 highlights the smallest eigenvalue λ_{\min} of the matrix S_Y as a way to monitor the convergence.



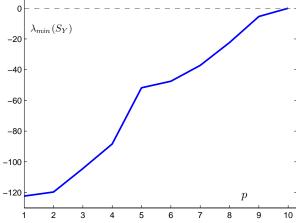
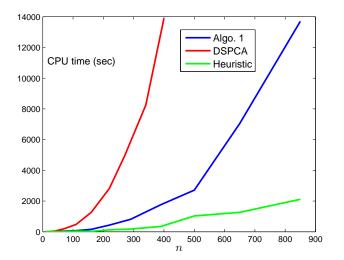


Figure 3: Left: monotone increase of $f(Y) = \text{Tr}(Y^T \Sigma Y) - \rho \sum_{i,j} h_{\kappa}((YY^T)_{ij})$ through the iterations (bottom abscissa) and with the rank p (top abscissa). The dashed horizontal line represents the maximum of the nonsmooth cost function in (22). Right: evolution of the smallest eigenvalue of S_Y .

Figure 4 provides some insight on the computational time required by a Matlab implementation of Algorithm 1 that solves (23). Square gaussian matrices A have been considered,

i.e., m = n. On the left hand plot, Algorithm 1 is compared with the above mentioned heuristic and the DSPCA algorithm. The right hand plot highlights the quadratic complexity of Algorithm 1 with the problem size n.



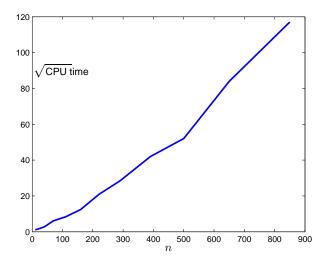


Figure 4: Right: Computational time for solving (23) versus the problem size in the case p = n. Left: Square root of the computational time versus n.

6.2 A second convex relaxation to the sparse PCA problem

Problem (20) is shown in [dBE07] to be strictly equivalent to

$$\max_{z \in \mathbb{R}^m} \quad \sum_{i=1}^n ((a_i^T z)^2 - \rho)_+,$$

s.t. $z^T z = 1,$ (24)

where a_i is the i^{th} column of A and the function x_+ corresponds to $\max(0, x)$. The auxiliary variable z enables to reconstruct the vector x: the component x_i is active if $(a_i^T z)^2 - \rho \ge 0$. As for the relaxation previously derived in Section 6.1, the vector z is lifted into a matrix Z of the spectahedron,

$$\max_{Z \in \mathbb{S}^m} \quad \sum_{i=1}^n \text{Tr}(a_i^T Z a_i - \rho)_+$$
s. t.
$$\text{Tr}(Z) = 1,$$

$$Z \succeq 0,$$
(25)

This program is equivalent to (24) in case of rank one matrices $Z = zz^T$. Program (25) maximizes a convex function and is thus nonconvex. The authors of [dBE07] have shown that, in case of rank one matrices Z, the convex cost function in (25) equals the concave function

$$f(Z) = \sum_{i=1}^{n} \text{Tr}(Z^{\frac{1}{2}}(a_i^T a_i - \rho I)Z^{\frac{1}{2}})_+, \tag{26}$$

where the function $Tr(X)_+$ stands for the sum of the positive eigenvalues of X. This gives the following nonsmooth convex relaxation of (20),

$$\max_{Z \in \mathbb{S}^{m}} \sum_{i=1}^{n} \text{Tr}(Z^{\frac{1}{2}}(a_{i}^{T}a_{i} - \rho I)Z^{\frac{1}{2}})_{+}$$
s. t. $\text{Tr}(Z) = 1$, (27)
$$Z \succeq 0$$
,

that is tight in case of rank-one solutions. This program is solved via the factorization $Z = YY^T$ and optimization on the quotient manifold $\mathcal{M}_{\mathcal{S}}$. In the case $Z = YY^T$, function (26) equals

$$f(Y) = \sum_{i=1}^{n} \text{Tr}(Y^{T}(a_{i}^{T} a_{i} - \rho I)Y)_{+},$$

which is a spectral function [dBE07]. The evaluation of the gradient and Hessian of f(Y) are based on explicit formulae derived in the papers [Lew96, LS01] to compute the first and second derivatives of a spectral function. Since we are not aware of any smoothing method that would preserve the convexity of (27), Algorithm 1 has been directly applied in this non-smooth context. In practice, no trouble has been observed since all numerical simulations converge successfully to the solution of (27). The computational complexity of Algorithm 1 for solving (27) is of order $O(nm^2p)$. The convex relaxation (27) of the sparse PCA problem (20) appears thus well suited to treat large scale data with $m \ll n$, such as gene expression data are.

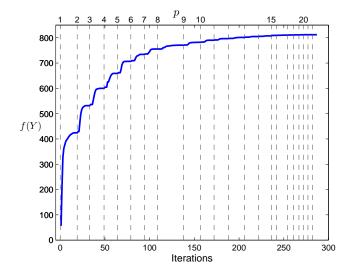
Figure 5 displays the convergence of Algorithm 1 for solving (27) with a random gaussian matrix A of size m = 100 and n = 500. The sparsity parameter ρ is chosen at 5 percent of the upper bound $\bar{\rho} = \max_{i} a_i^T a_i$, that is derived in [dBE07]. The smallest eigenvalue λ_{\min} of the matrix S_Y presents a monotone decrease once it gets sufficiently close to zero.

Figure 6 plots the CPU time required by a Matlab implementation of Algorithm 1 versus the dimension n of the matrix A. The dimension p has been fixed at 50 and A is chosen according to a gaussian distribution. Figure 6 illustrates the linear complexity in n of the proposed sparse PCA method.

6.3 Projection on rank one matrices

Both convex relaxations (23) and (27) are derived from the reformulation of a problem defined on unit norm vectors x into a problem with matrices $X = xx^T$, which is an equivalent formulation if X belongs to the spectahedron and has rank one. Within the derivation of both convex relaxations, the rank one condition has been dropped. The solutions of (23) and (27) are therefore expected to present a rank larger than one.

As previously mentioned, all numerical experiments performed with the DSPCA algorithm [dEJL07], which solves the nonsmooth convex program (22), led to a rank one solution. Thus,



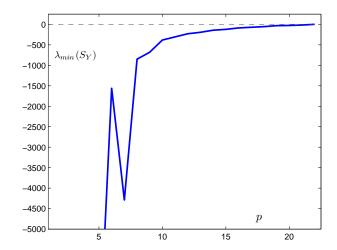


Figure 5: Left: monotone increase of the cost function through the iterations (bottom abscissa) and with the rank p (top abscissa). Right: evolution of the smallest eigenvalue of S_Y .

the solution of the smooth convex relaxation (22) is expected to tend to a rank one matrix once the smoothing parameter κ gets sufficiently close to zero. Figure 7 illustrates this fact. It should be mentioned that a matrix X of the spectahedron has nonnegative eigenvalues whose sum is one. Hence, X is rank one if and only if its largest eigenvalue equals one. In order to deal with potential numerical problems in case of very small κ , we sequentially solve problems of the type of (23) with a decreasing value of κ . The solution of each problem initializes a new program (23) with a reduced κ .

In contrast to (22), the convex relaxation (27) usually provides solutions with a rank that is larger than one. The solution matrix X has to be projected onto the rank one matrices of the spectahedron in order to recover a vector variable x. A convenient heuristic is to compute the dominant eigenvector of the matrix X. A vector x that achieves a higher objective value in (20) might, however, be obtained with the following homotopy method. We consider the program

$$\max_{Z \in \mathbb{S}^m} \mu f_{cvx}(Z) + (1 - \mu) f_{ccv}(Z)$$
s. t. $\operatorname{Tr}(Z) = 1$, (28)
$$Z \succeq 0$$
,

with the concave function,

$$f_{ccv}(Z) = \sum_{i=1}^{n} \text{Tr}(Z^{\frac{1}{2}}(a_i^T a_i - \rho I)Z^{\frac{1}{2}})_+$$

and the convex function,

$$f_{cvx}(Z) = \sum_{i=1}^{n} \text{Tr}(a_i^T Z a_i - \rho)_+,$$

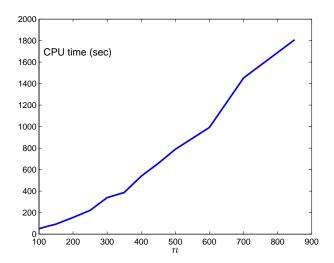


Figure 6: Computational time for solving (27) versus the problem size n in the case p = 50.

and for the parameter $0 \le \mu \le 1$. As previously mentioned, in case of rank one matrices $Z = zz^T$, the functions $f_{ccv}(Z)$ and $f_{cvx}(Z)$ are identical and equal to the cost function (24). For $\mu = 0$, program (28) is the convex relaxation (27) and the solution has typically a rank larger than one. If $\mu = 1$, solutions of (28) are extreme points of the spectahedron, i.e., rank one matrices. Hence, by solving a sequence of problems (28) with the parameter μ that increases from zero to one, the solution of (27) is projected onto the rank one matrices of the spectahedron. Program (28) is no longer convex once $\mu > 0$. The optimization method proposed in this paper then converges towards a local maximizer of (28).

Figure 8 presents computational results obtained on a random gaussian matrix $A \in \mathbb{R}^{150 \times 50}$. This projection method is compared with the usual approach that projects the symmetric positive semidefinite matrix Z onto its dominant eigenvector, i.e., $\tilde{Z} = zz^T$ where z is the unit-norm dominant eigenvector of Z. Let $f_{EVD}(Z)$ denotes the function,⁴

$$f_{EVD}(Z) = f_{ccv}(\tilde{Z}) = f_{cvx}(\tilde{Z}).$$

Figure 8 uses the maximum eigenvalue of a matrix Z of the spectahedron to monitor its rank. As previously mentioned, any rank one matrix Z of the spectahedron satisfies $\lambda_{\max}(Z) = 1$. The continuous plots of Figure 8 display the evolution of the functions $f_{ccv}(Z)$ and $f_{EVD}(Z)$ during the resolution of the convex program (27), i.e., $\mu = 0$ in (28). Point A represents the solution obtained with Algorithm 1 by solving (27) at the rank p = 1, whereas B and B' stands for the exact solution of (27), which is of rank larger than one. The dashed plots illustrate the effect of the parameter μ , that is linearly increased by steps of 0.05 between the points B and C. For a sufficiently large μ , program (28) presents a rank one solution, which is displayed by the point C. One clearly notices that the objective function of the original problem (24), which equals $f_{EVD}(Z)$, is larger at C than at B'. Hence, the projection method

 $^{^4\}mathrm{EVD}$ stands for eigenvalue decomposition.

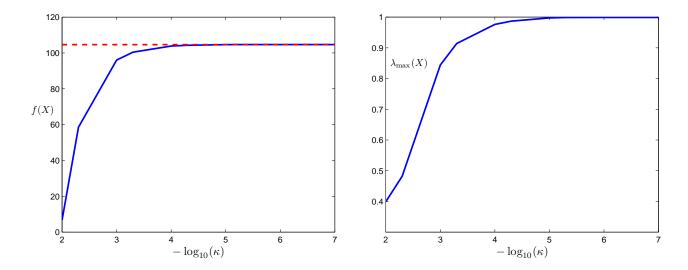


Figure 7: Left: evolution of the maximum the cost in (23) with the smoothing parameter κ . The dashed horizontal line represents the maximum of the nonsmooth cost function in (22). Right: evolution of the largest eigenvalue of the solution of (23).

based on (28) outperforms the projection based on the eigenvalue decomposition of Z in terms of achieved objective value.

7 Conclusion

We have proposed an algorithm for solving a nonlinear convex program that is defined in terms of a symmetric positive semidefinite matrix and that is assumed to present a low-rank solution. The proposed algorithm solves a sequence of nonconvex programs of much lower dimension than the original convex one. It presents a monotone convergence towards the sought solution, uses superlinear second order optimization methods and provides a tool to monitor the convergence, which enables to evaluate the quality of approximate solutions for the original convex problem. The efficiency of the approach has been illustrated on several applications: the maximal cut of a graph and various problems in the context of sparse principal component analysis. The proposed algorithm can also deal with problems featuring a nonconvex cost function. It then converges toward a local optimizer of the problem.

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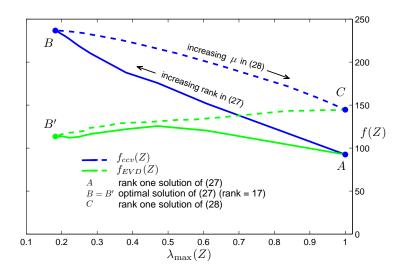


Figure 8: Evolution of the functions $f_{ccv}(Z)$ and $f_{EVD}(Z)$ in two situations. Continuous plots: resolution of the convex program (27) ($\mu = 0$ in (28)). Dashed plots: projection of the solution of (27) on a rank one matrix by gradual increase of μ .

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