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# Optimization schemes on manifolds for structured matrices with fixed eigenvalues

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## Abstract

Several manifold optimization schemes are presented and analyzed for solving a specialized inverse structured symmetric matrix problem with prescribed spectrum. Some entries in the desired matrix are assigned in advance and cannot be altered. The rest of the entries are free, some of them preferably away from zero. The reconstructed matrix must satisfy these requirements and its eigenvalues must be the given ones. This inverse eigenvalue problem is related to the problem of determining the graph, with weights on the undirected edges, of the matrix associated with its sparse pattern. Our optimization schemes are based on considering the eigenvector matrix as the only unknown and iteratively moving on the manifold of orthogonal matrices, forcing the additional structural requirements through a change of variables and a convenient differentiable objective function in the space of square matrices. We propose Riemannian gradient-type methods combined with two different well-known retractions, and with two well-known constrained optimization strategies: penalization and augmented Lagrangian. We also present a block alternating technique that takes advantage of a proper separation of variables. Convergence properties of the penalty alternating approach are established. Finally, we present initial numerical results to demonstrate the effectiveness of our proposals.

**Keywords:** Riemannian optimization, Stiefel manifold, inverse eigenvalue problems, spectral graph theory, augmented Lagrangian, alternating direction method of multipliers

**AMS Subject Classification:** 15A29, 65F18, 15A83, 15B10, 05C50, 90C30

## 1 Introduction

Given a set of real eigenvalues in no particular order, say  $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ , that defines a fixed diagonal matrix  $D$  whose diagonal entries are the given  $\lambda_i$ s, the problem of interest is to find a real symmetric  $n \times n$  matrix  $A$  with additional structural requirements, such that its eigenvalues are the given ones. In other words, we need to find  $A$  such that  $A = XDX^\top$  (Schur factorization) for an orthogonal matrix  $X$  whose columns are the eigenvectors of  $A$ .

There are, of course, some additional and fundamental requirements that add difficulty to the problem, otherwise  $A = D$  is a valid solution. For some specified pairs  $(i, j) \in I_0$  the  $a_{ij}$  entries must be zero at the solution. In addition, for some other specified pairs  $(i, j) \in I_{fix}$  the  $a_{ij}$  entries must have some given (nonzero) values at the solution. For all other pairs  $(i, j)$ , the  $a_{ij}$  entries are free. However, for a subset of these pairs (say  $(i, j) \in I_{nz}$ ), it is preferable to choose them as nonzero free variables. The complement of that subset (say  $(i, j) \in I_{free}$ ) contains entries that are completely free in  $\mathbb{R}$ . Here, the four given

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sets of indices:  $I_0, I_{fix}, I_{nz}$ , and  $I_{free}$  must form a partition of all possible pairs  $(i, j)$ , with  $i$  and  $j$  in  $\{1, 2, 3, \dots, n\}$ , and they need to reflect the symmetry of the desired matrix  $A$ .

The desired pattern, described above for the unknown symmetric matrix  $A$ , can be associated with a weighted undirected graph with  $n$  vertices, in which two vertices  $i$  and  $j$  are connected (adjacent) if and only if  $a_{ij}$  is not zero. The described inverse problem and the connection between the undirected graph and the matrix  $A$  with preset eigenvalues appear in several real-life applications related to quantum chemistry, information theory, social networks, and combinatorial optimization; see, e.g., [9, 10, 36, 37] and the references cited therein. It is worth noting that not every arbitrary assignment of real eigenvalues can guarantee the existence of a certain structure of the associated symmetric matrix. This is a topic of recent interest in matrix analysis. For a unified theoretical development of whether a predetermined distribution of eigenvalues can be achieved with a given graph, and also how the graph of a symmetric matrix influences the possible multiplicities of its eigenvalues, we refer to the book by Johnson and Saiago [19].

In the last few decades, numerous publications have addressed the general topic of Inverse Eigenvalue Problems (IEP), which share some relationship with the problem at hand and the optimization techniques used in our proposal. For instance, a Cayley transform based iterative method for solving IEP was developed in [2]. Similarly, Bai et. al. [3] introduced an iterative approach equipped with the Cayley transform for inverse singular value problems. In [35] some numerical optimization ideas on manifolds are indicated for a more rigorous structured IEP problem. Moreover, stochastic IEP with incomplete eigendata have been addressed in [38] via a Riemannian conjugate gradient method. Other Riemannian conjugate gradient methods have also been developed to solve stochastic IEP; see, e.g., [33, 40]. For a full review on structured IEP see [11] and references in there.

The rest of this document is organized as follows. In Section 2, we present the proposed continuously differentiable optimization model that considers the eigenvector matrix  $X$  as the only unknown, such that the orthogonality of  $X$  is a key constraint that needs to be imposed on the optimization problem. The rest of the structural matrix requirements are included in the objective function using a penalization strategy. In Section 3, we describe in detail the proposed iterative method for solving the orthogonality constrained optimization problem. In particular, we apply a fast and robust Riemannian gradient scheme, using two well-understood retractions and a suitable non-monotone globalization strategy. To enhance the practical behavior of the overall procedure, in Section 4, we introduce a block alternating minimization algorithm that takes advantage of a convenient variable splitting. The proposed procedure iterates alternatively solving an optimization problem with orthogonality constraints, using the development of Section 3, and a linearly constrained quadratic problem for which a closed formula is obtained. In Section 5, we establish the convergence properties of the algorithm described in Section 4 under some mild assumptions. Furthermore, in Section 6 we develop an alternating direction scheme that, instead of using a penalization strategy, uses an augmented Lagrangian approach. In Section 7, we report the obtained numerical results, and give further insights into the proposed schemes. Finally, in Section 8 we present some concluding remarks.

## 2 Manifold approach and penalization strategy

The main idea is to minimize a conveniently defined function that only depends on the matrix of eigenvectors  $X$  for solving the problem described in Section 1. Since the matrix of eigenvectors must be orthogonal, one constraint to be considered is  $X^\top X = I$ . The set formed by this constraint, that is  $\mathcal{O}(n) := \{X \in \mathbb{R}^{n \times n} : X^\top X = I\}$  is known as the *orthogonal group* [1, 8, 31]. Optimization problems over the orthogonal group has been recently studied, and for which a variety of effective iterative methods have been proposed; see, e.g., [18, 25, 27, 29]. Now, to consider only  $X$  as the variable matrix and to incorporate all the requirements described in Section 1, we need to introduce several suitable matrix operators and notations. In here, the Hadamard product  $M_1 \circ M_2$  between matrices  $M_1$  and  $M_2$  of the same dimensions will play a key role. Additionally, the trace of  $M \in \mathbb{R}^{m \times n}$ , i.e., the sum of its

diagonal elements, is denoted by  $tr(M)$ . The standard inner product between two matrices  $M_1 \in \mathbb{R}^{m \times n}$  and  $M_2 \in \mathbb{R}^{m \times n}$  is defined as  $\langle M_1, M_2 \rangle = tr(M_1^\top M_2)$ . The Frobenius norm of  $M \in \mathbb{R}^{m \times n}$  is defined as  $\|M\|_F = \sqrt{\langle M, M \rangle}$ . The main objective is to force the eigenvalues to be the given ones by building up a convenient continuously differentiable constrained optimization model that guarantees that the eigenvalues of any element of its feasible set are always the diagonal entries of the given diagonal matrix  $D$ .

Let  $P \in \mathbb{R}^{n \times n}$  be the matrix such that its entry  $(i, j)$  is given by

$$P_{ij} = \begin{cases} 0 & \text{if } (i, j) \in I_0, \\ 1 & \text{else} \end{cases}$$

This square matrix will be used to force the zero entries in the set of indices  $I_0$ . Similarly, we need a matrix  $Q$  with entries 1 if  $(i, j) \in I_{nz}$ , and zero elsewhere. The matrix  $Q$  will be used to maximize those entries in the obtained iterates while ensuring that at least one of them is nonzero. We also need a matrix  $R$  with entries 1 if  $(i, j) \in I_{fix}$ , and zero elsewhere. The matrix  $R$  will be employed to force the given specified nonzero entries, that will be represented by  $C$ , i.e.,  $C_{ij} = A_{ij}$  if the pair  $(i, j)$  belong to  $I_{fix}$ , and zero elsewhere. All these matrices can be seen as pattern matrices, and clearly they satisfy:  $P \circ P = P$ ,  $R \circ C = C$ ,  $Q \circ Q = Q$ , and  $R \circ R = R$ . These properties will be used to establish the gradient expression of a penalty objective function to be considered.

Our optimization model, to solve the specialized IEP described above, is given by

$$\min_{X \in \mathcal{O}(n)} F(X) \quad \text{s.t.} \quad P \circ (\Phi(X)) - \Phi(X) = 0, \quad R \circ (\Phi(X)) - C = 0, \quad (1)$$

where  $\Phi(X) := X^\top D X$  and  $F : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$  is defined by  $F(X) = -\|Q \circ \Phi(X)\|_F^2$ .

In order to solve this challenging problem, we can incorporate a penalization strategy. First, let us recall the main ideas of the classical and straightforward penalty approach for solving a constrained optimization problem. Penalty methods transform optimization problems with constraints into a sequence of unconstrained subproblems, whose solutions ideally converge to a minimizer of the original optimization problem. In our case, the constraints to be included in the cost function are

$$P \circ (\Phi(X)) - \Phi(X) = 0 \quad \text{and} \quad R \circ (\Phi(X)) - C = 0, \quad (2)$$

Thus, our penalization strategy is to execute the following iterative process until convergence

$$X_{k+1} = \arg \min_{X \in \mathcal{O}(n)} F_k(X), \quad (3a)$$

$$(\mu_{k+1}, \sigma_{k+1}) = (\rho_1 \mu_k, \rho_2 \sigma_k) \quad (3b)$$

where  $\rho_1 > 1$ ,  $\rho_2 > 1$  and

$$F_k(X) := -\|Q \circ \Phi(X)\|_F^2 + \mu_k \|P \circ (\Phi(X)) - \Phi(X)\|_F^2 + \sigma_k \|R \circ (\Phi(X)) - C\|_F^2, \quad (4)$$

and  $\mu_k > 0$ ,  $\sigma_k > 0$  are the penalty parameters to penalize constraint violations. Starting from  $\mu_0 > 0$  and  $\sigma_0 > 0$ , if the monotonically increasing sequences  $\{\mu_k\}$  and  $\{\sigma_k\}$  tend to infinity, then the sequence of minimizers of (4), over the set  $X^\top X = I$ , converges to a solution of (1) for which (2) holds, when  $k$  goes to infinity; see, e.g., [23, Secc. 12.1].

We close this section with a result dedicated to obtaining the gradient of the function  $F_k(\cdot)$  in (4).

**Lemma 2.1** *Let us consider the functions  $f_1 : X \in \mathbb{R}^{n \times n} \mapsto -\|Q \circ \Phi(X)\|_F^2$ ,  $f_2 : X \in \mathbb{R}^{n \times n} \mapsto \|P \circ (\Phi(X)) - \Phi(X)\|_F^2$ ,  $f_3 : X \in \mathbb{R}^{n \times n} \mapsto \|R \circ (\Phi(X)) - C\|_F^2$ . It follows that*

- $\mathcal{D}\Phi(X)(Z) = X^\top DZ + Z^\top DX$ .
- $\nabla f_1(X) = -2(DX(Q \circ (X^\top DX)) + Q \circ (X^\top DX)X^\top D)$ .
- $\nabla f_2(X) = DX(X^\top DX - P \circ (X^\top DX)) + (X^\top DX - P \circ (X^\top DX))X^\top D$ .
- $\nabla f_3(X) = 2[DX(R \circ (X^\top DX) - C) + (R \circ (X^\top DX) - C)X^\top D]$ .

**Proof.** The function  $\Phi : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{n \times n}$  previously defined is differentiable and its Fréchet derivative along  $Z$ ,  $\mathcal{D}\Phi(X)(Z)$ , is identified as the second term of the right hand side of the following equality (see, e.g., [1, Section A.5]):

$$\Phi(X + Z) = \Phi(X) + \mathcal{D}\Phi(X)(Z) + o(\|Z\|).$$

Since  $\Phi(X + Z) = \Phi(X) + X^\top DZ + Z^\top DX + Z^\top DZ$ , then  $\mathcal{D}\Phi(X)(Z) = X^\top DZ + Z^\top DX$ .

The function  $f_2 : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$  defined above is differentiable and its gradient can be obtained as follows. Consider the auxiliary function  $g : \mathbb{R} \rightarrow \mathbb{R}$ , given by

$$g(t) = f_2(X + tZ),$$

for any arbitrary matrix  $Z$ . From basic calculus we know that  $g'(0) = \langle \nabla f_2(X), Z \rangle$ . After simple algebraic manipulations, using that  $D^\top = D$ ,  $P^\top = P$  and  $P \circ P = P$ , we obtain

$$\begin{aligned} g'(0) &= \langle X^\top DZ + Z^\top DX, X^\top DX - P \circ (X^\top DX) \rangle \\ &= \langle Z, DXW \rangle + \langle Z, WX^\top D \rangle, \end{aligned}$$

where  $W = X^\top DX - P \circ (X^\top DX)$ , and the expression of the gradient of  $f_2(\cdot)$  is obtained. In a similar way, the expressions for  $\nabla f_1(\cdot)$  and  $\nabla f_3(\cdot)$  can also be established. ■

We note that the computational work for building the gradient at any iteration  $k$ , given the matrix  $X_k$ , requires the products  $DX_k$  and  $X_k^\top D$ , and from any of them we can obtain  $X_k^\top DX_k$ . Using those 3 matrices, that appear several times each, the entire gradient matrix is obtained, which is nothing but the summation of the last 3 terms in Lemma 2.1 multiplying the last two by  $\mu_k$  and  $\sigma_k$ , respectively.

### 3 Optimization over the orthogonal group

In this section, we describe some iterative methods for solving the orthogonality constrained optimization problem (1). In particular, we briefly review two specialized Riemannian gradient methods to solve optimization problems with orthogonal constraints. Let  $X \in \mathcal{O}(n)$  be an arbitrary matrix, the tangent space of the orthogonal group at  $X$  is given by

$$T_X \mathcal{O}(n) = \{Z = XW \in \mathbb{R}^{n \times n} : W^\top = -W\} = X \mathcal{S}_{\text{skew}}(n),$$

where  $\mathcal{S}_{\text{skew}}(n)$  represents the set of all  $n \times n$  skew-symmetric matrices, see [1, 14, 29].

On the other hand, it is well-known that if we equip each tangent space  $T_X \mathcal{O}(n)$  with the standard matrix inner product  $\langle M_1, M_2 \rangle$ , then the pair  $(\mathcal{O}(n), \langle \cdot, \cdot \rangle)$  forms a Riemannian manifold [1, 8]. In this context, the inner product is so-called *Riemannian metric*, see [1, 8]. Under this specific Riemannian metric, the orthogonal projection operator over the tangent space  $T_X \mathcal{O}(n)$  is given by

$$P_X(V) = X \text{skew}(X^\top V) = \frac{1}{2}(V - XV^\top X),$$

where  $\text{skew}(M) := \frac{1}{2}(M - M^\top)$  is the skew-symmetric part of  $M \in \mathbb{R}^{n \times n}$ , for details see Example 3.6.2 in [1].

In view of  $\mathcal{O}(n)$  is an embedded Riemannian sub-manifold of the Euclidean space  $\mathbb{R}^{n \times n}$ , the Riemannian gradient of the objective function  $F : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$  can be easily computed as follows

$$\nabla_{\mathcal{O}(n)} F(X) = P_X(\nabla F(X)). \quad (5)$$

Here we are using  $\nabla_{\mathcal{O}(n)} F(\cdot)$  to denote the Riemannian gradient of  $F(\cdot)$  and  $\nabla F(\cdot)$  to denote the Euclidean (classical) gradient of  $F(\cdot)$ . The justification for formula (5) appears in (3.37) in [1].

The Riemannian gradient provides us a search direction that we can use to minimize the function  $F$  over the domain  $\mathcal{O}(n)$ , see [1, 18, 26, 27]. However, we need an additional tool to preserve the feasibility of all the iterates. For this purpose we need a mapping called *retraction* [1, 8, 26]. Roughly speaking, a retraction is a smooth function that sends vectors from  $T_X \mathcal{O}(n)$  to a point on the manifold  $\mathcal{O}(n)$ , with a local rigidity property that preserves gradients at  $X$ . See [1, 8, 26] for a rigorous definition of retraction.

For the orthogonal group there are several retractions. In this work, we only consider two specific retractions that to our knowledge are the ones that require the least computational cost to evaluate them. The first retraction is based on the QR factorization. Let  $X \in \mathcal{O}(n)$  and  $Z = XW \in T_X \mathcal{O}(n)$  the first retraction is defined as follows

$$R_X^{\text{qr}}(Z) = \text{qf}(X + Z),$$

where  $\text{qf}(P)$  denotes the function that sends the matrix  $P$  to the  $Q$  factor of its QR factorization such that its  $R$  factor has strictly positive diagonal entries. We emphasize that this particular QR factorization is unique.

The second considered retraction is given by,

$$R_X^{\text{cayley}}(Z) = X \left( I - \frac{1}{2}W \right) \left( I + \frac{1}{2}W \right)^{-1},$$

which is based on the Cayley transform [18]. Notice that since  $W \in \mathcal{S}_{\text{skew}}(n)$ , the matrix  $I + \frac{1}{2}W$  is non-singular. These two retractions are described in Example 4.1.2 in [1]. Notice that the computational cost of performing either of the two retractions is  $O(n^3)$ .

The Riemannian gradient method [1, 8, 16, 28] is a line-search iterative scheme, which constructs a sequence of iterates  $\{X_k\} \subset \mathcal{O}(n)$ , starting at  $X_0 \in \mathcal{O}(n)$ , by using the following recursion

$$X_{k+1} = R_{X_k}(-\tau_k \nabla_{\mathcal{O}(n)} F(X_k)),$$

where  $\tau_0 > 0$  is the step-size and  $R_{X_k}(\cdot)$  is any retraction. Typically, the step-size  $\tau_k$  is computed using a backtracking strategy in such a way that it satisfies the following non-monotone globalization rule

$$F(X_{k+1}) \leq T_k - c_1 \tau_k \|\nabla_{\mathcal{O}(n)} F(X_k)\|_F^2,$$

where  $c_1 \in (0, 1)$  and  $\{T_k\}$  corresponds to the Zhang-Hager non-monotone strategy [39], i.e.,

$$T_{k+1} = \frac{\eta q_k T_k + F(X_k)}{q_{k+1}}, q_{k+1} = \eta q_k + 1, \quad \eta \in (0, 1), \quad T_0 = F(X_0), \quad \text{and} \quad q_0 = 1.$$

In order to accelerate the convergence, the Barzilai-Borwein step-sizes [4, 17] are incorporated in this method; see, e.g., [16, 17, 25, 28].

## 4 Penalty alternating minimization methods

In this section we introduce a block alternating minimization algorithm to solve problem (1). Using the combination of variable splitting and a penalty scheme, the proposed procedure solves the inverse eigenvalue problem by iteratively optimizing manifold problems and linearly constrained quadratic problems. Let us start by reformulating problem (1) as follows

$$\min_{X \in \mathbb{R}^{n \times n}} F(X) \quad \text{s.t.} \quad X^\top X = I, \quad P_{I_{\text{knw}}}[\Phi(X) - A] = 0, \quad (6)$$

where  $I_{\text{knw}} = I_0 \cup I_{\text{fix}}$  and  $P_{I_{\text{knw}}}[M]$  is the projection onto the subspace of  $n$ -by- $n$  sparse matrices with nonzero values in the entries indexed by  $I_{\text{knw}}$ , that is,

$$P_{I_{\text{knw}}}[M] = \begin{cases} M_{ij} & \text{if } (i, j) \in I_{\text{knw}}, \\ 0 & \text{otherwise.} \end{cases}$$

An important property of the projection operator  $P_{I_{\text{knw}}}[\cdot]$  is

$$P_{I_{\text{knw}}}[M_1 + \beta M_2] = P_{I_{\text{knw}}}[M_1] + \beta P_{I_{\text{knw}}}[M_2], \quad \forall M_1, M_2 \in \mathbb{R}^{n \times n}, \forall \beta \in \mathbb{R},$$

which indicates that  $P_{I_{\text{knw}}}[\cdot]$  is a linear operator. In addition, observe that the proposed optimization model (6) is well-defined because of the compactness of the feasible set  $\{X \in \mathcal{O}(n) : P_{I_{\text{knw}}}[\Phi(X) - A] = 0\}$  and the continuity of the objective function, which guarantees the existence of global minimizers (even maximizers) for problem (6).

On the other hand, by applying the variable splitting technique to Problem (6), we obtain

$$\min_{X, Y \in \mathbb{R}^{n \times n}} F(X) \quad \text{s.t.} \quad X^\top X = I, \quad P_{I_{\text{knw}}}[Y - A] = 0, \quad Y = \Phi(X). \quad (7)$$

To solve the above problem, we can use the quadratic penalty method to deal with the non-linear constraint  $Y = \Phi(X)$ . It is well-known that, starting from  $(X_0, Y_0)$ , the classic quadratic penalization method solves

$$\min_{X, Y \in \mathbb{R}^{n \times n}} F(X) + \frac{\mu_k}{2} \|Y - \Phi(X)\|_F^2 \quad \text{s.t.} \quad X^\top X = I, \quad P_{I_{\text{knw}}}[Y - A] = 0, \quad (8)$$

at the  $k$ -th iteration for  $(X_{k+1}, Y_{k+1})$ , until convergence, where  $\{\mu_k\}$  is an increasing sequence of positive real numbers such that  $\mu_k \rightarrow \infty$ . However, solving (8) for  $(X, Y)$  simultaneously is challenging because of the complicated form of the constraints. Additionally, the sub-problems (8) cannot be solved analytically due to the non-linearity and non-convexity of the feasible domain.

Using the idea of the classical alternating minimization methods [5], we solve problem (8) with respect to each matrix variable  $X$  and  $Y$  separately, while fixing the other at its previous values, and then the penalty parameter is incremented. Particularly, starting from  $(X_0, Y_0)$  and  $\mu_0 = 1$ , we propose the following framework

$$X_{k+1} = \arg \min_X F(X) + \frac{\mu_k}{2} \|\Phi(X) - Y_k\|_F^2 \quad \text{s.t.} \quad X^\top X = I \quad (9a)$$

$$Y_{k+1} = \arg \min_Y \frac{\mu_k}{2} \|Y - \Phi(X_{k+1})\|_F^2 \quad \text{s.t.} \quad P_{I_{\text{knw}}}[Y - A] = 0 \quad (9b)$$

$$\mu_{k+1} = \rho \mu_k, \quad (9c)$$

where  $\rho > 1$  is a global parameter. The orthogonality constrained sub-problems have no closed solution, thus inner iterations are needed to solve (9a) approximately. In practice, we employ the Riemannian gradient method discussed in Section 3. Nevertheless, the advantage of the iterative process (9a)-(9b)-(9c) is that the second optimization sub-problem has an analytical solution (see Lemma 4.1) given by

$$Y_{k+1} = \Phi(X_{k+1}) + P_{I_{\text{knw}}}[A - \Phi(X_{k+1})]. \quad (10)$$

The following lemma provides the closed-form solution for the optimization problem (9b).

**Lemma 4.1** *Let  $A, B \in \mathbb{R}^{n \times n}$  be two given square matrices. Then, the global solution of the problem*

$$\min_{Y \in \mathbb{R}^{n \times n}} \frac{1}{2} \|Y - B\|_F^2 \quad \text{s.t.} \quad P_{I_{\text{knw}}}[Y - A] = 0, \quad (11)$$

has the following closed-form

$$Y = B + P_{I_{\text{knw}}}[A - B].$$

**Proof.** By introducing a Lagrange multiplier  $\hat{\Lambda} \in \mathbb{R}^{n \times n}$ , so that  $\hat{\Lambda} = P_{I_{\text{knw}}}[\hat{\Lambda}]$ , the Lagrangian function associated with (11) is defined as

$$\mathcal{L}(Y, \hat{\Lambda}) = \frac{1}{2} \|Y - B\|_F^2 - \text{tr}(\hat{\Lambda}^\top P_{I_{\text{knw}}}[Y - A]).$$

Now, differentiating this function, we obtain the Karush-Kuhn-Tucker conditions for Problem (11):

$$Y - B - \hat{\Lambda} = 0 \quad (12)$$

and

$$P_{I_{\text{knw}}}[Y - A] = 0. \quad (13)$$

In view of (12)-(13) and  $P_{I_{\text{knw}}}[\hat{\Lambda}] = \hat{\Lambda}$ , we have

$$\hat{\Lambda} = P_{I_{\text{knw}}}[Y - B] = P_{I_{\text{knw}}}[Y] - P_{I_{\text{knw}}}[B] = P_{I_{\text{knw}}}[A] - P_{I_{\text{knw}}}[B] = P_{I_{\text{knw}}}[A - B].$$

Merging this last result with (12), we arrive at  $Y = B + P_{I_{\text{knw}}}[A - B]$ . Therefore, the pair  $(Y, \hat{\Lambda}) = (B + P_{I_{\text{knw}}}[A - B], P_{I_{\text{knw}}}[A - B])$  is a critical point of the Lagrangian function associated with the linearly constrained optimization problem (11). Finally, since (11) is convex, this critical point is also the global solution. ■

In numerical optimization, proximal-type algorithms [30, 29] are derived by incorporating a proximal term in the objective function to enforce that the new iterate does not stray too far from the previous iterate, such a property will be fundamental in our convergence analysis. Inspired by this strategy, we propose the following modification of the method (9a)-(9b)-(9c),

$$X_{k+1} = \arg \min_X F(X) + \frac{\mu_k}{2} \|\Phi(X) - Y_k\|_F^2 \quad \text{s.t.} \quad X^\top X = I \quad (14a)$$

$$Y_{k+1} = \arg \min_Y \frac{\mu_k}{2} \|Y - \Phi(X_{k+1})\|_F^2 + \frac{\alpha_k}{2} \|Y - Y_k\|_F^2 \quad \text{s.t.} \quad P_{I_{\text{knw}}}[Y - A] = 0 \quad (14b)$$

$$\mu_{k+1} = \rho \mu_k, \quad (14c)$$

where  $\{\alpha_k\} \subset \mathbb{R}^+$ , is a sequence of proximal parameters. The sub-problem (14b) is equivalent to

$$Y_{k+1} = \arg \min_Y \frac{1}{2} \|Y - (\tau_k \Phi(X_{k+1}) + (1 - \tau_k) Y_k)\|_F^2 \quad \text{s.t.} \quad P_{I_{\text{knw}}}[Y - A] = 0,$$

where  $\tau_k := \frac{\mu_k}{\mu_k + \alpha_k} \in (0, 1]$ . Therefore, it follows from Lemma 4.1 that the global solution of (14b) is given by

$$\begin{aligned} Y_{k+1} &= (\tau_k \Phi(X_{k+1}) + (1 - \tau_k) Y_k) + P_{I_{\text{knw}}}[A - (\tau_k \Phi(X_{k+1}) + (1 - \tau_k) Y_k)] \\ &= \tau_k (\Phi(X_{k+1}) + P_{I_{\text{knw}}}[A - \Phi(X_{k+1})]) + (1 - \tau_k) Y_k. \end{aligned} \quad (15)$$

Notice that  $Y_{k+1}$  is the convex combination between the previous iterate and the  $Y_{k+1}$  matrix of the non-altered sub-problem in variable  $Y$  (9b). Later we will see that for suitable choices of  $\alpha_k$ , the sequence  $\{Y_k\}$  generated by the proximal variant satisfies that  $\lim_{k \rightarrow \infty} \|Y_{k+1} - Y_k\|_F = 0$ , this property is crucial in our analysis, and it is not fulfilled for the original iterative scheme (9a)-(9b)-(9c). It is precisely this property that motivates the modification of the original alternating proposal.

## 5 Convergence analysis

This section begins by establishing the necessary first-order optimality conditions of Problem (7). The Lagrangian function associated with this problem is defined by

$$\mathcal{L}(X, Y, \Lambda, \hat{\Lambda}, \tilde{\Lambda}) = F(X) - \frac{1}{2} \langle \Lambda, X^\top X - I \rangle - \langle \hat{\Lambda}, P_{I_{\text{knw}}}[Y - A] \rangle - \langle \tilde{\Lambda}, Y - \Phi(X) \rangle, \quad (16)$$

where the matrices  $\Lambda$ ,  $\hat{\Lambda}$ ,  $\tilde{\Lambda}$  represent the dual variables and satisfy  $\Lambda^\top = \Lambda$  and  $\hat{\Lambda} = P_{I_{knw}}[\hat{\Lambda}]$ , due to the symmetry of the constraint  $X^\top X = I$  and the structure of the restriction  $P_{I_{knw}}[Y - A] = 0$ . By differentiating the mapping (16) with respect to all its block variables, we derive the Karush-Kuhn-Tucker (KKT) conditions (also known as the first-order optimality conditions) for problem (7),

$$\nabla F(X) - X\Lambda + DX(\tilde{\Lambda}^\top + \tilde{\Lambda}) = 0, \quad (17a)$$

$$\hat{\Lambda} + \tilde{\Lambda} = 0, \quad (17b)$$

$$X^\top X - I = 0, \quad (17c)$$

$$P_{I_{knw}}[Y - A] = 0, \quad (17d)$$

$$Y - \Phi(X) = 0. \quad (17e)$$

Let us recall that  $D$  denotes the diagonal matrix formed by the pre-established eigenvalues of  $A$ .

**Proposition 5.1** *The sequences  $\{X_k\}$ ,  $\{Y_k\}$ , generated by the iterative scheme (9a)-(9c), are bounded.*

**Proof.** Since  $X_k^\top X_k = I$  for all  $k \geq 0$ , we have directly that  $\|X_k\|_F = \sqrt{n}$ . Thus, the sequence  $\{X_k\}$  is bounded. In addition, from the updating formula (10), for all  $k$ , we get

$$\begin{aligned} \|Y_{k+1}\|_F &= \|\Phi(X_{k+1}) + P_{I_{knw}}[A - \Phi(X_{k+1})]\|_F \\ &\leq \|\Phi(X_{k+1})\|_F + \|P_{I_{knw}}[A - \Phi(X_{k+1})]\|_F \\ &= \|D\|_F + \|P_{I_{knw}}[A - \Phi(X_{k+1})]\|_F \\ &\leq \|D\|_F + \|A - \Phi(X_{k+1})\|_F \\ &\leq \|D\|_F + \|A\|_F + \|\Phi(X_{k+1})\|_F \\ &= 3\|D\|_F. \end{aligned}$$

Therefore,  $\{Y_k\}$  is also bounded. ■

Now, let  $\{(X_k, Y_k)\}$  be any sequence generated by the alternating scheme (9a)-(9c). From the optimality of the iterates  $X_k$  and  $Y_k$ , for each  $k \geq 0$  there must exist matrices  $\Theta_k$  and  $\hat{\Theta}_k$  (Lagrange multipliers) verifying the following equations

$$\nabla F(X_k) - X_k\Theta_k + 2\mu_{k-1}DX_k(\Phi(X_k) - Y_{k-1}) = 0, \quad (18)$$

and

$$\mu_{k-1}(Y_k - \Phi(X_k)) - \hat{\Theta}_k = 0, \quad (19)$$

respectively.

Before presenting our convergence result for the scheme (9a)-(9c), we need the following remark.

**Remark 5.2** *Notice that all the given eigenvalues, that defines the fixed diagonal matrix  $D$ , can be moved to the positive side of the real line by a constant shift  $\alpha > 0$  for a sufficiently large  $\alpha$ . In this case, the new positive eigenvalues correspond to the eigenvalues of  $A + \alpha I$ , which has the same eigenvectors of  $A$ . Moreover, the structural conditions on the diagonal elements of  $A$  must be adapted according to the sum of  $\alpha > 0$ . Once the problem is solved we can always recover the desired solution matrix  $A$  by subtracting  $\alpha I$ . Hence, for theoretical reasons and without any loss of generality we can assume that the given eigenvalues  $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$  are all positive and that the given matrix  $D$  is non-singular.*

**Theorem 5.3** *Let  $\{(X_k, Y_k)\}$  be a sequence generated by the iterative scheme (9a)-(9c). Let us assume that  $\{\Theta_k\}$  is a bounded sequence and that  $\lim_{k \rightarrow \infty} \|Y_{k+1} - Y_k\|_F = 0$ . Let  $(X_*, Y_*, \Theta_*)$  be a limit point of the sequence  $\{(X_k, Y_k, \Theta_k)\}$ . Then, the pair  $(X_*, Y_*)$  is a KKT point for problem (7).*

**Proof.** It follows from equation (18) that

$$\nabla F(X_{k+1}) - X_{k+1}\Theta_{k+1} + 2\mu_k DX_{k+1}(\Phi(X_{k+1}) - Y_k) = 0, \quad (20)$$

or equivalently

$$2\mu_k DX_{k+1}[(\Phi(X_{k+1}) - Y_{k+1}) + (Y_{k+1} - Y_k)] = X_{k+1}\Theta_{k+1} - \nabla F(X_{k+1}).$$

Then, using the fact that  $X_k \in \mathcal{O}(n)$  for each  $k \geq 0$  and that  $D$  is non-singular (Remark 5.2), we get

$$\Phi(X_{k+1}) - Y_{k+1} = \frac{1}{2\mu_k} X_{k+1}^\top D^{-1} X_{k+1} (\Theta_{k+1} - \nabla F(X_{k+1})) + (Y_k - Y_{k+1}).$$

Applying the Frobenius norm on both sides of the last result, we obtain

$$\begin{aligned} \|\Phi(X_{k+1}) - Y_{k+1}\|_F &= \left\| \frac{1}{2\mu_k} X_{k+1}^\top D^{-1} X_{k+1} (\Theta_{k+1} - \nabla F(X_{k+1})) + (Y_k - Y_{k+1}) \right\|_F \\ &\leq \left\| \frac{1}{2\mu_k} X_{k+1}^\top D^{-1} X_{k+1} (\Theta_{k+1} - \nabla F(X_{k+1})) \right\|_F + \|Y_k - Y_{k+1}\|_F \\ &= \frac{1}{2\mu_k} \|D^{-1} X_{k+1} (\Theta_{k+1} - \nabla F(X_{k+1}))\|_F + \|Y_k - Y_{k+1}\|_F \\ &\leq \frac{1}{2\mu_k} \|D^{-1}\|_F \|\Theta_{k+1} - \nabla F(X_{k+1})\|_F + \|Y_k - Y_{k+1}\|_F, \\ &\leq \frac{1}{2\mu_k} \|D^{-1}\|_F (\|\Theta_{k+1}\|_F + \|\nabla F(X_{k+1})\|_F) + \|Y_k - Y_{k+1}\|_F. \end{aligned} \quad (21)$$

Since  $F(\cdot)$  is continuous and  $\mathcal{O}(n)$  is compact then there exists  $C_1 > 0$  such that  $\|\nabla F(X_k)\|_F \leq C_1$ , for all  $k$ . In addition, from the hypothesis there also exists a constant  $C_2 > 0$  such that  $\|\Theta_k\|_F \leq C_2$ , for any  $k$ . Substituting these two inequalities in (21) we arrive at

$$\|\Phi(X_{k+1}) - Y_{k+1}\|_F \leq \frac{(C_1 + C_2)}{2\mu_k} \|D^{-1}\|_F + \|Y_k - Y_{k+1}\|_F.$$

Applying limits in this last relation, we conclude that

$$\lim_{k \rightarrow \infty} \|\Phi(X_{k+1}) - Y_{k+1}\|_F = 0.$$

Notice that this result directly implies that  $\Phi(X_*) - Y_* = 0$ , which indicates that the pair  $(X_*, Y_*)$  satisfies the KKT condition (17e).

On the other hand, let us introduce the notations  $\tilde{\Lambda}_{k+1} := \mu_k(\Phi(X_{k+1}) - Y_k)$  and  $\hat{\Lambda}_{k+1} := \hat{\Theta}_{k+1} + \mu_k(Y_k - Y_{k+1})$ , where  $\hat{\Theta}_k$  is the matrix that appears in (19). Thus, equation (18) can be rewritten as

$$\nabla F(X_{k+1}) - X_{k+1}\Theta_{k+1} + 2DX_{k+1}\tilde{\Lambda}_{k+1} = 0,$$

which implies that

$$\tilde{\Lambda}_{k+1} = \frac{1}{2} X_{k+1}^\top D^{-1} (X_{k+1}\Theta_{k+1} - \nabla F(X_{k+1})).$$

Hence by taking the limit as  $k \in \mathcal{K}$  goes to  $\infty$ , we find that

$$\tilde{\Lambda}_* := \lim_{k \in \mathcal{K}} \tilde{\Lambda}_{k+1} = \frac{1}{2} X_*^\top D^{-1} (X_*\Theta_* - \nabla F(X_*)).$$

Additionally, observe that the equation (19) can be reformulated as

$$\begin{aligned}
0 &= \mu_k(Y_{k+1} - \Phi(X_{k+1})) - \hat{\Theta}_{k+1} \\
&= \mu_k(Y_k - \Phi(X_{k+1}) + Y_{k+1} - Y_k) - \hat{\Theta}_{k+1} \\
&= -\mu_k(\Phi(X_{k+1}) - Y_k) - (\hat{\Theta}_{k+1} + \mu_k(Y_k - Y_{k+1})) \\
&= -\tilde{\Lambda}_{k+1} - \hat{\Lambda}_{k+1},
\end{aligned}$$

which leads us to

$$\hat{\Lambda}_{k+1} = -\tilde{\Lambda}_{k+1}, \quad \forall k \geq 0. \quad (22)$$

By taking limits in (22), we conclude that

$$\hat{\Lambda}_* := \lim_{k \in \mathcal{K}} \hat{\Lambda}_{k+1} = -\tilde{\Lambda}_*,$$

and consequently

$$\hat{\Lambda}_* + \tilde{\Lambda}_* = 0$$

which establishes the existence of two matrices satisfying the KKT condition (17b).

Similarly, since  $\tilde{\Lambda}_{k+1}$  is a symmetric matrix for all  $k \geq 0$ , the equation (20) can be posed as

$$\nabla F(X_{k+1}) - X_{k+1}\Lambda_{k+1} + DX_{k+1}(\tilde{\Lambda}_{k+1}^\top + \tilde{\Lambda}_{k+1}) = 0,$$

where we are using the notation  $\Lambda_{k+1} := \Theta_{k+1}$ . Here, it is important to note that  $\Lambda_* := \lim_{k \in \mathcal{K}} \Lambda_{k+1} = \Theta_*$ . Hence, applying limits in the previous equality we have

$$\nabla F(X_*) - X_*\Lambda_* + DX_*(\tilde{\Lambda}_*^\top + \tilde{\Lambda}_*) = 0.$$

This indicates that the KKT condition (17a) is also satisfied in the limit. Finally, notice that the KKT condition (17c) is easily verified at  $X^*$  because  $\{X_k\} \subset \mathcal{O}(n)$  and  $\mathcal{O}(n)$  is a closed set; and the condition KKT (17d) is fulfilled trivially by applying the limit, since  $P_{I_{knw}}[Y_k - A] = 0$ , for all  $k \geq 0$ . Therefore the theorem is proved. ■

Let us now analyze the proximal alternating scheme defined by (14a)-(14c).

**Proposition 5.4** *Let  $\{(X_k, Y_k)\}$  be a sequence generated by the iterative scheme (14a)-(14c), starting from a given  $Y_0 \in \mathbb{R}^{n \times n}$  such that  $\|Y_0\|_F \leq 3\|D\|_F$ . Then, the sequences  $\{X_k\}$  and  $\{Y_k\}$  are bounded.*

**Proof.** Clearly the sequence  $\{X_k\}$  is bounded because  $X_k^\top X_k = I$ , for all  $k \geq 0$ . Now we prove that  $\{Y_k\}$  is also bounded. In particular we are going to prove that

$$\|Y_k\|_F \leq 3\|D\|_F, \quad \forall k \geq 0. \quad (23)$$

The proof is by induction. In view of the initialization, (23) is trivially fulfilled for  $k = 0$ . Let us now assume that, for an index  $k \geq 0$ ,  $\|Y_k\|_F \leq 3\|D\|_F$ . Employing (15) and the inductive hypothesis, we obtain

$$\begin{aligned}
\|Y_{k+1}\|_F &= \|\tau_k(\Phi(X_{k+1}) + P_{I_{knw}}[A - \Phi(X_{k+1})]) + (1 - \tau_k)Y_k\|_F \\
&\leq \tau_k\|\Phi(X_{k+1}) + P_{I_{knw}}[A - \Phi(X_{k+1})]\|_F + (1 - \tau_k)\|Y_k\|_F \\
&\leq 3\tau_k\|D\|_F + 3(1 - \tau_k)\|D\|_F \\
&= 3\|D\|_F,
\end{aligned}$$

proving the inequality (23). Therefore  $\{Y_k\}$  is bounded. ■

**Proposition 5.5** *Let  $\{(X_k, Y_k)\}$  be a sequence generated by the iterative process defined by (14a)-(14c), starting from  $Y_0$  such that  $\|Y_0\|_F \leq 3\|D\|_F$ . Assume that the proximal parameter is given by  $\alpha_k = \sigma\mu_k^2$ , for some  $\sigma > 0$ . Then,*

$$\lim_{k \rightarrow \infty} \|Y_{k+1} - Y_k\|_F = 0.$$

**Proof.** It follows from the definition of  $X_{k+1}$  in (14a) that

$$F(X_{k+1}) + \frac{\mu_k}{2} \|Y_k - \Phi(X_{k+1})\|_F^2 \leq F(X_k) + \frac{\mu_k}{2} \|Y_k - \Phi(X_k)\|_F^2. \quad (24)$$

Similarly, from the definition of  $Y_{k+1}$  in (14b), we have

$$\frac{\mu_k}{2} \|Y_{k+1} - \Phi(X_{k+1})\|_F^2 + \frac{\alpha_k}{2} \|Y_{k+1} - Y_k\|_F^2 \leq \frac{\mu_k}{2} \|Y_k - \Phi(X_{k+1})\|_F^2. \quad (25)$$

Combining the inequalities (24) and (25) we get

$$F(X_{k+1}) + \frac{\mu_k}{2} \|Y_{k+1} - \Phi(X_{k+1})\|_F^2 \leq F(X_k) + \frac{\mu_k}{2} \|Y_k - \Phi(X_k)\|_F^2 - \frac{\alpha_k}{2} \|Y_{k+1} - Y_k\|_F^2. \quad (26)$$

By rearranging the inequality (26) we obtain

$$\begin{aligned} \frac{\alpha_k}{2} \|Y_{k+1} - Y_k\|_F^2 &\leq F(X_k) - F(X_{k+1}) + \frac{\mu_k}{2} \|Y_k - \Phi(X_k)\|_F^2 - \frac{\mu_k}{2} \|Y_{k+1} - \Phi(X_{k+1})\|_F^2 \\ &\leq F(X_k) - F(X_{k+1}) + \frac{\mu_k}{2} \|Y_k - \Phi(X_k)\|_F^2 \\ &\leq -F(X_{k+1}) + \frac{\mu_k}{2} \|Y_k - \Phi(X_k)\|_F^2 \\ &\leq \|Q \circ \Phi(X_{k+1})\|_F^2 + \frac{\mu_k}{2} \|Y_k - \Phi(X_k)\|_F^2. \end{aligned}$$

As a consequence,

$$\frac{\alpha_k}{2\mu_k^2} \|Y_{k+1} - Y_k\|_F^2 \leq \frac{1}{\mu_k^2} \|Q \circ \Phi(X_{k+1})\|_F^2 + \frac{1}{2\mu_k} \|Y_k - \Phi(X_k)\|_F^2.$$

It follows from Proposition 5.4 that  $\|Y_k\| \leq 3\|D\|_F$ , for all  $k$ . Using this bound and the formula  $\alpha_k = \sigma\mu_k^2$  provided by the hypothesis, we obtain

$$\begin{aligned} \|Y_{k+1} - Y_k\|_F^2 &\leq \frac{2}{\sigma} \left( \frac{1}{\mu_k^2} \|Q \circ \Phi(X_{k+1})\|_F^2 + \frac{1}{2\mu_k} \|Y_k - \Phi(X_k)\|_F^2 \right) \\ &\leq \frac{2}{\sigma} \left( \frac{1}{\mu_k^2} \|\Phi(X_{k+1})\|_F^2 + \frac{1}{2\mu_k} (\|Y_k\|_F + \|\Phi(X_k)\|_F)^2 \right) \\ &\leq \frac{2}{\sigma} \left( \frac{1}{\mu_k^2} \|D\|_F^2 + \frac{1}{2\mu_k} (3\|D\|_F + \|D\|_F)^2 \right) \\ &= \frac{2}{\sigma} \left( \frac{1}{\mu_k^2} \|D\|_F^2 + \frac{8}{\mu_k} \|D\|_F^2 \right) \\ &\leq \frac{2(1 + 8\mu_k)}{\sigma\mu_k^2} \|D\|_F^2. \end{aligned}$$

By taking limits in both sides of the above relation, and using (14c) we conclude that

$$\lim_{k \rightarrow \infty} \|Y_{k+1} - Y_k\|_F^2 = 0.$$

■

From the optimality of the iterates, for the proximal alternating minimization approach there must exist, at the  $k$ -th iteration, a matrix  $\hat{\Theta}_k$  (Lagrange multiplier) such that for all  $k$

$$\mu_{k-1}(Y_k - \Phi(X_k)) + \alpha_{k-1}(Y_k - Y_{k-1}) - \hat{\Theta}_k = 0.$$

Finally, using Propositions 5.4 and 5.5, and repeating the steps of the proof of Theorem 5.3 with a few slight modifications, we obtain our convergence result for the proximal-type algorithm.

**Theorem 5.6** *Let  $\{(X_k, Y_k)\}$  be a sequence generated by the iterative scheme (14a)-(14c), starting from  $Y_0$  such that  $\|Y_0\|_F \leq 3\|D\|_F$ . Let us assume that  $\{\hat{\Theta}_k\}$  is a bounded sequence. Let  $(X_*, Y_*, \hat{\Theta}_*)$  be a limit point of the sequence  $\{(X_k, Y_k, \hat{\Theta}_k)\}$ . Then, the pair  $(X_*, Y_*)$  is a KKT point for problem (7).*

## 6 A manifold ADMM

In this section we design a Riemannian alternating direction method of multipliers (RADMM) as an alternative to recover the matrix  $A$ . Let us recall the optimization model (7). Instead of penalizing the equality constraint  $Y = \Phi(X)$  to obtain the model (8), we now consider the Lagrangian function associated with (7), given by

$$\begin{aligned} \mathcal{L}_\mu(X, Y, \tilde{\Theta}) &= F(X) + \langle \tilde{\Theta}, Y - \Phi(X) \rangle + \frac{\mu}{2} \|Y - \Phi(X)\|_F^2 \\ &= F(X) + \frac{\mu}{2} \|Y - \Phi(X) + \mu^{-1}\tilde{\Theta}\|_F^2 - \frac{1}{2\mu} \|\tilde{\Theta}\|_F^2, \end{aligned}$$

where  $\tilde{\Theta} \in \mathbb{R}^{n \times n}$  represents the dual variable related to the constraint  $Y = \Phi(X)$ . Starting from  $\tilde{\Theta}_0 = 0$  and  $\mu_0 = 1$ , the classic augmented Lagrangian method (ALM) [6, 7] generates a sequence  $\{(X_k, Y_k, \tilde{\Theta}_k)\}$  by

$$(X_k, Y_k) = \arg \min_{X, Y} \mathcal{L}_{\mu_k}(X, Y, \tilde{\Theta}_k) \quad \text{s.t.} \quad X^\top X = I, \quad P_{I_{\text{knw}}}[Y - A] = 0, \quad (27)$$

then updates the multiplier matrix  $\tilde{\Theta}$  by the recursive formula

$$\tilde{\Theta}_{k+1} = \tilde{\Theta}_k + \mu_k(Y_{k+1} - \Phi(X_{k+1})),$$

and set  $\mu_{k+1} = \rho\mu_k$ , for some global parameter  $\rho > 1$  selected by the user. An efficient approach to solve the subproblem (27) is the well-known alternating direction method of multipliers ADMM [12, 13, 15]. Specifically, we propose the following iterative process:

$$X_{k+1} = \arg \min_X \mathcal{L}_{\mu_k}(X, Y_k, \tilde{\Theta}_k) \quad \text{s.t.} \quad X^\top X = I \quad (28a)$$

$$Y_{k+1} = \arg \min_Y \mathcal{L}_{\mu_k}(X_{k+1}, Y, \tilde{\Theta}_k) \quad \text{s.t.} \quad P_{I_{\text{knw}}}[Y - A] = 0 \quad (28b)$$

$$\tilde{\Theta}_{k+1} = \tilde{\Theta}_k + \mu_k(Y_{k+1} - \Phi(X_{k+1})) \quad (28c)$$

$$\mu_{k+1} = \rho\mu_k, \quad (28d)$$

Here, the subproblem (28a) can be solved by using the Riemannian gradient method described in Section 3, while using Lemma 4.1 the subproblem (28b) has an exact solution given by

$$Y_{k+1} = \Phi(X_{k+1}) - \mu_k^{-1}\tilde{\Theta}_k + P_{I_{\text{knw}}}[A - (\Phi(X_{k+1}) - \mu_k^{-1}\tilde{\Theta}_k)]. \quad (29)$$

We close this section with some remarks. The ALM is an effective tool for solving constrained optimization problems, which has been well studied and enjoys global convergence under certain assumptions, see, e.g., [6, 7] as two standard references. The alternating direction method of multipliers (ADMM) given

by (28) can be seen as an approximated ALM specially designed to solve the non-convex problem (7). In fact, at every cycle, our proposed ADMM scheme (28) needs to solve two optimization subproblems: (28a) and (28b). Problem (28b) is solved exactly using (29), and (28a) minimizes a continuous function on a (non-convex) compact set, and so it has global solutions. We note that the ADMM has been successfully adapted to solve several non-convex problems; see, e.g., matrix completion [32, 34], noisy color image restoration [21], and clustering in pattern recognition [24]. In addition, the global convergence of ADMM for a class of non-convex and non-smooth optimization problems has been established; see, e.g., [12, 13, 15]. Moreover, the ADMM strategy has been extended to solve optimization problems on a manifold, see [20, 22].

## 7 Numerical Results

To give further insight into the inverse structured symmetric matrix problem with given eigenvalues, and to illustrate the practical performance of the proposed algorithms, we present the results of some numerical experiments. We compare several proposed methods: the penalization strategy (3a)-(3b) combined with the Riemannian gradient method based on the QR retraction (R-QR), the same penalization strategy combined with the Riemannian gradient method based on the Cayley retraction (R-Cayley); the proximal alternating approach defined by equations (14a)-(14c) described in Section 4 (Alternating-P); and the Riemannian alternating direction method of multipliers described in Section 6 (Alternating-AL). All considered methods were implemented in Matlab with double precision. The experiments were executed in a laptop computer with CPU Intel core i7, 4.7 GHz, RAM memory of 16 GB.

All runs are terminated as soon as one of the following three conditions holds: a maximum number of iterations (*maxiter*) is reached, the difference in norm of two consecutive iterates is less than or equal to a given tolerance (*tol* > 0), or the Riemannian gradient norm is less than or equal to *tol*. To guarantee that the initial matrix  $X_0$  belongs to the Stiefel manifold, we generate a random symmetric matrix  $W$  such that  $w_{i,j} = 0$  for all pairs  $(i, j) \in I_0$ , and set  $X_0$  to be the orthogonal factor  $Q$  of the  $QR$  factorization of  $W$ . The required input parameters in our algorithms are fixed as follows: *maxiter* = 500, *tol* =  $10^{-5}$ , the growing factor ( $\rho$ ) for the penalty parameters is 1.5, and any of the penalty parameters stop growing when they reach the value  $10^{20}$ . The selected values of *maxiter* and *tol* are sufficient to demonstrate the behavior of the iterative methods and evaluate the obtained solutions. The entries of the matrices  $\hat{\Theta}_k$ , in (28c), are kept between the bounds  $-10^{20}$  and  $10^{20}$ . In our experiments, we report the number of required iterations (Iter), the value of the functions  $f_1(X)$ ,  $f_2(X)$ , and  $f_3(X)$  ( $f_1, f_2, f_3$ ) defined in Lemma 2.1, the orthogonality (Orth) given by  $\|X^\top X - I\|_F$ , and the smallest entry in  $I_{nz}$  in absolute value ( $\min(|NZ|)$ ) at the solution matrix. We also report the final value of the penalty parameters  $\mu_k$  and  $\sigma_k$ , and the required running time in seconds (Time). When a method reaches *maxiter* iterations and the Riemannian gradient norm is still greater than *tol*, we report the symbol (\*\*) under  $f_1$ .

For our first set of experiments, we fix the diagonal entries of  $D$  to be the eigenvalues of the tridiagonal symmetric positive definite  $n \times n$  matrix obtained by discretizing the second-order derivative, over a closed interval in one variable, with zero values at the extreme points. In other words, the given  $\lambda_i$ s are the eigenvalues of the matrix  $tridiag(-1, 2, -1)$ , which can be seen as a special case of the so-called Laplacian matrices that have an impact in chemical graph theory [9, 36]. It is well-known that, for any  $n \geq 2$ , the eigenvalues of  $tridiag(-1, 2, -1)$  are given by  $\lambda_i = 2 - 2\cos(i\pi/(n+1))$  for  $1 \leq i \leq n$ . The considered structure is the following: The operator  $P$  is defined to guarantee that outside of the three main diagonals all entries are zero; i.e.,  $P = tridiag(1, 1, 1)$ . As for additional structural requirements, the entries in the main diagonal are all totally free variables (indicated with the symbol x); there are no nonzero preset values, so  $R = 0$ ,  $C = 0$  and  $\sigma_k = 0$  for all  $k$ ; and all the entries in the main sub-diagonals are free variables that must be nonzero (indicated with the symbol nz), thus the matrix  $Q$  has 1 at the entries of the two main sub-diagonals and zero elsewhere. For example, the given matrix pattern for  $n = 6$  is given

by:

$$\begin{bmatrix} x & \text{nz} & 0 & 0 & 0 & 0 \\ \text{nz} & x & \text{nz} & 0 & 0 & 0 \\ 0 & \text{nz} & x & \text{nz} & 0 & 0 \\ 0 & 0 & \text{nz} & x & \text{nz} & 0 \\ 0 & 0 & 0 & \text{nz} & x & \text{nz} \\ 0 & 0 & 0 & 0 & \text{nz} & x \end{bmatrix},$$

which is identified with a simple undirected graph of 6 vertices [19, pp. 5-8]. For this tridiagonal matrix and for several values of  $n$ , in Table 1 we report the performance of the 4 considered methods: R-QR, R-Cayley, Alternating-P, and Alternating-AL. We note that the eigenvalues of the obtained matrix (although each method obtains a different matrix) are the eigenvalues of  $\text{tridiag}(-1, 2, -1)$ . From Table 1 we also see that, even when the penalty parameter  $\mu_k$  reaches the upper bound  $10^{20}$  or a near-by value, the corresponding method works but it requires many more iterations; see, e.g., the behavior of the R-QR and the Alternating-P schemes for  $n = 10$ . Finally, as expected, for the Alternating-AL scheme the parameter  $\mu_k$  reaches a much smaller value than the one reached by the Alternating-P method.

Table 1: Performance of the 4 considered methods for the inverse structured tridiagonal matrix case.

$n$	Method	Iter	$f_1$	$f_2$	$f_3$	$\mu_k$	Orth	$\min( NZ )$	Time
4	R-QR	47	-4.58	$10^{-11}$	—	$10^6$	$10^{-16}$	0.16	21.8
	R-Cayley	48	-4.51	$10^{-11}$	—	$10^6$	$10^{-13}$	0.13	20.5
	Alternating-P	42	-5.65	$10^{-10}$	—	$10^7$	$10^{-16}$	0.72	2.3
	Alternating-AL	41	-5.33	$10^{-12}$	—	$10^4$	$10^{-16}$	0.37	9.1
7	R-QR	42	-7.86	$10^{-11}$	—	$10^6$	$10^{-15}$	0.28	21.4
	R-Cayley	68	-5.62	$10^{-16}$	—	$10^{10}$	$10^{-12}$	0.06	35.7
	Alternating-P	172	-3.23	$10^{-12}$	—	$10^{18}$	$10^{-16}$	0.15	41.4
	Alternating-AL	38	-8.73	$10^{-10}$	—	$10^5$	$10^{-16}$	0.18	13.6
10	R-QR	143	-2.23	$10^{-15}$	—	$10^{20}$	$10^{-15}$	0.08	77.4
	R-Cayley	47	-7.2	$10^{-12}$	—	$10^7$	$10^{-12}$	0.11	23.8
	Alternating-P	126	-2.87	$10^{-16}$	—	$10^{18}$	$10^{-15}$	0.1	39.6
	Alternating-AL	76	-11.2	$10^{-16}$	—	$10^{10}$	$10^{-15}$	0.12	26.2

For  $n = 4$  we now present the obtained matrices  $A_4^{\text{Alt-P}}$  (left) and  $A_4^{\text{Alt-AL}}$  (right), produced by the Alternating-P and the Alternating-AL methods, respectively. We note that the matrices are different, but they have the same 4 eigenvalues: 0.382, 1.382, 2.618, and 3.618.

$$\begin{bmatrix} 2.1483 & -1.2175 & 0 & 0 \\ -1.2175 & 1.7251 & -0.9095 & 0 \\ 0 & -0.9095 & 2.4111 & -0.7188 \\ 0 & 0 & -0.7188 & 1.7155 \end{bmatrix}, \quad \begin{bmatrix} 2.2188 & -1.5093 & 0 & 0 \\ -1.5093 & 1.7435 & -0.4979 & 0 \\ 0 & -0.4979 & 2.5473 & -0.3709 \\ 0 & 0 & -0.3709 & 1.4903 \end{bmatrix}.$$

For the second experiment, we consider the  $7 \times 7$  symmetric Laplacian matrix described in [36, Table II, p. 369]. These matrices have a potential for use in chemical graph theory. We fix the diagonal entries of  $D$  to be the eigenvalues of the matrix displayed in [36], i.e., the given eigenvalues are: 0, 0.3672, 1.0571,

2.3745, 4.4681, 7.0357, and 8.6973. The required structural pattern is the following:

$$\begin{bmatrix} x & nz & 0 & 0 & 0 & 0 & 0 \\ nz & x & nz & 0 & 0 & 0 & -3 \\ 0 & nz & x & nz & 0 & -3 & 0 \\ 0 & 0 & nz & x & nz & 0 & 0 \\ 0 & 0 & 0 & nz & x & 0 & 0 \\ 0 & 0 & -3 & 0 & 0 & x & 0 \\ 0 & -3 & 0 & 0 & 0 & 0 & x \end{bmatrix},$$

which is identified with the undirected weighted graph (a linear tree in this case) of the 2,3-Dimethyl pentane, shown in Figure 1. In Table 2 we report the behavior of the 4 considered methods for this  $7 \times 7$  Laplacian matrix. In all cases, the structural requirements are satisfied and the 7 eigenvalues are the given ones.

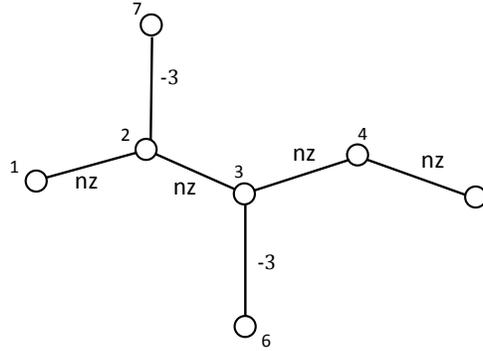


Figure 1: Structural pattern graph of the symmetric Laplacian matrix (2,3-Dimethyl pentane).

Table 2: Performance of the 4 considered methods for the  $7 \times 7$  symmetric Laplacian case.

Method	Iter	$f_1$	$f_2$	$f_3$	$\mu_k$	$\sigma_k$	Orth	$\min( NZ )$	Time
R-QR	142	-18.3	$10^{-15}$	$10^{-19}$	$10^{20}$	$10^{20}$	$10^{-15}$	0.33	49.7
R-Cayley	198	-16.5	$10^{-14}$	$10^{-17}$	$10^{20}$	$10^{20}$	$10^{-12}$	0.26	91.5
Alternating-P	169	-4.42	$10^{-10}$	$10^{-12}$	$10^{20}$	—	$10^{-16}$	0.12	50.2
Alternating-AL	59	-13.9	$10^{-12}$	$10^{-14}$	$10^6$	—	$10^{-15}$	0.15	23.4

We notice that, for the 4 methods, the structural requirements are satisfied and the 7 eigenvalues are the given ones. As an example, we now present the matrix  $A_7^{Alt-AL}$  obtained by the Alternating-AL method:

$$\begin{bmatrix} 2.3980 & 1.0306 & 0 & 0 & 0 & 0 & 0 \\ 1.0306 & 6.5352 & -1.0112 & 0 & 0 & 0 & -3 \\ 0 & -1.0112 & 5.4677 & -0.1578 & 0 & -3 & 0 \\ 0 & 0 & -0.1578 & 1.9569 & 2.2133 & 0 & 0 \\ 0 & 0 & 0 & 2.2133 & 2.5202 & 0 & 0 \\ 0 & 0 & -3 & 0 & 0 & 2.9671 & 0 \\ 0 & -3 & 0 & 0 & 0 & 0 & 2.1548 \end{bmatrix}.$$

For our third experiment, let us consider the  $4 \times 4$  symmetric matrix indicated in [35, p. 265], in which the only nonzero fixed value is  $\pi$  at the  $(2, 2)$  entry.

$$\begin{bmatrix} x & x & \text{nz} & 0 \\ x & \pi & \text{nz} & x \\ \text{nz} & \text{nz} & x & 0 \\ 0 & x & 0 & \text{nz} \end{bmatrix}.$$

We note that the associated undirected graph is not a tree since it has a cycle (vertices 1, 2, and 3). In this case, we fix the given eigenvalues to be 1, 2, 3, and 4. Since the four eigenvalues are different, the existence of a symmetric matrix with the described pattern is guaranteed [19, Chapter 11]. In Table 3 we report the behavior of the 4 considered methods for this  $4 \times 4$  matrix. In all cases, all the structural requirements are satisfied and the 4 obtained eigenvalues are the given ones. We present the 4 different obtained solution matrices  $A_4^{R-QR}$  (up-left),  $A_4^{R-Cayley}$  (up-right),  $A_4^{Alt-P}$  (down-left), and  $A_4^{Alt-AL}$  (down-right), produced by the R-QR, R-Cayley, Alternating-P, and Alternating-AL methods:

$$\begin{bmatrix} 1.0447 & 0.3031 & 0.1156 & 0 \\ 0.3031 & 3.1416 & 0.8863 & -0.4011 \\ 0.1156 & 0.8863 & 2.7724 & 0 \\ 0 & -0.4011 & 0 & 3.0414 \end{bmatrix}, \begin{bmatrix} 1.8230 & -0.3693 & -1.2722 & 0 \\ -0.3693 & 3.1416 & 0.2045 & 0.0326 \\ -1.2722 & 0.2045 & 3.0345 & 0 \\ 0 & 0.0326 & 0 & 2.001 \end{bmatrix}$$

$$\begin{bmatrix} 1.1665 & -0.1108 & 0.3620 & 0 \\ -0.1108 & 3.1416 & 0.1030 & 0.3614 \\ 0.3620 & 0.1030 & 1.8456 & 0 \\ 0 & 0.3614 & 0 & 3.8464 \end{bmatrix}, \begin{bmatrix} 3.0773 & -0.2011 & 0.4089 & 0 \\ -0.2011 & 3.1416 & -1.0775 & 0.5837 \\ 0.4089 & -1.0775 & 1.6742 & 0 \\ 0 & 0.5837 & 0 & 2.1069 \end{bmatrix}.$$

Table 3: Performance of the 4 methods for the  $4 \times 4$  symmetric matrix indicated above.

Method	Iter	$f_1$	$f_2$	$f_3$	$\mu_k$	$\sigma_k$	Orth	$\min( NZ )$	Time
R-QR	50	-10.8	$10^{-12}$	$10^{-20}$	$10^6$	$10^8$	$10^{-16}$	0.115	17.8
R-Cayley	62	-7.3	$10^{-14}$	$10^{-22}$	$10^6$	$10^8$	$10^{-13}$	0.204	20.6
Alternating-P	128	-14.8	$10^{-12}$	$10^{-20}$	$10^{12}$	—	$10^{-16}$	0.103	17.1
Alternating-AL	58	-14.9	$10^{-12}$	$10^{-20}$	$10^7$	—	$10^{-16}$	0.4	3.5

For the fourth and last experiment, we consider the  $10 \times 10$  symmetric matrix described in [19, p. 150], which is identified with the undirected graph shown in Figure 2. This graph is the smallest possible nonlinear tree; see [19, Section 5]. Following the description in [19, p. 150], we fix the given eigenvalues to be -3, -2, -2, 0, 0, 0, 0, 2, 2, and 3. These 5 eigenvalues together with their multiplicity guarantee that there are possible solutions to the inverse structural matrix problem; see [19, Section 6]. The required structural pattern is the following:

$$\begin{bmatrix} 0 & 0 & \text{nz} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \text{nz} & \sqrt{2} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \sqrt{2} & 0 & 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & \text{nz} & \text{nz} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \text{nz} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \text{nz} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 & \text{nz} & \text{nz} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \text{nz} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \text{nz} & 0 & 0 \end{bmatrix}.$$

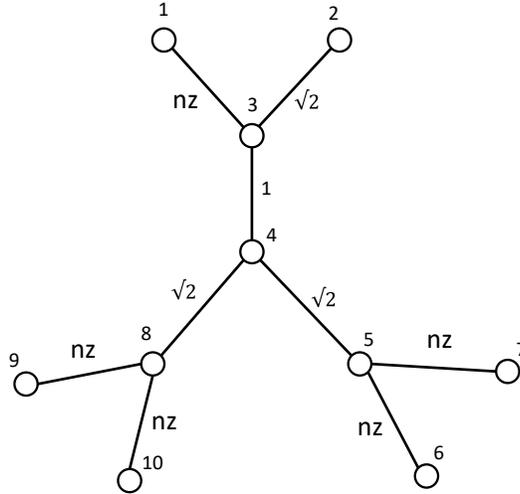


Figure 2: Structural pattern graph of the symmetric matrix described in [19, p. 150].

In Table 4 we report the behavior of the 4 considered methods for this  $10 \times 10$  matrix. It can be observed that the methods R-QR and R-Cayley could not find a solution after 500 iterations, while the Alternating schemes were able to find a solution for which all the structural requirements are satisfied and the 10 obtained eigenvalues are the given ones. We note that after 500 iterations for both R-QR and R-Cayley the achieved eigenvalues are already the right ones, however the Riemannian gradient norm is still of the order of  $10^{-2}$ , and so when the process is stopped the values of  $f_2$  and  $f_3$  are not sufficiently close to zero. We now present the matrix  $A_{10}^{Alt-AL}$  obtained after 50 iterations by the Alternating-AL method:

$$A_{10}^{Alt-AL} = \begin{bmatrix} 0 & 0 & 1.4142 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.4142 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1.4142 & 1.4142 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1.4142 & 0 & 0 & 0 & 1.4142 & 0 & 0 \\ 0 & 0 & 0 & 1.4142 & 0 & -0.1893 & 1.991 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.1893 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.991 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.4142 & 0 & 0 & 0 & 0 & -1.1971 & 1.6022 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1.1971 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.6022 & 0 & 0 \end{bmatrix}.$$

We also present the matrix  $A_{10}^{Alt-P}$  obtained after 55 iterations by the Alternating-P method, by simply showing the entries that differ with respect to  $A_{10}^{Alt-AL}$ :  $A_{10}^{Alt-P}(5, 6) = A_{10}^{Alt-P}(6, 5) = -0.0375$ ,  $A_{10}^{Alt-P}(5, 7) = A_{10}^{Alt-P}(7, 5) = 1.9996$ ,  $A_{10}^{Alt-P}(8, 9) = A_{10}^{Alt-P}(9, 8) = -0.712$ , and  $A_{10}^{Alt-P}(8, 10) = A_{10}^{Alt-P}(10, 8) = 1.869$ . It should be noted that [19, p. 127] presents yet another solution, which was obtained manually using the interlacing theorem and other useful matrix analysis results.

Table 4: Performance of the 4 considered methods for the  $10 \times 10$  matrix described in [35, p. 150].

Method	Iter	$f_1$	$f_2$	$f_3$	$\mu_k$	$\sigma_k$	Orth	$\min( NZ )$	Time
R-QR	500	**	$10^{-1}$	$10^{-2}$	$10^{20}$	$10^{20}$	$10^{-15}$	**	**
R-Cayley	500	**	$10^{-1}$	$10^{-2}$	$10^{20}$	$10^{20}$	$10^{-12}$	**	**
Alternating-P	55	-19.8	$10^{-11}$	$10^{-11}$	$10^9$	—	$10^{-15}$	0.037	23.8
Alternating-AL	50	-19.9	$10^{-11}$	$10^{-11}$	$10^5$	—	$10^{-15}$	0.189	23.5

## 8 Concluding Remarks

We have focused on the inverse structured symmetric matrix problem for which certain entries have preassigned values, including a sparse pattern, and such that the desired matrix eigenvalues are given in advance. In principle, the variables of the problem are the rest of the entries, but it is desired that some of them are nonzero, while the others are completely free. For this problem, we have presented a continuously differentiable optimization model in the space of square matrices, which attempts to achieve all the stated objectives only using the orthogonal eigenvector matrix of the solution as a variable. It should be noted that with only this matrix as an unknown a solution can be achieved, even though this matrix alone has no explicit value once the problem is solved.

To solve these challenging problems, we have developed several iterative methods that keep the iterations on the Stiefel manifold of orthogonal matrices. In particular, we have combined a Riemmanian gradient-type method with a non-monotone line search globalization strategy and with two types of retraction operators to stay on the manifold: QR and Cayley. The proposed Riemmanian gradient schemes have been applied as internal methods of a penalty machinery that enforces the structural requirements by imposing the orthogonality of the variable matrix as the only constraint, producing the R-QR and the R-Cayley methods. In our numerical experiments we have observed the standard tendency of the penalty parameters to grow to very high values to guarantee convergence. As a remedy to this numerical difficulty, we have also proposed a block alternating scheme based on a suitable variable splitting. One of the alternating steps is combined with either a penalty or an augmented Lagrangian strategy, and the other alternating step is solved by a conveniently obtained closed formula.

In our numerical section we add understanding to the topic by illustrating the connection between the desired symmetric matrix and the associated undirected graph. In particular, we take advantage of knowledge recently developed in this line of research known as a spectral graph theory. First, as expected from the formulation of the original inverse matrix problem and the non-convexity of our optimization model, we note that if the problem has a solution, then it has many different solutions. In our experiments, we have observed that the 4 considered methods tend to produce 4 different solutions for each matrix problem and for each initial  $X_0$ . This is a positive outcome for the user's choice. Moreover, although our experiments only involved cases where we knew that solutions existed for the structure under consideration, the proposed numerical methods can also be applied to problems where the existence of a solution is uncertain. Indeed, the optimization problems considered involve a continuous function over a compact set. In this sense, the proposed schemes can be a useful tool for researchers in the field of spectral graph theory to conjecture and discover achievable structures. This line of thought deserves further investigation.

We have also observed that the Alternating-P and the Alternating-AL schemes present better practical performance compared to the R-QR and R-Cayley methods, especially when the size of the matrices increases. Furthermore, in the case of the nonlinear tree with  $n = 10$ , only the alternating methods were able to find a solution with few iterations, the other two exhibit a slow convergence and reached the limit of 500 iterations without driving the norm of the Riemmanian gradient below the preestablished tolerance. In general, we have observed that the alternating schemes are effective up to  $n = 20$ , which includes all the graphs analyzed in [19, Appendix A], and require a significant number of iterations and a high computational cost when  $n > 20$ . To address potential large-scale cases in the future, it may be necessary to adapt the ideas presented in this work or develop other optimization schemes to avoid the  $O(n^3)$  computational cost of each retraction.

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**Data availability.** The codes and data sets generated during the current study are available from the corresponding author on reasonable request.

**Conflicts of interest.** No potential conflict of interest was reported by the authors.

**Consent for publication.** All authors read and approved the submission of the final manuscript.

**Author's contributions.** JPC: study, conception, design, data collection, conceptualization, methodology and formal analysis. HO: study, conception, design, data collection, conceptualization, methodology and formal analysis. MR: study, conception, design, data collection, conceptualization, methodology and formal analysis.

## References

- [1] P. A. Absil, R. Mahony, and R. Sepulchre [2008], *Optimization algorithms on matrix manifolds*, Princeton University Press. DOI: <https://doi.org/10.1515/9781400830244>
- [2] Z.-J. Bai, R. H. Chan, and B. Morini [2004], *An inexact Cayley transform method for inverse eigenvalue problems*, *Inverse Problems*, 20(5): 1675. DOI: 10.1088/0266-5611/20/5/022
- [3] Z.-J. Bai, B. Morini, and S.-F. Xu [2007], *On the local convergence of an iterative approach for inverse singular value problems*, *Journal of Computational and Applied Mathematics*, 198: 344–360. DOI: 10.1016/j.cam.2005.06.050
- [4] J. Barzilai and J. M. Borwein [1988], *Two-point step size gradient methods*, *IMA J. Numer. Anal.*, 8: 141–148. DOI: <https://doi.org/10.1093/imanum/8.1.141>
- [5] A. Beck [2015], *On the convergence of alternating minimization for convex programming with applications to iteratively reweighted least squares and decomposition schemes*, *SIAM J. Optim.*, 25(1): 185–209. DOI: <https://doi.org/10.1137/13094829X>
- [6] D. Bertsekas [1982], *Constrained optimization and Lagrange multiplier methods*, Academic Press, New York.
- [7] E. Birgin and J. M. Martínez [2014], *Practical augmented Lagrangian methods for constrained optimization*, SIAM, Philadelphia.
- [8] N. Boumal [2023], *An introduction to optimization on smooth manifolds*, Cambridge University Press, Cambridge. DOI: <https://doi.org/10.1017/9781009166164>
- [9] D. Cvetković, P. Rowlinson, and S. L. Simić [2009], *An Introduction to the Theory of Graph Spectra*, Cambridge University Press, Cambridge. DOI: <https://doi.org/10.1017/CB09780511801518>
- [10] M. T. Chu [1998], *Inverse eigenvalue problems*, *SIAM Rev.*, 40(1): 1–39. DOI: <https://doi.org/10.1137/S0036144596303984>

- [11] M. T. Chu and G. H. Golub [2002], *Structured inverse eigenvalue problems*, Acta Numerica, 1(1): 1–71. DOI: [10.1017/S0962492902000014](https://doi.org/10.1017/S0962492902000014)
- [12] W. Deng and W. Yin [2016], *On the global and linear convergence of the generalized alternating direction method of multipliers.*, J. Sci. Comput., 66: 889–916. DOI: <https://doi.org/10.1007/s10915-015-0048-x>
- [13] J. Eckstein and W. Yao [2015], *Understanding the convergence of the alternating direction method of multipliers: Theoretical and computational perspectives*, Pac. J. Optim., 11(4): 619–644.
- [14] A. Edelman, T. Arias and S. Smith [1998], *The geometry of algorithms with orthogonality constraints*, SIAM J. Matrix Anal. Appl., 20(2): 303–353. DOI: <https://doi.org/10.1137/S0895479895290954>
- [15] M. Hong and Z. Luo [2017], *On the linear convergence of the alternating direction method of multipliers.*, Math. Program., 162(1-2): 165–199. DOI: <https://doi.org/10.1007/s10107-016-1034-2>
- [16] J. Hu, X. Liu, Z. Wen and Y.-X. Yuan [2020], *A brief introduction to manifold optimization*, Journal of the Operations Research Society of China, 8: 199–248. DOI: <https://doi.org/10.1007/s40305-020-00295-9>
- [17] B. Iannazzo and M. Porcelli [2018], *The Riemannian Barzilai-Borwein method with nonmonotone line search and the matrix geometric mean computation*, IMA Journal of Numerical Analysis, 38(1): 495–517. DOI: <https://doi.org/10.1093/imanum/drx015>
- [18] B. Jiang and Y.-H. Dai [2015], *A framework of constraint preserving update schemes for optimization on Stiefel manifold*, Mathematical Programming, 153(2): 535–575. DOI: <https://doi.org/10.1007/s10107-014-0816-7>
- [19] C. R. Johnson and C. M. Saiago [2018], *Eigenvalues, multiplicities and graphs*, volume 211 of Cambridge Tracts in Mathematics, Cambridge University Press, Cambridge. DOI: <https://doi.org/10.1017/9781316155158>
- [20] A. Kovnatsky, K. Glashoff and M. Bronstein [2016], *MADMM: a generic algorithm for non-smooth optimization on manifolds.*, In: Computer Vision-ECCV 2016, 14th European Conference, Amsterdam, The Netherlands, October 11-14, 2016, Proceedings, Part V14 (pp. 680–696).
- [21] R. Lai and S. Osher [2014], *A splitting method for orthogonality constrained problems.* J. Sci. Comput., 58: 431–449. DOI: <https://doi.org/10.1007/s10915-013-9740-x>
- [22] J. Li, S. Ma and T. Srivastava [2022], *A Riemannian ADMM*, arXiv preprint arXiv:2211.02163.
- [23] D.G. Luenberger [1984], *Linear and Nonlinear Programming*, Addison-Wesley, Menlo Park, CA. DOI: <https://doi.org/10.1007/978-0-387-74503-9>
- [24] C. Lu, J. Feng, Z. Lin and S. Yan [2018], *Nonconvex sparse spectral clustering by alternating direction method of multipliers and its convergence analysis.* In Proceedings of the AAAI Conference on Artificial Intelligence (Vol. 32, No. 1). DOI: <https://doi.org/10.1609/aaai.v32i1.11658>
- [25] H. Oviedo, H. Lara, and O. Dalmau [2019], *A non-monotone linear search algorithm with mixed direction on Stiefel manifold*, Optimization Methods and Software, 34(2): 437–457. DOI: <https://doi.org/10.1080/10556788.2017.1415337>
- [26] H. Oviedo and H. Lara [2021], *Spectral residual method for nonlinear equations on Riemannian manifolds*, Computational and Applied Mathematics, 40(238): 1–23. DOI: <https://doi.org/10.1007/s40314-021-01630-3>

- [27] H. Oviedo, H. Lara and O. Dalmau [2021], *Two adaptive scaled gradient projection methods for Stiefel manifold constrained optimization*, Numerical Algorithms, 87: 1107–1127. DOI: <https://doi.org/10.1007/s11075-020-01001-9>
- [28] H. Oviedo [2022], *Global convergence of Riemannian line search methods with a Zhang-Hager-type condition*, Numerical Algorithms, 91(3): 1183–1203. DOI: <https://doi.org/10.1007/s11075-022-01298-8>
- [29] H. Oviedo [2023], *Proximal Point Algorithm with Euclidean Distance on the Stiefel Manifold*, Mathematics, 11(11): 2414. DOI: <https://doi.org/10.3390/math11112414>
- [30] N. Parikh and S. Boyd [2014], *Proximal Algorithms*, Foundations and Trends in Optimization, 1(3): 127–239. DOI: <http://dx.doi.org/10.1561/24000000003>
- [31] M. Plumbley [2004], *Lie group methods for optimization with orthogonality constraints*, In: Independent Component Analysis and Blind Signal Separation: Fifth International Conference, ICA 2004, Granada, Spain, September 22–24, 2004. Proceedings 5 (pp. 1245–1252). Springer Berlin Heidelberg. DOI: [https://doi.org/10.1007/978-3-540-30110-3\\_157](https://doi.org/10.1007/978-3-540-30110-3_157)
- [32] Y. Shen, Z. Wen and Y. Zhang [2014], *Augmented Lagrangian alternating direction method for matrix separation based on low-rank factorization* Optim. Methods Softw., 29(2): 239–263. DOI: <https://doi.org/10.1080/10556788.2012.700713>
- [33] G. Steidl and M. Winklery [2022], *A New Constrained Optimization Model for Solving the Nonsymmetric Stochastic Inverse Eigenvalue Problem*, Linear and Multilinear Algebra, 70(18): 3419–3448. DOI: <https://doi.org/10.1080/03081087.2020.1841077>
- [34] D. L. Sun and C. Fevotte [2014], *Alternating direction method of multipliers for non-negative matrix factorization with the beta-divergence*. In 2014 IEEE international conference on acoustics, speech and signal processing (ICASSP) (pp. 6201–6205).
- [35] B. Sutton [2019], *Numerical construction of structured matrices with given eigenvalues*, Spec. Matrices, 7: 263–271. DOI: <https://doi.org/10.1515/spma-2019-0020>
- [36] N. Trinajstić, D. Babić, S. Nikolić, D. Plavšić, D. Amić, and Z. Mihalić [1994], *The Laplacian matrix in chemistry*, J. Chem. Znf. Comput. Sci., 34: 386–376. DOI: <https://doi.org/10.1021/ci00018a023>
- [37] S. Wasserman and K. Kaust [1994], *Social Networks Analysis– Methods and Applications*, Cambridge University Press, Cambridge. DOI: <https://doi.org/10.1017/CB09780511815478>
- [38] T.-T. Yao, Z.-J. Bai and Z. Zhao [2019], *A Riemannian variant of the Fletcher-Reeves conjugate gradient method for stochastic inverse eigenvalue problems with partial eigendata*, Numer Linear Algebra Appl., 26: e2221. DOI: <https://doi.org/10.1002/nla.2221>
- [39] H. Zhang and W. W. Hager [2004], *A nonmonotone line search technique and its application to unconstrained optimization*, SIAM J. Optim., 14: 1043–1056. DOI: <https://doi.org/10.1137/S1052623403428208>
- [40] Z. Zhao, X.-Q. Jin, and Z.-J. Bai [2016], *A geometric nonlinear conjugate gradient method for stochastic inverse eigenvalue problems*, SIAM J. Numer. Anal., 54(4): 2015–2035. DOI: <https://doi.org/10.1137/140992576>