

Factorization of completely positive matrices using iterative projected gradient steps

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Abstract. We aim to factorize a completely positive matrix by using an optimization approach which consists in the minimization of a nonconvex smooth function over a convex and compact set. To solve this problem we propose a projected gradient algorithm with parameters that take into account the effects of relaxation and inertia. Both projection and gradient steps are simple in the sense that they have explicit formulas and do not require inner loops. Furthermore, no expensive procedure to find an appropriate starting point is needed. The convergence analysis shows that the whole sequence of generated iterates converges to a critical point of the objective function and it makes use of the Lojasiewicz inequality. Its rate of convergence expressed in terms of the Lojasiewicz exponent of a regularization of the objective function is also provided. Numerical experiments demonstrate the efficiency of the proposed method, in particular in comparison to other factorization algorithms, and emphasize the role of the relaxation and inertial parameters.

Key Words. matrix factorization, completely positive matrices, nonconvex optimization, relaxed-inertial projected gradient algorithm, Lojasiewicz inequality

AMS subject classification. 15A23, 15B48, 65K10, 90C26, 90C30

1 Introduction

A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is called *completely positive* if there exists an entrywise nonnegative matrix $X \in \mathbb{R}_+^{n \times r}$ such that

$$A = XX^T.$$

Let

$$\mathcal{CP}_n := \{A \in \mathbb{R}^{n \times n} : A = XX^T \text{ with } X \in \mathbb{R}_+^{n \times r}, r \geq 1\} \quad (1.1)$$

denote the set of $n \times n$ completely positive matrices. This set is a *proper cone* whose extreme rays are the rank-one matrices xx^T with $x \in \mathbb{R}_+^n$ (see [10]), thus

$$\mathcal{CP}_n = \text{conv} \{xx^T : x \in \mathbb{R}_+^n\},$$

where conv stands for the convex hull operator.

The factorization of a nonzero completely positive matrix A is never unique. Moreover, the number of columns of the factor X can vary (see [25, 33]), which gives rise to the following notion.

Let $A \in \mathbb{R}^{n \times n}$. The *cp-rank* of A is defined as

$$\text{cpr}(A) := \inf \{r \geq 1 : \exists X \in \mathbb{R}_+^{n \times r}, A = XX^T\}.$$

The majority of the known numerical methods aiming to factorize a completely positive matrix are sensitive to its cp-rank.

The *cp⁺-rank* of A is defined as

$$\text{cpr}^+(A) := \inf \{r \geq 1 : \exists X \in \mathbb{R}_{++}^{n \times r}, A = XX^T\},$$

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where $\mathbb{R}_{++}^{n \times r}$ denotes the set of matrices in $\mathbb{R}_+^{n \times r}$ which have at least one positive column. The cp^+ -rank is useful when characterizing the interior of the cone of completely positive matrices. Indeed, as showed by Dickinson in [25, Theorem 3.8], this can be characterized as

$$\text{int}(\mathcal{CP}_n) = \{A \in \mathbb{R}^{n \times n} : \text{rank}(A) = n, A = XX^T, X \in \mathbb{R}_{++}^{n \times r}\}. \quad (1.2)$$

The problem of computing the cp-rank of a matrix is in general open (see [11]). However, upper bounds for the cp-rank have been derived by Bomze, Dickinson and Still in [17, Theorem 4.1], namely, for $A \in \mathcal{CP}_n$, it holds

$$\text{cpr}(A) \leq \text{cp}_n := \begin{cases} n & \text{for } n \in \{2, 3, 4\}, \\ \frac{1}{2}n(n+1) - 4 & \text{for } n \geq 5. \end{cases}$$

Moreover, if $A \in \text{int}(\mathcal{CP}_n)$, then

$$\text{cpr}^+(A) \leq \text{cp}_n^+ := \begin{cases} n+1 & \text{for } n \in \{2, 3, 4\}, \\ \frac{1}{2}n(n+1) - 3 & \text{for } n \geq 5. \end{cases}$$

Notice that there exists matrices $A \in \text{int}(\mathcal{CP}_n)$ such that $\text{cpr}(A) \neq \text{cpr}^+(A)$.

Closely related to the completely positive matrices is the class of *copositive matrices*

$$\mathcal{COP}_n := \{A \in \mathbb{S}^{n \times n} : x^T A x \geq 0 \quad \forall x \in \mathbb{R}_+^n\},$$

where $\mathbb{S}^{n \times n}$ denotes the set of $n \times n$ symmetric matrices. In fact, \mathcal{CP}_n is the *dual cone* of \mathcal{COP}_n (see, for instance, [10]), namely,

$$\mathcal{CP}_n = (\mathcal{COP}_n)^* := \{A \in \mathbb{S}^{n \times n} : \langle A, B \rangle \geq 0 \quad \forall B \in \mathcal{COP}_n\}.$$

Here, $\langle \cdot, \cdot \rangle$ denotes the *Frobenius inner product* (see Section 2 for the precise definition).

Many relaxations of combinatorial optimization problems and of nonconvex quadratic optimization problems can be formulated as linear problems over \mathcal{CP}_n or \mathcal{COP}_n . Since the objective function and the constraint functions are linear, the challenge when addressing these is entirely transferred in the proper handling of the cone constraints. Consequently, copositive and completely positive matrices have received considerable attention in recent years (see, for instance, [16, 22, 31]). The application fields, where copositive and completely positive matrices appear, include block design, complementarity problems, projections in energy demand, the Markovian modelling of DNA evolutions, and maximin efficiency robust tests, see [10] and the references therein.

We illustrate this approach for a nonconvex quadratic programming problem

$$\begin{aligned} & \min_{x \in \mathbb{R}^n} x^T M x. \\ & \text{s.t. } \mathbf{j}_n^T x = 1, \\ & \quad x \in \mathbb{R}_+^n, \end{aligned} \quad (1.3)$$

where $M \in \mathbb{S}^{n \times n}$ and \mathbf{j}_n denotes the all-ones vector in \mathbb{R}^n . If M is not a positive semidefinite matrix, then (1.3) is a nonconvex optimization problem which is usually NP-hard and exhibits numerous local minima. Observe that the objective function of (1.3) can be rewritten in terms of the Frobenius inner product as for $X = xx^T$, it holds $x^T M x = \langle M, xx^T \rangle = \langle M, X \rangle$. In the same fashion, the constraint $\mathbf{j}_n^T x = 1$ implies $\langle \mathbf{j}_n \mathbf{j}_n^T, X \rangle = 1$. Therefore, the optimization problem

$$\begin{aligned} & \min_{X \in \mathbb{R}^{n \times n}} \langle M, X \rangle. \\ & \text{s.t. } \langle \mathbf{j}_n \mathbf{j}_n^T, X \rangle = 1, \\ & \quad X \in \mathcal{CP}_n, \end{aligned} \quad (1.4)$$

is a convex relaxation of the nonconvex quadratic problem (1.3). In [18] it has been shown how optimal solutions of (1.4) can be related to optimal solutions of (1.3). Let X_* be an optimal solution of (1.4). If X_* is of rank one, then it can be expressed as $X_* = x_* x_*^T$ and therefore x_* is an optimal solution

of (1.3). If $\text{rank}(X_*) > 1$, then X_* can be factorized as $X_* = \sum_{i=1}^r x_i x_i^T$ and it can be shown that an appropriately scaled version of each x_i is an optimal solution of (1.3).

Another class of matrices related to the completely positive matrices is the one of *doubly nonnegative matrices*, which are real positive semidefinite square matrices with nonnegative entries, namely, $\mathcal{DN}\mathcal{N}_n := \mathbb{S}^{n \times n} \cap \mathbb{R}_+^{n \times n}$. One has in general

$$\mathcal{CP}_n \subseteq \mathcal{DN}\mathcal{N}_n,$$

whereas, for $n \leq 4$, the inclusion becomes an equality (see [10, 31]). However, for $n \geq 5$, the inclusion is strict; for example (see [11])

$$A := \begin{pmatrix} 1 & 1 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 3 \end{pmatrix} \in \mathcal{DN}\mathcal{N}_5 \setminus \mathcal{CP}_5.$$

Checking membership of a matrix to \mathcal{CP}_n is known to be a NP-hard problem, as it has been proved by Dickinson and Gijben in [27]. Jarre and Schmallowsky proposed in [34] a method which provides a certificate for a given matrix to be completely positive. Their approach is based on an augmented primal-dual method and aims to solve a certain second order cone problem. Eventually, it is necessary to solve Lyapunov equations to obtain a completely positive factorization.

One of the main challenge when dealing with completely positive matrices is their efficient factorization ([10, 26, 33]). This is a question of high relevance in many applications, as, for example, in the statistics of multivariate extremes. Cooley and Thibaud have shown in [24] that the tail dependence of a multi-variate regularly-varying random vector can be summarized in a so-called tail pairwise dependence matrix Σ of pairwise dependence metrics. This matrix Σ can be shown to be completely positive, and a nonnegative factorization of it can be used to estimate probabilities of extreme events or to simulate realizations with pairwise dependence summarized by Σ . This approach is used in [24] to study data describing daily precipitation measurements. Further applications of the nonnegative factorization of completely positive matrices can be found in data mining and clustering ([28]), and in automatic control ([13, 44]).

Sponsel and Dür developed in [57] an algorithm for determining the projection of a matrix onto the copositive cone \mathcal{COP}_n . This method can be also used to compute completely positive factorizations, however, for reasonably big input matrices, the algorithm runs into memory problems. In [49], Nie treats the completely positive factorization problem as a special case of an \mathcal{A} -truncated K -moment problem, for which an algorithm is developed based on the solving of a sequence of semidefinite optimization problems. From the numerical point of view this method is expensive, the reported numerical experiments demonstrate the factorization of completely positive matrices only up to order 8×8 .

Recently, Groetzner and Dür proposed in [33] a novel approach to the nonnegative factorization problem which consists of formulating it as a nonconvex split feasibility problem and, consequently, in solving it via the *method of alternating projections*. It is known that when the initial point is sufficiently close to the feasible set, then the sequence generated by the nonconvex method of alternating projections converges to an feasible element. The drawback of this algorithm is that it requires in every iteration two projections, which both have in general to be approximately calculated via inner loops, since they amount to solve a second order cone problem (SOCP) and to find a singular value decomposition of a matrix, respectively. In the same article, a modification of this method has been suggested, which replaces the solving of the SOCP by a simple projection on the nonnegative orthant, but keeps the singular value decomposition, however, without a theoretical evidence of its convergence. Also very recently, Chen, Pong, Tan and Zeng proposed in [23] another approach which consists of reformulating the split feasibility problem as a *difference-of-convex optimization problem* and, consequently, in solving it via a specific algorithm, which also requires the singular valued decomposition of a matrix in every iteration. We will present these approaches in more detail later.

In this paper we develop a different approach for the nonnegative factorization of a completely positive matrix, which amounts to the minimization of a nonconvex smooth function over a convex and compact set. To solve this problem we propose a *projected gradient algorithm* with parameters that take into account the effects of *relaxation* and *inertia*. The gradient and the projection steps are expressed by simple explicit formulas and thus do not require any inner loops. We prove the global convergence of the generated sequence for any starting point, which is another advantage over the methods discussed above,

which make use of expensive computing procedures to find the points where the algorithms start. We provide rates of convergence for both the sequences of objective function values and of iterates in terms of the Lojasiewicz exponent of a regularization of the objective function. Numerical experiments show that our algorithm outperforms the other iterative factorization methods and emphasize the influence of the relaxation and inertial parameters on its performances.

Relaxation techniques have been introduced to provide more flexibility to iterative schemes ([7]), while inertial effects in order to accelerate the convergence of numerical methods ([47, 12, 6]) and to allow the detection of different critical points ([53]). Inertial proximal gradient algorithms for nonconvex optimization problems have been proposed and studied in [19, 20, 38, 50, 52]; their global convergence has been shown in the framework of the Kurdyka-Lojasiewicz property ([2, 3, 14, 15, 35, 42]). For convex optimization problems, *relaxed inertial algorithms* have been proved to combine the advantages of both relaxation techniques and inertial effects (see [4, 5, 36]). One of the aims of this work is to investigate, also in the nonconvex setting, to which extent the interplay between relaxation and inertial parameters influence the numerical performances of projected/proximal gradient algorithms.

Solution methods for nonsmooth nonconvex optimization problems have been already used in the literature for *nonnegative matrix factorization*. We recall here PALM, introduced by Bolte, Sabach, and Teboulle in [15], which is a block coordinate projection gradient method, and its inertial variant studied by Pock and Sabach in [52], for which also numerical experiments were reported. Recently, the *symmetric nonnegative matrix factorization* has been addressed by Dragomir, d'Aspremont and Bolte in [29] from the perspective of a non-Euclidean first-order method. We also want to mention [32] where nonnegative matrix factorizations are computed in an alternating manner.

In what concerns *sparse matrix factorizations* ([48]), this can be formulated as the feasibility problem of finding an element in the intersection of two nonconvex sets. In [23] a difference-of-convex optimization approach was used to develop a solution method for it, as alternatives one could use approaches based on the method of alternating projections ([30]) or on the Douglas-Rachford algorithm for feasibility problems ([1, 40]).

2 Preliminaries

2.1 Notations

We will write for a $n \times r$ matrix $X := (x_{i,j})_{1 \leq i \leq n, 1 \leq j \leq r}$ if we want to specify its elements, and neglect the subscripts if there is no risk of confusion. The *Frobenius inner product* of $X, Y \in \mathbb{R}^{n \times r}$ is defined by $\langle X, Y \rangle := \text{trace}(X^T Y) = \sum_{i=1}^n \sum_{j=1}^r x_{i,j} y_{i,j}$. Due to the definition of trace operator it holds

$$\text{trace}(X^T Y) = \text{trace}(XY^T) = \text{trace}(Y^T X) = \text{trace}(YX^T). \quad (2.1)$$

For $X \in \mathbb{R}^{n \times r}$ we will denote its *Frobenius norm* by

$$\|X\|_F := \sqrt{\langle X, X \rangle} = \sqrt{\text{trace}(X^T X)} = \sqrt{\sum_{i=1}^n \sum_{j=1}^r |x_{i,j}|^2}, \quad (2.2)$$

and its *2-norm* by

$$\|X\|_2 := \sup_{\|\xi\| \neq 0} \frac{\|X\xi\|}{\|\xi\|},$$

where $\|\cdot\|$ denotes the usual *Euclidean norm* of a vector. If $X := [X_1 | \dots | X_r]$ is the column representation of the matrix X , then we have

$$\|X\|_F = \sqrt{\sum_{j=1}^r \|X_j\|^2}.$$

For every $X, Y \in \mathbb{R}^{n \times r}$ we have

$$\|X + Y\|_F^2 = \|X\|_F^2 + \|Y\|_F^2 + 2\langle X, Y \rangle, \quad (2.3a)$$

$$\|X\|_2 \leq \|X\|_F, \quad (2.3b)$$

$$\|X^T Y\|_2 \leq \|X\|_2 \cdot \|Y\|_2, \quad (2.3c)$$

$$\|X^T Y\|_F \leq \|X\|_F \cdot \|Y\|_F. \quad (2.3d)$$

In addition, for every $\eta \in \mathbb{R}$, it holds

$$\|\eta X + (1 - \eta) Y\|_{\mathbb{F}}^2 = \eta \|X\|_{\mathbb{F}}^2 + (1 - \eta) \|Y\|_{\mathbb{F}}^2 - \eta(1 - \eta) \|X - Y\|_{\mathbb{F}}^2. \quad (2.4)$$

For a symmetric positive semidefinite matrix $A \in \mathbb{R}^{n \times n}$ we denote by

$$\lambda_{\max}(A) := \lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A) := \lambda_{\min}(A) \geq 0$$

its *eigenvalues*. Therefore,

$$\text{trace}(A) = \sum_{i=1}^n \lambda_i(A) \geq \lambda_{\max}(A) = \|A\|_2 \geq \lambda_{\min}(A). \quad (2.5)$$

The following two estimates, which we also prove for the sake of completeness, will be useful later on.

Lemma 1. *Let $X, Y \in \mathbb{R}^{n \times r}$.*

(i) *It holds*

$$\|X^T Y\|_{\mathbb{F}} \leq \|X\|_2 \cdot \|Y\|_{\mathbb{F}}. \quad (2.6)$$

(ii) *If $A \in \mathbb{R}^{n \times n}$ is a symmetric positive semidefinite matrix, then*

$$\lambda_{\min}(A) \|X\|_{\mathbb{F}}^2 \leq \langle A, X X^T \rangle \leq \|A\|_2 \cdot \|X\|_{\mathbb{F}}^2. \quad (2.7)$$

Proof. (i) Using the column representation of $Y := [Y_1 | \cdots | Y_r]$, we have $X^T Y = [X^T Y_1 | \cdots | X^T Y_r]$.

Thus

$$\|X^T Y\|_{\mathbb{F}}^2 = \sum_{j=1}^r \|X^T Y_j\|^2 \leq \|X\|_2^2 \sum_{j=1}^r \|Y_j\|^2 = \|X\|_2^2 \|Y\|_{\mathbb{F}}^2.$$

Notice that, in view of (2.3b), inequality (2.6) is sharper than (2.3d).

(ii) For two positive semidefinite matrices $A, B \in \mathbb{R}^{n \times n}$ we have the following consequence of the Von Neumann's trace inequality (see [43, pp. 340–341])

$$\sum_{i=1}^n \lambda_i(A) \lambda_{n+1-i}(B) \leq \text{trace}(AB) \leq \sum_{i=1}^n \lambda_i(A) \lambda_i(B). \quad (2.8)$$

The inequality (2.7) follows by applying (2.8) for the positive semidefinite matrices A and $X X^T$, and by noticing further that $\sum_{i=1}^n \lambda_i(X X^T) = \text{trace}(X X^T) = \|X\|_{\mathbb{F}}^2$. \square

The *open ball* around $Z \in \mathbb{R}^{n \times r}$ with radius $\varepsilon > 0$ is denoted by $\mathring{\mathbb{B}}_{\mathbb{F}}(Z; \varepsilon) := \{X \in \mathbb{R}^{n \times r} : \|X - Z\|_{\mathbb{F}} < \varepsilon\}$ and the *closed ball* by $\mathbb{B}_{\mathbb{F}}(Z; \varepsilon) := \overline{\mathring{\mathbb{B}}_{\mathbb{F}}(Z; \varepsilon)}$, where the closure is taken with respect to the topology induced by the Frobenius norm. The *indicator function* of a set $\mathcal{D} \subseteq \mathbb{R}^{n \times r}$ is defined as $\delta_{\mathcal{D}}(X) = 0$, if $X \in \mathcal{D}$, and $\delta_{\mathcal{D}}(X) = +\infty$, otherwise. We say that an element $Z \in \mathcal{D}$ is a *projection* of an element X onto a nonempty closed subset \mathcal{D} of $\mathbb{R}^{n \times r}$, if $\|X - Z\|_{\mathbb{F}} = \inf_{Y \in \mathcal{D}} \|X - Y\|_{\mathbb{F}}$. If the set \mathcal{D} is also convex, then the projection of an element X is uniquely defined and we will denote it by $\mathbf{Pr}_{\mathcal{D}}(X)$. It is characterized by

$$\mathbf{Pr}_{\mathcal{D}}(X) \in \mathcal{D} \quad \text{and} \quad \langle X - \mathbf{Pr}_{\mathcal{D}}(X), Y - \mathbf{Pr}_{\mathcal{D}}(X) \rangle \leq 0 \quad \forall Y \in \mathcal{D}. \quad (2.9)$$

Example 1. For every $X \in \mathbb{R}^{n \times r}$,

(i) if $\mathcal{D} := \mathbb{R}_+^{n \times r}$, then it holds

$$\mathbf{Pr}_{\mathcal{D}}(X) = [X]_+ := \max\{X, \mathbf{0}\},$$

where the max operator is understood entrywise;

(ii) if $\mathcal{D} := \mathbb{B}_{\mathbb{F}}(\mathbf{0}; \varepsilon)$ for $\varepsilon > 0$, we have

$$\mathbf{Pr}_{\mathcal{D}}(X) = \frac{\varepsilon}{\max\{\|X\|_{\mathbb{F}}, \varepsilon\}} X.$$

In general, it is challenging to compute the projection onto the intersection of two sets, even if these are both convex and explicit forms for the projections onto the sets are available. To this end one can either use the method of alternating projections [8, 30] or the Douglas-Rachford algorithm for feasibility problems [1, 40]. Cyclic formulations of these iterative methods can be used to determine the projection onto the intersection of more than two sets.

In the following example we provide one particular pair of two convex sets for which the projection onto their intersection can be expressed by a closed formula. We will make use of this formula in our algorithm, which means that it will require a reduced computational effort when calculating this projection.

Example 2. Let $\varepsilon > 0$ and K be a nonempty closed convex cone in $\mathbb{R}^{n \times r}$. Then the projection onto the intersection $K \cap \mathbb{B}_F(0, \varepsilon)$ is given by (see [9, Theorem 7.1])

$$\mathbf{Pr}_{K \cap \mathbb{B}_F(0, \varepsilon)}(X) = \mathbf{Pr}_{\mathbb{B}_F(0, \varepsilon)} \circ \mathbf{Pr}_K(X) = \frac{\varepsilon}{\max\{\|\mathbf{Pr}_K(X)\|_F, \varepsilon\}} \mathbf{Pr}_K(X) \quad \forall X \in \mathbb{R}^{n \times r}. \quad (2.10)$$

Notice that in general $\mathbf{Pr}_{\mathbb{B}_F(0, \varepsilon)} \circ \mathbf{Pr}_K(X) \neq \mathbf{Pr}_K(X) \circ \mathbf{Pr}_{\mathbb{B}_F(0, \varepsilon)}$ (see [9, Example 7.5]).

For later comparison we discuss two more examples of projections on some particular sets which were used in the nonnegative factorization of completely positive matrices.

Example 3. Let $B \in \mathbb{R}^{n \times r}$ and consider the following set associated to B

$$\mathcal{P}(B) := \{X \in \mathbb{R}^{r \times r} : BX \in \mathbb{R}_+^{n \times r}\}. \quad (2.11)$$

The set $\mathcal{P}(B)$ is a polyhedral cone and thus a closed convex subset of $\mathbb{R}^{r \times r}$. The projection of $X \in \mathbb{R}^{r \times r}$ onto the set $\mathcal{P}(B)$ is the unique solution of the optimization problem

$$\begin{aligned} \min_{Y \in \mathbb{R}^{r \times r}} & \|Y - X\|_F. \\ \text{s.t.} & BY \in \mathbb{R}_+^{n \times r}. \end{aligned} \quad (2.12)$$

It was shown in [33] that (2.12) is equivalent to the second order cone problem (SOCP)

$$\begin{aligned} \min_{t \in \mathbb{R}, Z \in \mathbb{R}^{r \times r}} & t. \\ \text{s.t.} & B(X + Z) \in \mathbb{R}_+^{n \times r}, \\ & \|Z\|_F \leq t. \end{aligned} \quad (\text{SOCP})$$

Second order cone problems have been intensively studied in the literature from both theoretical and numerical perspectives.

Example 4. Let \mathcal{O}_r be the set of orthogonal matrices in $\mathbb{R}^{r \times r}$

$$\mathcal{O}_r := \{X \in \mathbb{R}^{r \times r} : XX^T = X^T X = \mathbb{I}_r\}, \quad (2.13)$$

where \mathbb{I}_r denotes $r \times r$ identity matrix. The set \mathcal{O}_r is compact but nonconvex, so projections on this set always exist, but may not be unique. A projection of an element $X \in \mathbb{R}^{r \times r}$ on \mathcal{O}_r can be found by polar decomposition of X (see, for instance, [33, Lemma 4.1]). In particular, for every $X \in \mathbb{R}^{r \times r}$, there exist a positive semidefinite matrix $T \in \mathbb{R}^{r \times r}$ and an orthogonal matrix $Y \in \mathbb{R}^{r \times r}$ such that

$$X = TY \quad \text{and} \quad \|X - Y\|_F \leq \|X - Z\|_F \quad \forall Z \in \mathcal{O}_r.$$

Therefore, the matrix Y is a projection of X onto \mathcal{O}_r and it can be computed by means of the singular value decomposition of $X = U\Sigma V^T$. Indeed, for $T := U\Sigma U^T$ and $Y := UV^T$ it holds

$$X = U\Sigma V^T = U\Sigma U^T UV^T = TY.$$

2.2 Variational analysis tools

In the following we will introduce some tools from variational analysis which will play an important role in the convergence analysis.

Let $\Psi: \mathbb{R}^{n \times r} \rightarrow \mathbb{R} \cup \{+\infty\}$ be a proper and lower semicontinuous function and X an element of its *effective domain* $\text{dom} \Psi := \{Y \in \mathbb{R}^{n \times r} : \Psi(Y) < +\infty\}$. The *Fréchet (viscosity) subdifferential* of Ψ at X is

$$\widehat{\partial} \Psi(X) := \left\{ V \in \mathbb{R}^{n \times r} : \liminf_{Y \rightarrow X} \frac{\Psi(Y) - \Psi(X) - \langle V, Y - X \rangle}{\|Y - X\|_F} \geq 0 \right\}$$

and the *limiting (Mordukhovich) subdifferential* ([45, 54]) of Ψ at X is

$$\begin{aligned} \partial \Psi(X) := \{ & V \in \mathbb{R}^{n \times r} : \text{exist sequences } X_k \rightarrow X \text{ and } V_k \rightarrow V \text{ as } k \rightarrow +\infty \\ & \text{such that } \Psi(X_k) \rightarrow \Psi(X) \text{ as } k \rightarrow +\infty \text{ and } V_k \in \widehat{\partial} \Psi(X_k) \text{ for any } k \geq 0\}. \end{aligned}$$

For $X \notin \text{dom} \Psi$, we set $\widehat{\partial} \Psi(X) = \partial \Psi(X) := \emptyset$.

The inclusion $\widehat{\partial} \Psi(X) \subseteq \partial \Psi(X)$ holds for each $X \in \mathbb{R}^{n \times r}$. If Ψ is convex, then the two subdifferentials coincide with the *convex subdifferential* of Ψ

$$\widehat{\partial} \Psi(X) = \partial \Psi(X) = \{V \in \mathbb{R}^{n \times r} : \Psi(Y) \geq \Psi(X) + \langle V, Y - X \rangle \ \forall Y \in \mathbb{R}^{n \times r}\} \text{ for any } X \in \mathbb{R}^{n \times r}.$$

If $X \in \mathbb{R}^{n \times r}$ is a local minimum of Ψ , then $0 \in \partial \Psi(X)$. We denote by $\text{crit}(\Psi) := \{X \in \mathbb{R}^{n \times r} : 0 \in \partial \Psi(X)\}$ the set of *critical points* of Ψ . The limiting subdifferential fulfils the following closedness criterion: if $\{X_k\}_{k \geq 0}$ and $\{V_k\}_{k \geq 0}$ are sequence in $\mathbb{R}^{n \times r}$ such that $V_k \in \partial \Psi(X_k)$ for any $k \geq 0$ and $(X_k, V_k) \rightarrow (X, V)$ and $\Psi(X_k) \rightarrow \Psi(X)$ as $k \rightarrow +\infty$, then $V \in \partial \Psi(X)$. We also have the following subdifferential sum formula (see [45, Proposition 1.107], [54, Exercise 8.8]): if $\Phi: \mathbb{R}^{n \times r} \rightarrow \mathbb{R}$ is a continuously differentiable function, then $\partial(\Psi + \Phi)(X) = \partial \Psi(X) + \nabla \Phi(X)$ for any $X \in \mathbb{R}^{n \times r}$.

The *normal cone* to a nonempty convex subset \mathcal{D} of $\mathbb{R}^{n \times r}$ is defined as

$$\mathbf{N}_{\mathcal{D}}(X) := \{V \in \mathbb{R}^{n \times r} : \langle V, Y - X \rangle \leq 0 \quad \forall Y \in \mathcal{D}\},$$

for $X \in \mathcal{D}$, and as $\mathbf{N}_{\mathcal{D}}(X) = \emptyset$ for $X \notin \mathcal{D}$. It holds $\mathbf{N}_{\mathcal{D}}(X) = \partial \delta_{\mathcal{D}}(X)$ for every $X \in \mathbb{R}^{n \times r}$. If $\mathcal{D} \subseteq \mathbb{R}^{n \times r}$ is a nonempty convex closed set and $X \in \mathbb{R}^{n \times r}$, then

$$Z = \mathbf{Pr}_{\mathcal{D}}(X) \Leftrightarrow X - Z \in \mathbf{N}_{\mathcal{D}}(Z). \quad (2.14)$$

2.3 Nonnegative factorization of completely positive matrices via projection onto the orthogonal set \mathcal{O}_r

In the following we will revisit some recent iterative approaches for finding a nonnegative factorization of completely positive matrices.

In [33] this problem was reformulated as a feasibility problem. For a given matrix $A \in \mathbb{R}^{n \times n}$, in a first step, a not necessarily entrywise nonnegative matrix $B \in \mathbb{R}^{n \times r}$ such that $A = BB^T$ was considered. The aim was

$$\text{to find a } r \times r \text{ square matrix } Q \text{ such that } Q \in \mathcal{P}(B) \cap \mathcal{O}_r, \quad (2.15)$$

where $\mathcal{P}(B)$ and \mathcal{O}_r are the polyhedral cone associated to B and the set of $r \times r$ orthogonal matrices given in (2.11) and in (2.13), respectively. This approach was motivated by the observation that, for every $B_1, B_2 \in \mathbb{R}^{n \times r}$, it holds $B_1 B_1^T = B_2 B_2^T$ if and only if there exists $Q \in \mathcal{O}_r$ such that $B_1 Q = B_2$ (see [33, Lemma 2.6]).

To solve (2.15), naturally, the method of alternating projections was used.

(The Method of Alternating Projections ([33])). Let $A \in \mathcal{CP}_n$ and r be a positive integer value.

Input:

- a given $B \in \mathbb{R}^{n \times r}$ such that $A = BB^T$;
- a given starting point $Q_0 \in \mathcal{O}_r$.

Main iterate: Set $k := 0$.

Step1 : Compute

$$\begin{cases} P_k & := \mathbf{Pr}_{\mathcal{P}(B)}(Q_k), \\ Q_{k+1} & \in \mathbf{Pr}_{\mathcal{O}_r}(P_k). \end{cases} \quad (\text{MAP})$$

Step2 : If a stopping criterion is not met, then set $k := k + 1$ and go to **Step1**.

Output: $Q_{k+1} \in \mathcal{O}_r$, which provides a completely positive factorization $A = (BQ_{k+1})(BQ_{k+1})^T$.

The stopping criterion used in [33] for this scheme, as well as for the other two methods that will be described later in this section, reads

$$\min_{1 \leq i \leq n, 1 \leq j \leq r} (BQ_{k+1})_{i,j} \geq -\text{To1}_{\text{fea}}, \quad (2.16)$$

where To1_{fea} is a positive very small tolerance number.

The nonconvex method of alternating projections is known to converge *locally*, which means that convergence can be guaranteed if the initial point is sufficiently close to $\mathcal{P}(B) \cap \mathcal{O}_r$.

As noticed in Example 3, the first step in (MAP) amounts to solve a second-order cone problem, which usually can be done only in an approximate way and requires an inner loop. To avoid this drawback, another algorithm was proposed in [33], which, in every iteration, calculates an approximation of $\text{Pr}_{\mathcal{P}(B)}(Q_k)$. This is done by using the projection on $\mathbb{R}_+^{n \times r}$, for which an exact formula exists, and an update step which uses the *Moore-Penrose-Inverse* of B , that is $B^+ := B^T (BB^T)^{-1}$.

This second algorithm has the following formulation.

(*The second Method of Alternating Projections ([33])*). Let $A \in \mathcal{CP}_n$ and r be a positive integer value.

Input:

- a given $B \in \mathbb{R}^{n \times r}$ such that $A = BB^T$;
- a given starting point $Q_0 \in \mathcal{O}_r$.

Main iterate: Set $k := 0$.

Step1 : Compute

$$\begin{cases} R_k & := \text{Pr}_{\mathbb{R}_+^{n \times r}}(BQ_k), \\ \hat{P}_k & := B^+ R_k + (\mathbb{I}_r - B^+ B) Q_k, \\ Q_{k+1} & \in \text{Pr}_{\mathcal{O}_r}(\hat{P}_k). \end{cases} \quad (\text{ModMAP})$$

Step2 : If a stopping criterion is not met, then set $k := k + 1$ and go to **Step1**.

Output: $Q_{k+1} \in \mathcal{O}_r$, which provides a completely positive factorization $A = (BQ_{k+1})(BQ_{k+1})^T$.

In [23], an alternative approach to (2.15) was considered, by reformulating the nonnegative factorization problem as a difference-of-convex optimization problem and by solving the latter via a nonmonotone linesearch algorithm. This can be found [23, Section 6.1], here we present for easy reference the iterative scheme with a fixed stepsize.

(*The Difference-of-Convex Approach with fixed stepsize ([23])*). Let $A \in \mathcal{CP}_n$ and r be a positive integer value.

Input:

- a given $B \in \mathbb{R}^{n \times r}$ such that $A = BB^T$;
- a fixed stepsize $L_B > \lambda_{\max}(B^T B)$;
- a given starting point $Q_0 \in \mathcal{O}_r$.

Main iterate: Set $k := 0$.

Step1 : Compute

$$\begin{cases} W_k & := \text{Pr}_{\mathbb{R}_+^{n \times r}}(BQ_k), \\ Q_{k+1} & \in \text{Pr}_{\mathcal{O}_r}\left(Q_k - \frac{1}{L_B} B^T (BQ_k - W_k)\right). \end{cases} \quad (\text{SpFeasDC})$$

Step2 : If a stopping criterion is not met, then set $k := k + 1$ and go to **Step1**.

Output: $Q_{k+1} \in \mathcal{O}_r$, which provides a completely positive factorization $A = (BQ_{k+1})(BQ_{k+1})^T$.

One can notice that all three iterative schemes require in every iteration the calculation of a projection onto the orthogonal set \mathcal{O}_r . To do this one basically needs to carry out a singular value decomposition of a matrix, as discussed in Example 4, which can be done in a subroutine that needs $\mathcal{O}(r^3)$ steps. Furthermore, all three algorithms ask for finding a matrix $B \in \mathbb{R}^{n \times r}$ such that $A = BB^T$. This can be done, for instance, by the Cholesky decomposition of A , in which case B is a lower triangular matrix, or by the spectral decomposition $A = V\Sigma V^T$ and then by setting $B := V\Sigma^{\frac{1}{2}}$. In either case, one needs an additional procedure to find an appropriate initial matrix B .

3 An optimization model with convergence guarantees

In this section we will propose a new approach for the nonnegative factorization of completely positive matrices, which consists of solving a nonconvex optimization problem by means of a projected gradient algorithm. We will also carry out for the iterative method a comprehensive convergence analysis, and even derive convergence rates.

3.1 The optimization model

For a given nonzero completely positive matrix $A \in \mathbb{R}^{n \times n}$, finding a factorization $A = XX^T$, where $X \in \mathbb{R}_+^{n \times r}$, can be cast as an optimization problem

$$\begin{aligned} \min_{X \in \mathbb{R}^{n \times r}} \mathcal{E}(X) &:= \frac{1}{2} \|A - XX^T\|_{\text{F}}^2, \\ \text{s.t. } X &\in \mathcal{D} := \mathbb{R}_+^{n \times r} \cap \mathbb{B}_{\text{F}}(\mathbf{0}, \sqrt{\text{trace}(A)}) \end{aligned} \quad (\text{P}_{\text{mod}})$$

Denoting by $\mathcal{E}_* := \inf_{X \in \mathcal{D}} \mathcal{E}(X)$ the optimal objective value of (P_{mod}) , it holds

$$A = X_* X_*^T \quad \text{with} \quad X_* \in \mathbb{R}_+^{n \times r} \Leftrightarrow [X_* \text{ solves } (\text{P}_{\text{mod}}) \quad \text{and} \quad \mathcal{E}_* = 0].$$

Notice that \mathcal{E} is a nonconvex objective function with continuous gradient $\nabla \mathcal{E}(X) = -2(A - XX^T)X$, which is however not Lipschitz continuous, but *locally* Lipschitz continuous. In order to be able to handle this situation in a proper way in the convergence analysis, we minimize the objective function $\mathcal{E}(X)$ over a meaningfully chosen bounded set, which, however, does not pose any restriction on the model. Indeed, if X satisfies $A = XX^T$, then

$$\|X\|_{\text{F}} \leq \sqrt{\text{trace}(A)},$$

since, according to the definition of the Frobenius norm and (2.1) - (2.2), we have

$$\|X\|_{\text{F}} = \sqrt{\text{trace}(X^T X)} = \sqrt{\text{trace}(X X^T)} = \sqrt{\text{trace}(A)}.$$

This explains the choice of \mathcal{D} as the intersection of $\mathbb{R}_+^{n \times r}$ and $\mathbb{B}_{\text{F}}(\mathbf{0}, \sqrt{\text{trace}(A)})$.

Proposition 2. *Let $A \in \mathcal{CP}_n$.*

(i) *The set \mathcal{D} is nonempty convex and closed, and for any $X \in \mathbb{R}^{n \times r}$ it holds*

$$\mathbf{Pr}_{\mathcal{D}}(X) := \frac{\sqrt{\text{trace}(A)}}{\max\{\|[X]_+\|_{\text{F}}, \sqrt{\text{trace}(A)}\}} [X]_+, \quad (3.1)$$

where $[X]_+ := \max\{X, \mathbf{0}\}$ and the max operator is understood entrywise.

(ii) *For $X, Y \in \mathbb{R}^{n \times r}$, the following inequalities are true*

$$-\|A\|_2 \cdot \|X - Y\|_{\text{F}}^2 \leq \mathcal{E}(X) - \mathcal{E}(Y) - \langle \nabla \mathcal{E}(Y), X - Y \rangle \leq \frac{L(X, Y)}{2} \|X - Y\|_{\text{F}}^2, \quad (3.2)$$

where

$$L(X, Y) := 2 \left(\|Y\|_2^2 - \lambda_{\min}(A) \right) + (\|X\|_2 + \|Y\|_2)^2. \quad (3.3)$$

Proof. (i) Since \mathcal{D} is the intersection of the cone $K := \mathbb{R}_+^{n \times r}$ with the ball $\mathbb{B}_F(0, \sqrt{\text{trace}(A)})$, it follows from (2.10) that

$$\mathbf{Pr}_{\mathcal{D}}(X) = \frac{\sqrt{\text{trace}(A)}}{\max\{\|\mathbf{Pr}_K(X)\|_F, \sqrt{\text{trace}(A)}\}} \mathbf{Pr}_K(X).$$

For $K = \mathbb{R}_+^{n \times r}$ it holds $\mathbf{Pr}_K(X) = \mathbf{Pr}_{\mathbb{R}_+^{n \times r}}(X) = [X]_+ = \max\{X, \mathbf{0}\}$.

(ii) We introduce the auxiliary function $\mathcal{Q}: \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$ defined as

$$\mathcal{Q}(Z) := \frac{1}{2} \|A - Z\|_F^2 \quad \forall Z \in \mathbb{R}^{n \times n}.$$

By the definition, $\mathcal{E}(X) = \mathcal{Q}(XX^T)$ for every $X \in \mathbb{R}^{n \times n}$. Since $\nabla \mathcal{Q}(Z) = -(A - Z)$, the following relation is true for every $Z, W \in \mathbb{R}^{n \times n}$

$$\mathcal{Q}(W) = \mathcal{Q}(Z) + \langle \nabla \mathcal{Q}(Z), W - Z \rangle + \frac{1}{2} \|W - Z\|_F^2. \quad (3.4)$$

Moreover, if Z is symmetric, then so is $\nabla \mathcal{Q}(Z)$.

Let $X, Y \in \mathbb{R}^{n \times r}$ be fixed. One can easily verify that

$$XX^T - YY^T = (X - Y)Y^T + Y(X - Y)^T + (X - Y)(X - Y)^T. \quad (3.5)$$

Applying (3.4) with $W := XX^T$ and $Z := YY^T$ and by taking into consideration (3.5), we get

$$\begin{aligned} \mathcal{Q}(XX^T) - \mathcal{Q}(YY^T) &= \langle \nabla \mathcal{Q}(YY^T), XX^T - YY^T \rangle + \frac{1}{2} \|XX^T - YY^T\|_F^2 \\ &= \langle \nabla \mathcal{Q}(YY^T), (X - Y)Y^T \rangle + \langle \nabla \mathcal{Q}(YY^T), Y(X - Y)^T \rangle \\ &\quad + \langle \nabla \mathcal{Q}(YY^T), (X - Y)(X - Y)^T \rangle + \frac{1}{2} \|XX^T - YY^T\|_F^2 \\ &= 2 \langle \nabla \mathcal{Q}(YY^T) Y, (X - Y) \rangle + \langle \nabla \mathcal{Q}(YY^T), (X - Y)(X - Y)^T \rangle \\ &\quad + \frac{1}{2} \|XX^T - YY^T\|_F^2. \end{aligned} \quad (3.6)$$

Since $2 \nabla \mathcal{Q}(YY^T) Y = -2(A - YY^T) Y = \nabla \mathcal{E}(Y)$, it remains to estimate the two last terms in (3.6). Observe that

$$\begin{aligned} &\langle \nabla \mathcal{Q}(YY^T), (X - Y)(X - Y)^T \rangle + \frac{1}{2} \|XX^T - YY^T\|_F^2 \\ &= - \langle A - YY^T, (X - Y)(X - Y)^T \rangle + \frac{1}{2} \|XX^T - YY^T\|_F^2 \\ &= - \langle A, (X - Y)(X - Y)^T \rangle + \|Y^T(X - Y)\|_F^2 + \frac{1}{2} \|XX^T - YY^T\|_F^2, \end{aligned} \quad (3.7)$$

where the last equation comes from the fact that trace operator is invariant under cyclic permutations, as we see below

$$\begin{aligned} \langle YY^T, (X - Y)(X - Y)^T \rangle &= \text{trace} \left[(YY^T)^T (X - Y)(X - Y)^T \right] \\ &= \text{trace} \left[YY^T (X - Y)(X - Y)^T \right] \\ &= \text{trace} \left[(X - Y)^T YY^T (X - Y) \right] \\ &= \text{trace} \left[(Y^T (X - Y))^T Y^T (X - Y) \right] \\ &= \|Y^T (X - Y)\|_F^2. \end{aligned}$$

Notice that, thanks to (2.7), $\langle A, (X - Y)(X - Y)^T \rangle \leq \|A\|_2 \|X - Y\|_F^2$. Plugging this estimate into (3.7), also neglecting the last two nonnegative terms, we obtain the left-hand side inequality in (3.2).

By applying (2.6) we can derive an upper bound for the last term in (3.7)

$$\begin{aligned} \|XX^T - YY^T\|_F &\leq \|(X - Y)X^T\|_F + \|Y(X - Y)^T\|_F \\ &\leq \|X\|_2 \|X - Y\|_F + \|Y\|_2 \|X - Y\|_F = (\|X\|_2 + \|Y\|_2) \|X - Y\|_F. \end{aligned} \quad (3.8)$$

By plugging (3.8) into (3.7) and recalling the inequalities (2.7) and (2.6), we get the right-hand side inequality in (3.2) with $L(X, Y)$ defined as in (3.3). \square

3.2 A projected gradient algorithm with relaxation and inertial parameters

We are now in the position to formulate the projected gradient algorithm we propose in this paper to solve (P_{mod}) .

Algorithm 1. Let $A \in \mathcal{CP}_n$ and r be a positive integer value.

Input:

- given starting points $X_1 := X_0 \in \mathcal{D}$ and;
- a sequence $\{\alpha_k\}_{k \geq 1} \subseteq [0, 1]$, for which we set $\alpha_+ := \sup_{k \geq 0} \alpha_k$ and

$$L_F(\alpha_+) := 2 \left[(3 + 8\alpha_+ + 6\alpha_+^2) \text{trace}(A) - \lambda_{\min}(A) \right] > 0; \quad (3.9)$$

- a relaxation parameter $\rho \in (0, 1]$ chosen such that

$$0 < \frac{\sqrt{L_F(\alpha_+) + 2\|A\|_2}}{\sqrt{L_F(\alpha_+) + 2\|A\|_2} + \sqrt{L_F(\alpha_+)}} < \rho < \frac{\sqrt{L_F(\alpha_+) + 2\|A\|_2}}{(1 + \alpha_+) \sqrt{L_F(\alpha_+) + 2\|A\|_2} - \sqrt{L_F(\alpha_+)}}. \quad (3.10)$$

Main iterate: Set $k := 1$.

Step1 : Compute

$$Y_k := X_k + \alpha_k (X_k - X_{k-1}), \quad (3.11a)$$

$$Z_{k+1} := \mathbf{Pr}_{\mathcal{D}} \left(Y_k - \frac{1}{L_F(\alpha_+)} \nabla \mathcal{E}(Y_k) \right), \quad (3.11b)$$

$$X_{k+1} := (1 - \rho) X_k + \rho Z_{k+1}. \quad (3.11c)$$

Step2 : If a stopping criterion is not met, then set $k := k + 1$ and go to **Step1**.

Output: $X_{k+1} \in \mathcal{D}$, which provides a factorization $A = X_{k+1} X_{k+1}^T$.

Remark 3. (i) In the analysis we will use, to ease the reading, L_F instead of $L_F(\alpha_+)$, however, we will return to this notation in subsection 4.1, where we will consider some particular choices of the sequence of inertial parameters, which will give different values for α_+ . To help the readers to understand the choice of the parameters, and the motivation behind the construction of L_F in (3.9), we formulate and prove Lemma 4 and Lemma 6 first and postpone the discussion on the feasibility of ρ in (3.10) to Remark 7.

- (ii) In the following theoretical investigations, we are interested on the convergence behaviour of the generated sequences as $k \rightarrow +\infty$, however, in the numerical experiments we will use as stopping criterion

$$\frac{\|A - X_k X_k^T\|_F^2}{\|A\|_F^2} < \text{To1}_{\text{val}},$$

where To1_{val} is a positive very small tolerance number.

- (iii) Recall that an explicit formula for the projection operator on \mathcal{D} has been given in (3.1).

(iv) For any $k \geq 1$, the following equivalent formulation of (3.11c) will be useful in the analysis

$$X_{k+1} = (1 - \rho) X_k + \rho Z_{k+1} \Leftrightarrow Z_{k+1} - X_k = \frac{1}{\rho} (X_{k+1} - X_k) \quad (3.12a)$$

$$\Leftrightarrow Z_{k+1} - X_{k+1} = \left(\frac{1}{\rho} - 1 \right) (X_{k+1} - X_k). \quad (3.12b)$$

The following result proves that the sequence $\{X_k\}_{k \geq 0}$ generated by Algorithm 1 belongs to \mathcal{D} and that $L_F(\alpha_+)$ is an upper bound for the sequence $\{L(Z_{k+1}, Y_k)\}_{k \geq 1}$.

Lemma 4. *Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1. For any $k \geq 1$*

(i) *it holds $X_{k+1} \in \mathcal{D}$ and $\|Y_k\|_F \leq (1 + 2\alpha_+) \sqrt{\text{trace}(A)}$;*

(ii) *it holds*

$$L(Z_{k+1}, Y_k) \leq L_F(\alpha_+) = 2 \left[(3 + 8\alpha_+ + 6\alpha_+^2) \text{trace}(A) - \lambda_{\min}(A) \right], \quad (3.13)$$

where $(X, Y) \mapsto L(X, Y)$ is defined in (3.3).

Proof. (i) Notice that $\{Z_k\}_{k \geq 2} \subseteq \mathcal{D}$ due to (3.11b). If we assume that $X_1 \in \mathcal{D}$, then, by induction arguments, $X_{k+1} \in \mathcal{D}$, since it is a convex combination of X_k and Z_{k+1} . Consequently, for any $k \geq 0$, $\|X_k\|_F \leq \sqrt{\text{trace}(A)}$. By the definition of Y_k in (3.11a), we have

$$\|Y_k\|_F \leq (1 + \alpha_k) \|X_k\|_F + \alpha_k \|X_{k-1}\|_F \leq (1 + 2\alpha_+) \sqrt{\text{trace}(A)} \quad \forall k \geq 1.$$

(ii) Since $\{Z_k\}_{k \geq 2} \subseteq \mathcal{D} \subseteq \mathbb{B}_F(\mathbf{0}; \sqrt{\text{trace}(A)})$ and $\{Y_k\}_{k \geq 1} \subseteq \mathbb{B}_F(\mathbf{0}; (1 + 2\alpha_+) \sqrt{\text{trace}(A)})$ it follows from the definition of $(X, Y) \mapsto L(X, Y)$ in (3.3) that

$$\begin{aligned} L(Z_{k+1}, Y_k) &= 2 \left(\|Y_k\|_2^2 - \lambda_{\min}(A) \right) + (\|Z_{k+1}\|_2 + \|Y_k\|_2)^2 \\ &= 3 \|Y_k\|_2^2 + \|Z_{k+1}\|_2^2 + 2 \|Z_{k+1}\|_2 \cdot \|Y_k\|_2 - 2\lambda_{\min}(A) \\ &\leq \left[3(1 + 2\alpha_+)^2 + 1 + 2(1 + 2\alpha_+) \right] \text{trace}(A) - 2\lambda_{\min}(A). \end{aligned}$$

□

Remark 5. In the nonconvex setting, the boundedness of the sequence of iterates plays an important role in the convergence analysis. As seen in Lemma 4 (i), the nature of Algorithm 1 ensures that $X_k \in \mathcal{D}$ for every $k \geq 0$, and thus the sequence $\{X_k\}_{k \geq 0}$ is bounded.

For readers' convenience we denote the objective function of (P_{mod}) by $\Psi := \mathcal{E} + \delta_{\mathcal{D}}$.

Lemma 6. *Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1. For every $k \geq 2$ it holds*

$$\Psi(Z_{k+1}) + \left(\frac{L_F - (L_F + 2\|A\|_2)\gamma}{2} + \frac{\tau}{2} \right) \|X_{k+1} - X_k\|^2 \leq \Psi(Z_k) + \frac{\tau}{2} \|X_k - X_{k-1}\|^2, \quad (3.14)$$

where

$$\gamma := \max \left\{ \left(\frac{1}{\rho} - 1 \right)^2, \left(1 + \alpha_+ - \frac{1}{\rho} \right)^2 \right\}, \quad (3.15a)$$

$$\tau := \frac{L_F(1 - \rho)}{\rho} + (L_F + 2\|A\|_2)\gamma. \quad (3.15b)$$

Proof. Let $k \geq 2$ be fixed. We first show that

$$\Psi(Z_{k+1}) + \frac{L_F}{2} \|Z_{k+1} - Z_k\|_F^2 \leq \Psi(Z_k) + \frac{L_F + 2\|A\|_2}{2} \|Z_k - Y_k\|_F^2. \quad (3.16)$$

The characterization of the projection (2.9) ensures that

$$\left\langle Y_k - \frac{1}{L_F} \nabla \mathcal{E}(Y_k) - Z_{k+1}, X - Z_{k+1} \right\rangle \leq 0 \quad \forall X \in \mathcal{D}. \quad (3.17)$$

In view of (3.11b), it is clear that $Z_k \in \mathcal{D}$, thus, setting $X := Z_k$ in (3.17) yields

$$\begin{aligned} 0 &\leq \langle \nabla \mathcal{E}(Y_k), Z_k - Z_{k+1} \rangle + L_F \langle Z_{k+1} - Y_k, Z_k - Z_{k+1} \rangle \\ &= \langle \nabla \mathcal{E}(Y_k), Z_k - Z_{k+1} \rangle - \frac{L_F}{2} \|Z_{k+1} - Y_k\|_F^2 - \frac{L_F}{2} \|Z_{k+1} - Z_k\|_F^2 + \frac{L_F}{2} \|Z_k - Y_k\|_F^2. \end{aligned} \quad (3.18)$$

The left-hand side inequality in (3.2) implies that

$$\mathcal{E}(Z_k) \geq \mathcal{E}(Y_k) + \langle \nabla \mathcal{E}(Y_k), Z_k - Y_k \rangle - \|A\|_2 \cdot \|Y_k - Z_k\|_F^2, \quad (3.19)$$

while the right-hand side inequality in (3.2) and (3.13) imply

$$\mathcal{E}(Z_{k+1}) \leq \mathcal{E}(Y_k) + \langle \nabla \mathcal{E}(Y_k), Z_{k+1} - Y_k \rangle + \frac{L_F}{2} \|Z_{k+1} - Y_k\|_F^2. \quad (3.20)$$

Summing up (3.18), (3.20) and (3.19), and noticing that $\delta_{\mathcal{D}}(Z_{k+1}) = \delta_{\mathcal{D}}(Z_k) = 0$, yield (3.16).

Next we will study the term $\|Z_{k+1} - Z_k\|_F^2$ in detail. From (3.12a) we have that

$$Z_{k+1} = \frac{1}{\rho} (X_{k+1} - X_k) + X_k,$$

and

$$Z_k = \frac{1}{\rho} (X_k - X_{k-1}) + X_{k-1},$$

thus

$$Z_{k+1} - Z_k = \frac{1}{\rho} (X_{k+1} - X_k) + \left(1 - \frac{1}{\rho}\right) (X_k - X_{k-1}). \quad (3.21)$$

Then, by using identity (2.4), it holds

$$\begin{aligned} \|Z_{k+1} - Z_k\|_F^2 &= \left\| \frac{1}{\rho} (X_{k+1} - X_k) + \left(1 - \frac{1}{\rho}\right) (X_k - X_{k-1}) \right\|_F^2 \\ &= \frac{1}{\rho} \|X_{k+1} - X_k\|_F^2 + \left(1 - \frac{1}{\rho}\right) \|X_k - X_{k-1}\|_F^2 \\ &\quad - \frac{1}{\rho} \left(1 - \frac{1}{\rho}\right) \|(X_{k+1} - X_k) - (X_k - X_{k-1})\|_F^2 \\ &\geq \frac{1}{\rho} \|X_{k+1} - X_k\|_F^2 - \left(\frac{1}{\rho} - 1\right) \|X_k - X_{k-1}\|_F^2. \end{aligned} \quad (3.22)$$

Combining (3.11a) and (3.12b) gives us further

$$Z_k - Y_k = Z_k - X_k - \alpha_k (X_k - X_{k-1}) = \left(\frac{1}{\rho} - 1 - \alpha_k\right) (X_k - X_{k-1}). \quad (3.23)$$

By plugging (3.22) and (3.23) into (3.16), we get

$$\begin{aligned} &\Psi(Z_{k+1}) + \frac{L_F}{2\rho} \|X_{k+1} - X_k\|_F^2 \\ &= \Psi(Z_{k+1}) + \left(\frac{L_F(1-\rho)}{2\rho} + \frac{L_F}{2}\right) \|X_{k+1} - X_k\|_F^2 \\ &\leq \Psi(Z_k) + \left(\frac{L_F(1-\rho)}{2\rho} + \frac{L_F + 2\|A\|_2}{2} \left(\frac{1}{\rho} - 1 - \alpha_k\right)^2\right) \|X_k - X_{k-1}\|_F^2 \\ &\leq \Psi(Z_k) + \left(\frac{L_F(1-\rho)}{2\rho} + \frac{(L_F + 2\|A\|_2)\gamma}{2}\right) \|X_k - X_{k-1}\|_F^2, \end{aligned} \quad (3.24)$$

which is nothing else than (3.14) with the constants τ and γ as defined in (3.15). Notice that (3.24) is true since γ is an upper bound for $\left(\frac{1}{\rho} - 1 - \alpha_k\right)^2$. Indeed, if $\frac{1}{\rho} - 1 \geq \alpha_k$, then

$$0 \leq \frac{1}{\rho} - 1 - \alpha_k \leq \frac{1}{\rho} - 1 \Rightarrow \left(\frac{1}{\rho} - 1 - \alpha_k\right)^2 \leq \left(\frac{1}{\rho} - 1\right)^2 \leq \gamma.$$

Otherwise, we have

$$0 < 1 + \alpha_k - \frac{1}{\rho} \leq 1 + \alpha_+ - \frac{1}{\rho} \Rightarrow \left(\frac{1}{\rho} - 1 - \alpha_k\right)^2 \leq \left(1 + \alpha_+ - \frac{1}{\rho}\right)^2 \leq \gamma,$$

which leads to the desired statement. \square

The estimate above remains true if we replace Ψ by \mathcal{E} . In fact, the indicator function was artificially inserted in the decreasing property (3.14), as it will help us to prove the convergence of the iterates later on. Now, with $\tau \geq 0$ introduced in (3.15b), we define the following function

$$\Psi_\tau: \mathbb{R}^{n \times r} \times \mathbb{R}^{n \times r} \rightarrow \mathbb{R} \cup \{+\infty\}, \quad \Psi_\tau(Z, X) := \Psi(Z) + \frac{\rho^2 \tau}{2} \|Z - X\|_F^2. \quad (3.25)$$

The objective function Ψ of (P_{mod}) is closely related to Ψ_τ in terms of their critical point. Indeed, if $\tau = 0$, which is the case when $\rho = 1$ and $\alpha_+ = 0$, then $\Psi_\tau(Z, X) = \Psi(Z)$ for any $(Z, X) \in \mathbb{R}^{n \times r} \times \mathbb{R}^{n \times r}$, thus $Z_* \in \text{crit}\Psi$ if and only if $(Z_*, X_*) \in \text{crit}\Psi_\tau$ for $X_* \in \mathbb{R}^{n \times r}$. On the other hand, one can easily verify that for every $\tau > 0$ we have

$$X_* \in \text{crit}\Psi \Leftrightarrow (X_*, X_*) \in \text{crit}\Psi_\tau. \quad (3.26)$$

Remark 7. In the view of (3.11c), it holds $X_{k+1} - X_k = \rho(Z_{k+1} - X_k)$ for every $k \geq 1$. Therefore, using the definition (3.25), the inequality (3.14) can be rewritten for any $k \geq 2$ as

$$\Psi_\tau(Z_{k+1}, X_k) + C_0 \|X_{k+1} - X_k\|_F^2 \leq \Psi_\tau(Z_k, X_{k-1}), \quad \text{where } C_0 := \frac{L_F - (L_F + 2\|A\|_2)\gamma}{2}. \quad (3.27)$$

We will show that $C_0 > 0$. It holds

$$L_F - (L_F + 2\|A\|_2)\gamma > 0 \Leftrightarrow \begin{cases} \left(\frac{1}{\rho} - 1\right)^2 < \frac{L_F}{L_F + 2\|A\|_2}, \\ \left(1 + \alpha_+ - \frac{1}{\rho}\right)^2 < \frac{L_F}{L_F + 2\|A\|_2}. \end{cases} \quad (3.28)$$

On the one hand, since $0 < \rho \leq 1$, we have

$$0 \leq \frac{1}{\rho} - 1 < \sqrt{\frac{L_F}{L_F + 2\|A\|_2}} \Leftrightarrow 1 \leq \frac{1}{\rho} < \frac{\sqrt{L_F + 2\|A\|_2} + \sqrt{L_F}}{\sqrt{L_F + 2\|A\|_2}}.$$

This is further equivalent to

$$\frac{\sqrt{L_F + 2\|A\|_2}}{\sqrt{L_F + 2\|A\|_2} + \sqrt{L_F}} < \rho \leq 1. \quad (3.29)$$

On the other hand, by setting $\xi := \frac{1}{\rho} > 0$, the second inequality in (3.28) can be equivalently expressed as

$$\xi^2 - 2(1 + \alpha_+)\xi + (1 + \alpha_+)^2 - \frac{L_F}{L_F + 2\|A\|_2} < 0. \quad (3.30)$$

Its reduced discriminant reads

$$\Delta' := (1 + \alpha_+)^2 - \left((1 + \alpha_+)^2 - \frac{L_F}{L_F + 2\|A\|_2}\right) = \frac{L_F}{L_F + 2\|A\|_2} > 0.$$

Thus, the inequality (3.30) is equivalent to

$$\begin{aligned} 1 + \alpha_+ - \sqrt{\frac{L_F}{L_F + 2\|A\|_2}} &= \frac{(1 + \alpha_+)\sqrt{L_F + 2\|A\|_2} - \sqrt{L_F}}{\sqrt{L_F + 2\|A\|_2}} \\ &< \xi = \frac{1}{\rho} < 1 + \alpha_+ + \sqrt{\frac{L_F}{L_F + 2\|A\|_2}} = \frac{(1 + \alpha_+)\sqrt{L_F + 2\|A\|_2} + \sqrt{L_F}}{\sqrt{L_F + 2\|A\|_2}}, \end{aligned}$$

which means

$$\frac{\sqrt{L_F + 2\|A\|_2}}{(1 + \alpha_+)\sqrt{L_F + 2\|A\|_2} + \sqrt{L_F}} < \rho < \frac{\sqrt{L_F + 2\|A\|_2}}{(1 + \alpha_+)\sqrt{L_F + 2\|A\|_2} - \sqrt{L_F}}. \quad (3.31)$$

Combining (3.29) and (3.31), we observe further that

$$\frac{\sqrt{L_F + 2\|A\|_2}}{(1 + \alpha_+) \sqrt{L_F + 2\|A\|_2} + \sqrt{L_F}} \leq \frac{\sqrt{L_F + 2\|A\|_2}}{\sqrt{L_F + 2\|A\|_2} + \sqrt{L_F}}.$$

Thus, in view of (3.10), $C_0 > 0$.

A direct consequence of Lemma 6 follows.

Proposition 8. *Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1. The following statements are true:*

- (i) *the sequence $\{\Psi_\tau(Z_k, X_{k-1})\}_{k \geq 2}$ is monotonically decreasing and convergent;*
- (ii) *it holds that $X_{k+1} - X_k \rightarrow 0$ as $k \rightarrow +\infty$, and so $X_{k+1} - Y_k \rightarrow 0$ and $Z_{k+1} - Y_k \rightarrow 0$ as $k \rightarrow +\infty$, hence the sequences $\{X_k\}_{k \geq 0}$, $\{Y_k\}_{k \geq 1}$ and $\{Z_k\}_{k \geq 2}$ have the same cluster points.*

Proof. Let $k \geq 2$ be fixed. In view of (3.27) we have

$$\Psi_\tau(Z_{k+1}, X_k) + C_0 \|X_{k+1} - X_k\|^2 \leq \Psi_\tau(Z_k, X_{k-1}).$$

It is clear that the sequence $\{\Psi(Z_k, X_{k-1})\}_{k \geq 2}$ is monotonically decreasing and, since it is nonnegative, is convergent. The fact that $C_0 > 0$ and telescoping arguments (see, for instance, [7, Lemma 5.31]) give $\sum_{k \geq 1} \|X_{k+1} - X_k\|^2 < +\infty$, thus $X_{k+1} - X_k \rightarrow 0$ as $k \rightarrow +\infty$. By taking into consideration (3.21), we deduce that $Z_{k+1} - Z_k \rightarrow 0$ as $k \rightarrow +\infty$. Using further (3.12a) and (3.11a), we have $Z_{k+1} - Y_k \rightarrow 0$ as $k \rightarrow +\infty$. According to (3.12), (3.11a) and (3.11c), the conclusion follows. \square

Now we show that every cluster point of $\{X_k\}_{k \geq 0}$ is a critical point of Ψ .

Theorem 9. *Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1. Then every cluster point of $\{X_k\}_{k \geq 0}$ is a critical point of Ψ .*

Proof. Let \bar{X} be a cluster point of $\{X_k\}_{k \geq 0}$, which means that there exists a subsequence $\{X_{k_i}\}_{i \geq 1}$ such that $X_{k_i} \rightarrow \bar{X}$ as $i \rightarrow +\infty$. We deduce further that $Z_{k_i} \rightarrow \bar{X}$ as $i \rightarrow +\infty$, due to (3.12b). By the characterization of the projection (2.14) and (3.11b), we get that for every $i \geq 1$

$$W_{k_i} := Y_{k_i-1} - Z_{k_i} - \frac{1}{L_F} \nabla \mathcal{E}(Y_{k_i-1}) \in \mathbf{N}_{\mathcal{D}}(Z_{k_i}).$$

From here,

$$L_F W_{k_i} = L_F(Y_{k_i-1} - Z_{k_i}) + \nabla \mathcal{E}(Z_{k_i}) - \nabla \mathcal{E}(Y_{k_i-1}) - \nabla \mathcal{E}(Z_{k_i}) \in \mathbf{N}_{\mathcal{D}}(Z_{k_i}) \quad \forall i \geq 1.$$

By passing to limit as $i \rightarrow +\infty$, and by taking into consideration the continuity of $\nabla \mathcal{E}$ and the fact that $Z_{k+1} - Y_k \rightarrow 0$ as $k \rightarrow +\infty$ (see Proposition 8 (ii)), we get

$$L_F W_{k_i} \rightarrow -\nabla \mathcal{E}(\bar{X}).$$

The closedness of the graph of the normal cone gives $-\nabla \mathcal{E}(\bar{X}) \in \mathbf{N}_{\mathcal{D}}(\bar{X})$. In other words, $\bar{X} \in \text{crit} \Psi$. \square

3.3 Global convergence thanks to the Lojasiewicz property

In this subsection we will prove that actually the whole sequence of iterates $\{X_k\}_{k \geq 0}$ generated by Algorithm 1 converges to a critical point of the objective function Ψ and even establish its rate of convergence. To this end we will use that the regularized objective function Ψ_τ fulfills the *Lojasiewicz property* (see [42]), since it is a *semialgebraic function* (see [2, Example 1], [14]). Recall that a function is called semialgebraic if its graph can be expressed as a semialgebraic set

$$\bigcup_{i=1}^p \bigcap_{j=1}^q \{x \in \mathbb{R}^n : P_{i,j} = 0, Q_{i,j} < 0\},$$

where $P_{i,j}, Q_{i,j} : \mathbb{R}^n \rightarrow \mathbb{R}$ are polynomials for all $1 \leq i \leq p, 1 \leq j \leq q$.

Let $\tau \geq 0$. The fact that Ψ_τ satisfies the *Lojasiewicz property* means that for any critical point (\bar{Z}, \bar{X}) of Ψ_τ there exist $C_L, \varepsilon_L > 0$ and $\theta \in [0, 1)$ such that

$$|\Psi_\tau(Z, X) - \Psi_\tau(\bar{Z}, \bar{X})|^\theta \leq C_L \cdot \text{dist}(\mathbf{0}, \partial\Psi_\tau(Z, X)) \quad \forall (Z, X) \in \mathring{\mathbb{B}}_F((\bar{Z}, \bar{X}), \varepsilon_L).$$

If Ω is a connected and compact subset of $\text{crit}\Psi_\tau$, then, according to [2, Lemma 1], Ψ_τ fulfills the *uniform Lojasiewicz property*, which means that there exist (global constants) $C, \varepsilon > 0$ and $\theta \in [0, 1)$ such that for all $(\bar{Z}, \bar{X}) \in \Omega$

$$|\Psi_\tau(Z, X) - \Psi_\tau(\bar{Z}, \bar{X})|^\theta \leq C \cdot \text{dist}(0, \partial\Psi_\tau(Z, X)) \quad \forall (Z, X) \in \mathbb{R}^{n \times r} \times \mathbb{R}^{n \times r} \text{ with } \text{dist}((Z, X), \Omega) < \varepsilon.$$

Next we will see that, for $\Omega := \Omega(\{(Z_k, X_{k-1})\}_{k \geq 2})$ the set of cluster points of the sequence $\{(Z_k, X_{k-1})\}_{k \geq 2}$, we actually are in the setting of the uniform Lojasiewicz property. Notice that $\Omega \neq \emptyset$ thanks to the boundedness of the sequences $\{X_k\}_{k \geq 0}$ and $\{Z_k\}_{k \geq 2}$.

Lemma 10. *Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1. The following statements are true:*

- (i) *it holds that $\Omega \subseteq \text{crit}\Psi_\tau = \{(X_*, X_*) \in \mathbb{R}^{n \times r} \times \mathbb{R}^{n \times r} : X_* \in \text{crit}\Psi\}$;*
- (ii) *it holds that $\lim_{k \rightarrow +\infty} \text{dist}[(Z_k, X_{k-1}), \Omega] = 0$;*
- (iii) *the set Ω is nonempty, connected and compact;*
- (iv) *the function Ψ_τ takes on Ω the value $\Psi_* := \lim_{k \rightarrow +\infty} \Psi_\tau(Z_k, X_{k-1})$.*

Proof. The item (i) follows from Theorem 9 and (3.26). The proof of (ii) - (iii) follows in the lines of [15, Theorem 5 (ii)-(iii)], by taking into consideration [15, Remark 5], according to which the properties in (ii) - (iii) are generic for sequences satisfying $Z_k - Z_{k-1} \rightarrow 0$ and $X_k - X_{k-1} \rightarrow 0$ as $k \rightarrow +\infty$, which is indeed our case due to Proposition 8 (ii).

Finally, to prove (iv), we consider an arbitrary element (\bar{X}, \bar{X}) in Ω , that is, there exists a subsequence $(Z_{k_i}, X_{k_i-1}) \rightarrow (\bar{X}, \bar{X})$ as $i \rightarrow +\infty$. It holds $\bar{X} \in \mathcal{D}$ and

$$\lim_{i \rightarrow +\infty} \Psi_\tau(Z_{k_i}, X_{k_i-1}) = \Psi_\tau(\bar{X}, \bar{X}).$$

As a consequence, since $\{\Psi(Z_k, X_{k-1})\}_{k \geq 2}$ converges due to Proposition 8 (i), it follows that Ψ_τ is a constant on Ω , namely, $\Psi_\tau(\bar{X}, \bar{X}) = \Psi_* = \lim_{k \rightarrow +\infty} \Psi_\tau(Z_k, X_{k-1})$ for every $(\bar{X}, \bar{X}) \in \Omega$. \square

As a last preparatory step we derive an upper bound for a subgradient of Ψ_τ .

Lemma 11. *Let $\{X_k\}_{k \geq 0}$ be a sequence generated by Algorithm 1. For any $k \geq 2$ we have*

$$V_k := (V'_k, V''_k) \in \partial\Psi_\tau(Z_k, X_{k-1}), \quad (3.32)$$

where

$$\begin{aligned} V'_k &:= L_F(Y_{k-1} - Z_k) + \nabla\mathcal{E}(Z_k) - \nabla\mathcal{E}(Y_{k-1}) + \rho^2\tau(Z_k - X_{k-1}) \\ V''_k &:= -\rho^2\tau(Z_k - X_{k-1}). \end{aligned}$$

In addition,

$$\|V_k\|_F \leq C_1 \|X_k - X_{k-1}\|_F + C_2 \|X_{k-1} - X_{k-2}\|_F \quad \forall k \geq 2, \quad (3.33)$$

where

$$\begin{aligned} L_{\mathcal{E}} &:= 2(\|A\|_2 + (3 + 6\alpha_+ + 4\alpha_+^2) \text{trace}(A)), \\ C_1 &:= \frac{L_F + L_{\mathcal{E}} + 2\rho^2\tau}{\rho} > 0, \\ C_2 &:= (L_F + L_{\mathcal{E}})\alpha_+ \geq 0. \end{aligned}$$

Proof. Let $k \geq 2$ be fixed. The calculus rules of the limiting subdifferential guarantee that for every $(Z, X) \in \mathbb{R}^{n \times r} \times \mathbb{R}^{n \times r}$ it holds

$$\begin{aligned} \partial_Z \Psi_\tau(Z, X) &= \partial\Psi(Z) + \rho^2\tau(Z - X) = \nabla\mathcal{E}(Z) + N_{\mathcal{D}}(Z) + \rho^2\tau(Z - X) \\ \nabla_X \Psi_\tau(Z, X) &= -\rho^2\tau(Z - X). \end{aligned}$$

By the characterization of the projection (2.14) and (3.11b), we have

$$W_k := Y_{k-1} - Z_k - \frac{1}{L_F} \nabla \mathcal{E}(Y_{k-1}) \in \mathbf{N}_{\mathcal{D}}(Z_k).$$

From this we deduce

$$L_F W_k = L_F (Y_{k-1} - Z_k) + \nabla \mathcal{E}(Z_k) - \nabla \mathcal{E}(Y_{k-1}) \in \nabla \mathcal{E}(Z_k) + \mathbf{N}_{\mathcal{D}}(Z_k),$$

which proves (3.32).

Further, we observe that

$$\begin{aligned} \|\nabla \mathcal{E}(Z_k) - \nabla \mathcal{E}(Y_{k-1})\|_F &= 2 \left\| (A - Z_k Z_k^T) Z_k - (A - Y_{k-1} Y_{k-1}^T) Y_{k-1} \right\|_F \\ &\leq 2 \|A\|_2 \|Z_k - Y_{k-1}\|_F + 2 \|Z_k Z_k^T Z_k - Y_{k-1} Y_{k-1}^T Y_{k-1}\|_F \\ &\leq 2 \|A\|_2 \|Z_k - Y_{k-1}\|_F + 2 \|Z_k Z_k^T\|_2 \|Z_k - Y_{k-1}\|_F \\ &\quad + 2 \|Z_k\|_2 \|Y_{k-1}\|_2 \|Z_k - Y_{k-1}\|_F + 2 \|Y_{k-1} Y_{k-1}^T\|_2 \|Z_k - Y_{k-1}\|_F \\ &\leq 2 (\|A\|_2 + (3 + 6\alpha_+ + 4\alpha_+^2) \text{trace}(A)) \|Z_k - Y_{k-1}\|_F \\ &= L_{\mathcal{E}} \|Z_k - Y_{k-1}\|_F, \end{aligned}$$

where the last inequality follows from (2.3b) - (2.3c) and the fact that $\{Z_k\}_{k \geq 1} \subseteq \mathcal{D} \subseteq \mathbb{B}(\mathbf{0}; \sqrt{\text{trace}(A)})$ and $\{Y_k\}_{k \geq 0} \subseteq \mathbb{B}(\mathbf{0}; (1 + \alpha_+) \sqrt{\text{trace}(A)})$ (see Lemma 4). From here we derive the following estimate which holds for all $k \geq 2$

$$\begin{aligned} \|V_k\|_F &= \sqrt{\|V_k'\|_F^2 + \|V_k''\|_F^2} \leq \|V_k'\|_F + \|V_k''\|_F \\ &= \|L_F (Y_{k-1} - Z_k) + \nabla \mathcal{E}(Z_k) - \nabla \mathcal{E}(Y_{k-1}) + \rho^2 \tau (Z_k - X_{k-1})\|_F + \rho^2 \tau \|Z_k - X_{k-1}\|_F \\ &\leq L_F \|Z_k - Y_{k-1}\|_F + \|\nabla \mathcal{E}(Z_k) - \nabla \mathcal{E}(Y_{k-1})\|_F + 2\rho^2 \tau \|Z_k - X_{k-1}\|_F \\ &= (L_F + L_{\mathcal{E}}) \|Z_k - Y_{k-1}\|_F + 2\rho^2 \tau \|Z_k - X_{k-1}\|_F \\ &\leq (L_F + L_{\mathcal{E}} + 2\rho^2 \tau) \|Z_k - X_{k-1}\|_F + (L_F + L_{\mathcal{E}}) \alpha_k \|X_{k-1} - X_{k-2}\|_F \\ &\leq \frac{L_F + L_{\mathcal{E}} + 2\rho^2 \tau}{\rho} \|X_k - X_{k-1}\|_F + (L_F + L_{\mathcal{E}}) \alpha_+ \|X_{k-1} - X_{k-2}\|_F, \end{aligned}$$

which yields the inequality (3.33). \square

To simplify the notation, let us define for every $k \geq 2$

$$\zeta_k := \Psi_{\tau}(Z_k, X_{k-1}) - \Psi_*, \quad (3.34)$$

where $\Psi_* = \lim_{k \rightarrow +\infty} \Psi_{\tau}(Z_k, X_{k-1})$. According to Proposition 8 (i), the sequence $\{\zeta_k\}_{k \geq 0}$ converges monotonically decreasing to 0.

We are now in the position to prove the global convergence of the sequence generated by Algorithm 1.

Theorem 12. *Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1. The sequence $\{X_k\}_{k \geq 0}$ converges to a critical point of Ψ .*

Proof. Let $(\bar{X}, \bar{X}) \in \Omega$. Then, according to Lemma 10 (iv), $\Psi_{\tau}(\bar{X}, \bar{X}) = \Psi_*$ and, for every $k \geq 2$, we have $\Psi_{\tau}(Z_k, X_{k-1}) - \Psi_{\tau}(\bar{X}, \bar{X}) = \zeta_k$. We will show that $\{X_k\}_{k \geq 0}$ has finite length, namely,

$$\sum_{k \geq 0} \|X_{k+1} - X_k\|_F < +\infty. \quad (3.35)$$

Form here it will follow that $\{X_k\}_{k \geq 0}$ is a Cauchy sequence, thus it converges to some X_* , which, according to Theorem 9, will be a critical point of (P_{mod}) .

In order to prove (3.35) we will consider two cases:

Case 1. There exists an integer $k_1 \geq 2$ such that $\zeta_k = 0 \Leftrightarrow \Psi_\tau(Z_{k_1}, X_{k_1-1}) = \Psi_*$. The monotonicity of $\{\zeta_k\}_{k \geq 0}$ implies that $\zeta_k = 0$ for all $k \geq k_1$ and, further, in view of (3.27) and (3.10), that $X_{k+1} - X_k = 0$ for all $k \geq k_1$. Hence

$$\sum_{k \geq 0} \|X_{k+1} - X_k\|_F = \sum_{k=0}^{k_1-1} \|X_{k+1} - X_k\|_F < +\infty.$$

Case 2. It holds $\zeta_k > 0$ for every $k \geq 2$. As Ψ_τ fulfills the uniform Łojasiewicz property, there exist $C, \varepsilon > 0$ and $\theta \in [0, 1)$ such that

$$|\Psi_\tau(Z, X) - \Psi_\tau(\bar{X}, \bar{X})|^\theta \leq C \cdot \text{dist}(0, \partial\Psi_\tau(Z, X)) \quad (3.36)$$

for all $(Z, X) \in \mathbb{R}^{n \times r} \times \mathbb{R}^{n \times r}$ with $\text{dist}[(Z, X), \Omega] < \varepsilon$. Since $\lim_{k \rightarrow +\infty} \text{dist}[(Z_k, X_{k-1}), \Omega] = 0$ (see Lemma 10 (ii)), there exists an integer $k_2 \geq 2$ such that

$$\text{dist}[(Z_k, X_{k-1}), \Omega] < \varepsilon \quad \forall k \geq k_2. \quad (3.37)$$

Combining (3.36) and (3.37), we deduce that for every $k \geq k_2$ it holds

$$\begin{aligned} |\Psi_\tau(Z_k, X_{k-1}) - \Psi_\tau(\bar{X}, \bar{X})|^\theta &= |\zeta_k|^\theta \leq C \cdot \text{dist}(0, \partial\Psi_\tau(Z_k, X_{k-1})) \\ &\leq C \|V_k\|_F \\ &\leq C \cdot C_1 \|X_k - X_{k-1}\|_F + C \cdot C_2 \|X_{k-1} - X_{k-2}\|_F, \end{aligned} \quad (3.38)$$

where the last two inequalities follow from Lemma 11. For the given exponent $\theta \in [0, 1)$, we define

$$\varphi: \mathbb{R}_+ \rightarrow \mathbb{R}, \quad s \mapsto s^{1-\theta}, \quad (3.39)$$

which is a nondecreasing function as $\varphi'(s) = \frac{s^{-\theta}}{1-\theta} > 0$. The concavity of φ gives, by taking into consideration (3.27), for all $k \geq 2$

$$\begin{aligned} \varphi(\zeta_k) - \varphi(\zeta_{k+1}) &\geq \varphi'(\zeta_k) \cdot (\zeta_k - \zeta_{k+1}) \\ &= \frac{(\zeta_k)^{-\theta}}{1-\theta} (\Psi_\tau(Z_k, X_{k-1}) - \Psi_\tau(Z_{k+1}, X_k)) \geq \frac{(\zeta_k)^{-\theta}}{1-\theta} \cdot C_0 \|X_{k+1} - X_k\|_F^2. \end{aligned}$$

From here we get that for every $k \geq k_2$

$$\begin{aligned} \|X_{k+1} - X_k\|_F &\leq \sqrt{\frac{1-\theta}{C_0} (\zeta_k)^\theta (\varphi(\zeta_k) - \varphi(\zeta_{k+1}))} \\ &\leq \frac{1}{2C \cdot (C_1 + C_2)} (\zeta_k)^\theta + \frac{(1-\theta)C \cdot (C_1 + C_2)}{2C_0} (\varphi(\zeta_k) - \varphi(\zeta_{k+1})) \\ &\leq \frac{C_1}{2(C_1 + C_2)} \|X_k - X_{k-1}\|_F + \frac{C_2}{2(C_1 + C_2)} \|X_{k-1} - X_{k-2}\|_F \\ &\quad + \frac{(1-\theta)C \cdot (C_1 + C_2)}{2C_0} (\varphi(\zeta_k) - \varphi(\zeta_{k+1})). \end{aligned} \quad (3.40)$$

By setting for every $k \geq k_2$

$$\begin{aligned} a_k &:= \|X_k - X_{k-1}\|_F, \\ b_k &:= C_3 (\varphi(\zeta_k) - \varphi(\zeta_{k+1})), \\ C_3 &:= \frac{(1-\theta)C \cdot (C_1 + C_2)}{2C_0}, \end{aligned}$$

the inequality (3.40) becomes

$$a_{k+1} \leq \chi_0 a_k + \chi_1 a_{k-1} + b_k,$$

with

$$\chi_0 := \frac{C_1}{2(C_1 + C_2)} \in (0, 1) \quad \text{and} \quad \chi_1 := \frac{C_2}{2(C_1 + C_2)} \in [0, 1).$$

Since $\chi_0 + \chi_1 = \frac{1}{2} < 1$, we obtain, by telescoping sum arguments, that $\sum_{k \geq k_2} \|X_k - X_{k-1}\|_F < +\infty$ (see, for instance, [19, Lemma 2.3] or [20, Lemma 3]). This leads to (3.35) and the proof is completed. \square

We will close this section by discussing the rates of convergence of the projected gradient algorithm with relaxation and inertial parameters. The nature of the rates is determined by the *Lojasiewicz exponent* θ of the function Ψ_τ , which cannot be calculated exactly. This is why we will cover in our statements all possible situations. Further discussions about the values the Lojasiewicz exponent take will be made in the last section of the paper.

An essential tool for deriving the rates of convergence is the following lemma, the proof of which can be found in [21, Lemma 15].

Lemma 13. *Let $\{\eta_k\}_{k \geq 0}$ be a monotonically decreasing sequence of nonnegative numbers converging 0. Assume further that there exists a natural number $\bar{k} \geq 2$ such that for any $k \geq \bar{k}$ it holds*

$$\eta_{k-2} - \eta_k \geq C_\eta \eta_k^{2\theta}, \quad (3.41)$$

where $C_\eta > 0$ and $\theta \in [0, 1)$. The following statements are true:

(i) if $\theta = 0$, then $\{\eta_k\}_{k \geq 0}$ converges in finite time;

(ii) if $\theta \in (0, 1/2]$, then there exist $C_{\eta,0} > 0$ and $Q \in [0, 1)$ such that for any $k \geq \bar{k}$

$$0 \leq \eta_k \leq C_{\eta,0} Q^k;$$

(iii) if $\theta \in (1/2, 1)$, then there exists $C_{\eta,1} > 0$ such that for any $k \geq \bar{k} + 2$

$$0 \leq \eta_k \leq C_{\eta,1} (k-1)^{-\frac{1}{2\theta-1}}.$$

We will show that the sequence $\{\zeta_k\}_{k \geq 0}$ defined in (3.34) satisfies the recursion inequality (3.41) in Lemma 13.

Lemma 14. *Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1 and $\{\zeta_k\}_{k \geq 2}$ the sequence defined in (3.34). Then there exists $k_3 \geq 2$ such that for any $k \geq k_3$*

$$\zeta_{k-2} - \zeta_k \geq C_4 \cdot \zeta_k^{2\theta}, \quad \text{where } C_4 := \frac{C_0}{2(C \cdot C_1)^2} > 0.$$

Proof. From (3.27) we get for any $k \geq 4$

$$\begin{aligned} \zeta_{k-2} - \zeta_k &= \Psi_\tau(Z_{k-2}, X_{k-3}) - \Psi_\tau(Z_{k-1}, X_{k-2}) + \Psi_\tau(Z_{k-1}, X_{k-2}) - \Psi_\tau(Z_k, X_{k-1}) \\ &\geq C_0 \|X_{k-1} - X_{k-2}\|_{\mathbb{F}}^2 + C_0 \|X_k - X_{k-1}\|_{\mathbb{F}}^2 \\ &\geq \frac{C_0}{2} (\|X_k - X_{k-1}\|_{\mathbb{F}} + \|X_{k-1} - X_{k-2}\|_{\mathbb{F}})^2 \\ &\geq \frac{C_0}{2C_1^2} (C_1 \|X_k - X_{k-1}\|_{\mathbb{F}} + C_2 \|X_{k-1} - X_{k-2}\|_{\mathbb{F}})^2 \end{aligned} \quad (3.42)$$

$$\geq \frac{C_0}{2C_1^2} \|V_k\|_{\mathbb{F}}^2, \quad (3.43)$$

where $V_k \in \partial\Psi_\tau(Z_k, X_{k-1})$ is the element defined in Lemma 11 and (3.42) holds true by taking into account further that $0 \leq \rho\alpha_+ \leq 1$, hence

$$C_1 = \frac{L_{\mathbb{F}} + L_{\mathcal{E}} + 2\rho^2\tau}{\rho} \geq \frac{L_{\mathbb{F}} + L_{\mathcal{E}}}{\rho} \geq (L_{\mathbb{F}} + L_{\mathcal{E}})\alpha_+ = C_2.$$

By the same argument as in the proof of Theorem 12, if we take $k_3 := k_2 \geq 2$ for which (3.37) holds, then according to (3.36) the following inequality holds for every $k \geq k_3$

$$|\Psi_\tau(Z_k, X_{k-1}) - \Psi_*|^\theta = \zeta_k^\theta \leq C \cdot \text{dist}(0, \partial\Psi_\tau(Z_k, X_{k-1})) \leq C \|V_k\|_{\mathbb{F}}.$$

The desired statement is a combination of this estimate and (3.43). \square

In order to transfer the convergence rates from $\{\zeta_k\}_{k \geq 0}$ to the sequence $\{X_k\}_{k \geq 0}$, we will need the following lemma.

Lemma 15. Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1 and $\{\zeta_k\}_{k \geq 2}$ the sequence defined in (3.34). Let X_* be the critical point of (P_{mod}) to which the sequence $\{X_k\}_{k \geq 0}$ converges as $k \rightarrow +\infty$ and $\varphi : \mathbb{R}_+ \rightarrow \mathbb{R}, \varphi(s) = s^{1-\theta}$. Then there exists $k_3 \geq 2$ such that for any $k \geq k_3$

$$\|X_k - X_*\|_{\mathbb{F}} \leq C_5 \max \left\{ \sqrt{\zeta_k}, \varphi(\zeta_k) \right\}, \quad \text{where } C_5 := \frac{4}{\sqrt{C_0}} + 2C_3 > 0. \quad (3.44)$$

Proof. By using the same arguments as in the proof of Theorem 12, there exists $k_3 \geq 2$ such that for any $k \geq k_3$ the following inequality is true

$$\|X_{k+1} - X_k\|_{\mathbb{F}} \leq \frac{C_1}{2(C_1 + C_2)} \|X_k - X_{k-1}\|_{\mathbb{F}} + \frac{C_2}{2(C_1 + C_2)} \|X_{k-1} - X_{k-2}\|_{\mathbb{F}} + C_3 (\varphi(\zeta_k) - \varphi(\zeta_{k+1})). \quad (3.45)$$

Let $k \geq k_3$ be fixed. By an induction argument one can prove that

$$\|X_k - X_*\|_{\mathbb{F}} \leq \|X_{k+1} - X_*\|_{\mathbb{F}} + \|X_{k+1} - X_k\|_{\mathbb{F}} \leq \dots \leq \sum_{i \geq k} \|X_{i+1} - X_i\|_{\mathbb{F}}. \quad (3.46)$$

For any $K \geq k + 2 \geq k_3$, by summing up (3.45) for $i = k + 2, \dots, K$, we get

$$\begin{aligned} \sum_{i=k+2}^K \|X_{i+1} - X_i\|_{\mathbb{F}} &\leq \frac{C_1}{2(C_1 + C_2)} \sum_{i=k+2}^K \|X_i - X_{i-1}\|_{\mathbb{F}} + \frac{C_2}{2(C_1 + C_2)} \sum_{i=k+2}^K \|X_{i-1} - X_{i-2}\|_{\mathbb{F}} \\ &\quad + C_3 \sum_{i=k+2}^K (\varphi(\zeta_i) - \varphi(\zeta_{i+1})). \end{aligned} \quad (3.47)$$

Notice that

$$\sum_{i=k+2}^K \|X_{i+1} - X_i\|_{\mathbb{F}} = \sum_{i=k}^K \|X_{i+1} - X_i\|_{\mathbb{F}} - \|X_{k+2} - X_{k+1}\|_{\mathbb{F}} - \|X_{k+1} - X_k\|_{\mathbb{F}}, \quad (3.48a)$$

$$\begin{aligned} \sum_{i=k+2}^K \|X_i - X_{i-1}\|_{\mathbb{F}} &= \sum_{i=k+1}^{K-1} \|X_{i+1} - X_i\|_{\mathbb{F}} \\ &= \sum_{i=k}^K \|X_{i+1} - X_i\|_{\mathbb{F}} - \|X_{k+1} - X_k\|_{\mathbb{F}} - \|X_{K+1} - X_K\|_{\mathbb{F}}, \end{aligned} \quad (3.48b)$$

$$\begin{aligned} \sum_{i=k+2}^K \|X_{i-1} - X_{i-2}\|_{\mathbb{F}} &= \sum_{i=k}^{K-2} \|X_{i+1} - X_i\|_{\mathbb{F}}, \\ &= \sum_{i=k}^K \|X_{i+1} - X_i\|_{\mathbb{F}} - \|X_K - X_{K-1}\|_{\mathbb{F}} - \|X_{K+1} - X_K\|_{\mathbb{F}}. \end{aligned} \quad (3.48c)$$

Plugging these relations into (3.47), neglecting the last two negative terms in (3.48b) and (3.48c), we get

$$\begin{aligned} \sum_{i=k}^K \|X_{i+1} - X_i\|_{\mathbb{F}} &\leq \frac{C_1}{2(C_1 + C_2)} \sum_{i=k+1}^K \|X_i - X_{i-1}\|_{\mathbb{F}} + \frac{C_2}{2(C_1 + C_2)} \sum_{i=k+1}^K \|X_{i-1} - X_{i-2}\|_{\mathbb{F}} \\ &\quad + \|X_{k+2} - X_{k+1}\|_{\mathbb{F}} + \|X_{k+1} - X_k\|_{\mathbb{F}} + C_3 \sum_{i=k+1}^K (\varphi(\zeta_i) - \varphi(\zeta_{i+1})) \\ &\leq \frac{1}{2} \sum_{i=k}^K \|X_{i+1} - X_i\|_{\mathbb{F}} + \|X_{k+2} - X_{k+1}\|_{\mathbb{F}} + \|X_{k+1} - X_k\|_{\mathbb{F}} + C_3 (\varphi(\zeta_{k+1}) - \varphi(\zeta_{K+1})). \end{aligned}$$

Thanks to (3.27) we can deduce that

$$\begin{aligned} \sum_{i=k}^K \|X_{i+1} - X_i\|_{\mathbb{F}} &\leq 2 \|X_{k+2} - X_{k+1}\|_{\mathbb{F}} + 2 \|X_{k+1} - X_k\|_{\mathbb{F}} + 2C_3 (\varphi(\zeta_{k+1}) - \varphi(\zeta_{K+1})) \\ &\leq \frac{2}{\sqrt{C_0}} \sqrt{\zeta_{k+1} - \zeta_{k+2}} + \frac{2}{\sqrt{C_0}} \sqrt{\zeta_k - \zeta_{k+1}} + 2C_3 (\varphi(\zeta_{k+1}) - \varphi(\zeta_{K+1})) \\ &\leq \frac{2}{\sqrt{C_0}} \sqrt{\zeta_{k+1}} + \frac{2}{\sqrt{C_0}} \sqrt{\zeta_k} + 2C_3 \varphi(\zeta_{k+1}). \end{aligned} \quad (3.49)$$

The fact that $\{\zeta_k\}_{k \geq 0}$ is monotonically decreasing implies $\sqrt{\zeta_{k+1}} \leq \sqrt{\zeta_k}$ and $\varphi(\zeta_{k+1}) \leq \varphi(\zeta_k)$. By passing $K \rightarrow +\infty$ in (3.49) and by using (3.46), we get the desired statement. \square

We can now formulate the rates of convergence for the sequences of *objective function values* and *iterates*.

Theorem 16. *Let $\{X_k\}_{k \geq 0}$ be the sequence generated by Algorithm 1 and $\{\zeta_k\}_{k \geq 2}$ the sequence defined in (3.34). Let X_* be the critical point of (P_{mod}) to which the sequence $\{X_k\}_{k \geq 0}$ converges as $k \rightarrow +\infty$. Then there exists $k_4 \geq 2$ such that the following statements are true:*

- (i) *if $\theta = 0$, then $\{\zeta_k\}_{k \geq 2}$ and $\{X_k\}_{k \geq 0}$ converge in finite time;*
- (ii) *if $\theta \in (0, 1/2]$, then there exist $C'_1, C'_2 > 0$ and $Q_1, Q_2 \in [0, 1)$ such that for any $k \geq k_4$*

$$0 \leq \mathcal{E}(Z_k) - \Psi_* \leq C'_1 Q_1^k \quad \text{and} \quad \|X_k - X_*\|_{\mathbb{F}} \leq C'_2 Q_2^k;$$

- (iii) *if $\theta \in (1/2, 1)$, then there exist $C'_3, C'_4 > 0$ such that for any $k \geq k_4 + 2$*

$$0 \leq \mathcal{E}(Z_k) - \Psi_* \leq C'_3 (k-1)^{-\frac{1}{2\theta-1}} \quad \text{and} \quad \|X_k - X_*\|_{\mathbb{F}} \leq C'_4 (k-1)^{-\frac{1-\theta}{2\theta-1}}.$$

Proof. Let $k_3 \geq 2$ be the index provided by previous lemma with the property that (3.44) holds for any $k \geq k_3$. Since $\{\zeta_k\}_{k \geq 0}$ converges to 0, there exists $k_4 \geq k_3$ such that for any $k \geq k_4$

$$\|X_k - X_*\|_{\mathbb{F}} \leq C_5 \max \left\{ \sqrt{\zeta_k}, \varphi(\zeta_k) \right\}, \quad (3.50)$$

$$\zeta_k \leq 1. \quad (3.51)$$

- (i) If $\theta = 0$, then $\{\zeta_k\}_{k \geq 1}$ converges in finite time. By similar arguments as in the proof of Theorem 12, we get that the sequence $\{X_k\}_{k \geq 0}$ becomes identical to X_* starting from a given index. In other words, the sequence $\{X_k\}_{k \geq 0}$ converges in finite time, too.
- (ii) If $\theta \in (0, 1/2]$, then, according to Lemma 13 (ii), there exist $C'_1 > 0$ and $Q_1 \in [0, 1)$ such that for any $k \geq k_4$

$$0 \leq \mathcal{E}(Z_k) - \Psi_* \leq \zeta_k \leq C'_1 Q_1^k.$$

Moreover, as $1 - 2\theta \geq 0$, due to (3.51) it holds

$$\zeta_k^{\frac{1-2\theta}{2}} = \zeta_k^{\frac{1}{2}-\theta} \leq 1 \Leftrightarrow \zeta_k^{1-\theta} \leq \sqrt{\zeta_k}.$$

Consequently, Lemma 15 implies that

$$\|X_k - X_*\|_{\mathbb{F}} \leq C_5 \sqrt{\zeta_k} \leq C_5 \sqrt{C'_1} \left(\sqrt{Q_1} \right)^k \quad \forall k \geq k_4,$$

which is nothing else than the second inequality of (ii) with $C'_2 := C_5 \sqrt{C'_1} > 0$ and $Q_2 := \sqrt{Q_1} \in (0, 1)$.

- (iii) If $\theta \in (1/2, 1)$, then we can use Lemma 13 (iii) to ensure that there exist $C'_3 > 0$ such that for any $k \geq k_4$

$$0 \leq \mathcal{E}(Z_k) - \Psi_* \leq \zeta_k \leq C'_3 (k-1)^{-\frac{1}{2\theta-1}}.$$

Since $2\theta - 1 > 0$ and $\zeta_k \leq 1$ due to (3.51), we have

$$\zeta_k^{\frac{2\theta-1}{2}} = \zeta_k^{\theta-\frac{1}{2}} \leq 1 \Leftrightarrow \sqrt{\zeta_k} \leq \zeta_k^{1-\theta}.$$

Then the second statement follows from (3.50) with $C'_4 := C_5 C'_3^{1-\theta} > 0$. \square

4 Particular instances and numerical experiments

4.1 Some particular instances of Algorithm 1

In the following we will discuss some particular instances of Algorithm 1. To this aim we will use again the notation $L_{\mathbf{F}}(\alpha_+)$, which will allow us to better underline the dependence of the step size from the inertial parameters.

Example 5. Choosing $\alpha_k = 0$ for all $k \geq 1$, Algorithm 1 reduces to the *relaxed projected gradient algorithm*

$$(\forall k \geq 1) \quad \begin{cases} Z_{k+1} := \mathbf{Pr}_{\mathcal{D}} \left(X_k - \frac{1}{L_{\mathbf{F}}(0)} \nabla \mathcal{E}(X_k) \right), \\ X_{k+1} := (1 - \rho) X_k + \rho Z_{k+1}. \end{cases}$$

In this case, $\alpha_+ = 0$ and condition (3.10) becomes

$$\frac{\sqrt{L_{\mathbf{F}}(0) + 2\|A\|_2}}{\sqrt{L_{\mathbf{F}}(0) + 2\|A\|_2} + \sqrt{L_{\mathbf{F}}(0)}} = \frac{\sqrt{3\text{trace}(A) + \|A\|_2 - \lambda_{\min}(A)}}{\sqrt{3\text{trace}(A) + \|A\|_2 - \lambda_{\min}(A)} + \sqrt{3\text{trace}(A) - \lambda_{\min}(A)}} < \rho \leq 1 < \frac{\sqrt{L_{\mathbf{F}}(0) + 2\|A\|_2}}{\sqrt{L_{\mathbf{F}}(0) + 2\|A\|_2} - \sqrt{L_{\mathbf{F}}(0)}}. \quad (4.1)$$

Notice that, according to (4.1), the choice $\rho = 1$ is allowed, which leads to the classical *projected gradient algorithm*.

Example 6. For $\rho = 1$, Algorithm 1 reduces to the *inertial projected gradient algorithm*

$$(\forall k \geq 1) \quad \begin{cases} Y_k := X_k + \alpha_k (X_k - X_{k-1}), \\ X_{k+1} := \mathbf{Pr}_{\mathcal{D}} \left(Y_k - \frac{1}{L_{\mathbf{F}}(\alpha_+)} \nabla \mathcal{E}(Y_k) \right). \end{cases}$$

In the nonconvex setting, algorithms with inertial effects proved to be helpful to detect critical points of minimization problems which cannot be found by their non-inertial variants (see, for instance, [20, 37]). For constant inertial parameters $\alpha_k = \alpha_+ \in [0, 1]$ for any $k \geq 1$, condition (3.10) is equivalent to

$$1 < \frac{\sqrt{L_{\mathbf{F}}(\alpha_+) + 2\|A\|_2}}{(1 + \alpha_+) \sqrt{L_{\mathbf{F}}(\alpha_+) + 2\|A\|_2} - \sqrt{L_{\mathbf{F}}(\alpha_+)}}$$

and further to

$$0 \leq \alpha_+ < \sqrt{\frac{L_{\mathbf{F}}(\alpha_+)}{L_{\mathbf{F}}(\alpha_+) + 2\|A\|_2}}. \quad (4.2)$$

Condition (4.2) is in implicit form, however, one can show that it is satisfied for every $0 < \alpha_+ \leq 0.967$. In order to find a larger α_+ , which fulfills (4.2), one can use a bisection routine starting from 0.967, as we did in our numerical experiments and will explain in the next subsection.

In order to see that for every $0 < \alpha_+ \leq 0.967$ the inequality (4.2) always holds true, one can rewrite (4.2) equivalently as

$$\alpha_+^2 (\|A\|_2 + (3 + 8\alpha_+ + 6\alpha_+^2) \text{trace}(A) - \lambda_{\min}(A)) \leq (3 + 8\alpha_+ + 6\alpha_+^2) \text{trace}(A) - \lambda_{\min}(A). \quad (4.3)$$

Relation (4.3) is definitively fulfilled if

$$w(\alpha_+) \leq 0,$$

where

$$w(\xi) := 6\text{trace}(A)\xi^4 + 8\text{trace}(A)\xi^3 - (\lambda_{\min}(A) + 2\text{trace}(A))\xi^2 - 8\xi\text{trace}(A) - 3\text{trace}(A) - \lambda_{\min}(A).$$

We have

$$w(\alpha_+) \leq \text{trace}(A)\phi(\alpha_+) - \lambda_{\min}(A)\alpha_+^2 - \lambda_{\min}(A) \leq \text{trace}(A)\phi(\alpha_+),$$

where

$$\phi(\xi) := 6\xi^4 + 8\xi^3 - 2\xi^2 - 8\xi - 3,$$

and this is why we will solve a more restricted yet easier inequality $\phi(\xi) \leq 0$ instead of (4.3). The derivative of ϕ reads

$$\phi'(\xi) = 24\xi^3 + 24\xi^2 - 4\xi - 8$$

and has exactly one root

$$\nu = \frac{1}{18} \sqrt[3]{594 - 54\sqrt{67}} + \frac{1}{6} \sqrt[3]{2(11 + \sqrt{67})} - \frac{1}{3} \approx 0.5253.$$

Since $\phi'(0) = -8 < 0$ and $\phi'(1) = 36 > 0$, we have that ϕ is decreasing on $(0, \nu)$ and increasing on $(\nu, 1)$. Moreover, as $\phi(0.967) = -0.00458574 < 0$, $\phi(0) = -3 < 0$ and $\phi(1) = 1 > 0$, we can conclude that $\phi(\xi) < 0$ for every $\xi \in [0, 0.967]$, which implies that (4.3) is fulfilled as a strict inequality for every $\alpha_+ \in [0, 0.967]$ as well. Since in the above approach we weakened (4.3) in order to simplify the computations, one cannot expect 0.967 to be the largest value for which this inequality is fulfilled. However, we will use in our numerical experiments 0.0967 as the starting point for a bisection procedure aimed to find larger values of α_+ which fulfill (4.3).

Example 7. An interesting choice of the variable inertial parameters $\{\alpha_k\}_{k \geq 1}$ in the context of the *inertial projected gradient algorithm* discussed in Example 6 is

$$\alpha_k := \kappa \cdot \frac{t_k - 1}{t_{k+1}}, \quad \text{where } \begin{cases} t_1 & := 1 \\ t_{k+1} & := \frac{1 + \sqrt{1 + 4t_k^2}}{2} \end{cases} \quad \forall k \geq 1. \quad (4.4)$$

Notice that, for $\kappa := 1$, this is exactly the update rule of the celebrated Nesterov/FISTA algorithm [47, 12]. This iterative scheme have attracted the interest of the optimization community and of many practitioners due to the fact that, in the convex setting, it improves for the sequence of objective function values the convergence rate over the one of the standard non-inertial method. In the nonconvex setting, no theoretical results, which emphasize an improvement in the convergence behaviour through this update rule, have been obtained so far, however, some empirical studies suggest that this might be the case (see, for instance, [52]).

Since $\alpha_+ = \sup_{k \geq 0} \alpha_k = \kappa$, one can find κ such that (3.10) holds by solving (see (4.2))

$$0 \leq \kappa < \sqrt{\frac{L_F(\kappa)}{L_F(\kappa) + 2\|A\|_2}}. \quad (4.5)$$

If one wants to choose larger values for κ , for instance to take κ close to 1, a restart mechanism can be adapted into the scheme (4.4), like, for example, in [51].

Example 8. If we set, again in the context of the *inertial projected gradient algorithm*,

$$\alpha_k := \frac{\kappa k}{k+3} \quad \forall k \geq 1, \quad \text{where } \kappa \in (0, 1),$$

then it holds $\alpha_+ = \kappa$. This is a setting considered by László in [37] for the inertial gradient algorithm, which is the scheme in Example 6 without the projection step. Our algorithm can be considered as an extension of the one in [37]. To guarantee convergence, in [37] is required that the step size fulfills

$$0 < \mu < \frac{2(1-\kappa)}{L_F},$$

where L_F denotes the Lipschitz constant of the gradient of the objective function. This condition excludes the case $\kappa = 1$ and allows $\mu = 1/L_F$ as stepsize when $\kappa = 1/2$. In our setting, we can have larger values of κ in combination with the stepsize $1/L_F$, namely, those for which (4.5) is fulfilled (see also the discussion at the end of Example 6).

Example 9. Other than for the classical inertial algorithms for convex optimization problems and monotone inclusions, for which the inertial parameters were not allowed to take values greater than 1/3, the interplay between relaxation and inertia gives us much more freedom when it comes to the choice of the latter. We have seen that as far as α_+ satisfies (4.2) we can choose $\rho = 1$. For α_+ close to 1 such that (4.2) is not satisfied, in other words

$$\sqrt{\frac{L_F(\alpha_+)}{L_F(\alpha_+) + 2\|A\|_2}} \leq \alpha_+,$$

we can take

$$0 < \frac{\sqrt{L_F(\alpha_+) + 2\|A\|_2}}{\sqrt{L_F(\alpha_+) + 2\|A\|_2} + \sqrt{L_F(\alpha_+)}} < \rho < \frac{\sqrt{L_F(\alpha_+) + 2\|A\|_2}}{(1 + \alpha_+)\sqrt{L_F(\alpha_+) + 2\|A\|_2} - \sqrt{L_F(\alpha_+)}} < 1. \quad (4.6)$$

This applies also for the case when $\alpha_k = 1$ for any $k \geq 1$, and thus $\alpha_+ = 1$, for which Algorithm 1 becomes

$$(\forall k \geq 1) \quad \begin{cases} Z_{k+1} := \mathbf{Pr}_{\mathcal{D}} \left(2X_k - X_{k-1} - \frac{1}{L_F(1)} \nabla \mathcal{E} (2X_k - X_{k-1}) \right), \\ X_{k+1} := (1 - \rho) X_k + \rho Z_{k+1}. \end{cases}$$

As we will see in the numerical results, the strategy of choosing α_+ close to 1 and ρ according to (4.6) yields to the best performances of the algorithm.

4.2 Numerical experiments

The aim of the numerical experiments we will present in this subsection is twofold: to compare the performances of our algorithm with those of other numerical methods for the nonnegative factorization of completely positive matrices, as are ModMAP and SpFeasDC from [33] and [23], respectively, and to show in which way and to which extent the algorithm parameters influence these performances.

A particular attention will be paid to the nonnegative factorization of matrices not belonging to the interior of \mathcal{CP}_n , for which the algorithms in [33, 23] perform rather poor.

Number of runs and starting points. In every numerical experiment, for $A \in \mathbb{R}^{n \times n}$ with $n < 100$, we run Algorithm 1 100 times for 100 randomly chosen initial matrices in \mathcal{D} (for instance, by choosing a random matrix in $\mathbb{R}^{n \times r}$ and then by using the projection formula (3.1)), and run the algorithms ModMAP and SpFeasDC also 100 times for 100 randomly chosen initial matrices in \mathcal{O}_r (for instance, by choosing a random matrix in $\mathbb{R}^{r \times r}$ and by computing a SVD decomposition); if $n \geq 100$, then we do this for each of the algorithms 10 times.

As noticed in Section 2.3, the algorithm ModMAP and SpFeasDC require, in addition, a matrix B , which we compute by the Cholesky decomposition. If the Cholesky decomposition fails, then we use the eigenvalue decomposition. Here we follow the approach described in [33, Section 3], see also [23, Section 6].

Parameter choice. We will choose the constant α_+ , which will then determine the sequence of inertial parameters $\{\alpha_k\}_{k \geq 1}$, with two different aims:

- by running a simple bisection routine which starts at 0.967 in order to find greater values for α_+ that satisfy (4.2), namely,

$$0 \leq \alpha_+ < \sqrt{\frac{L_F(\alpha_+)}{L_F(\alpha_+) + 2\|A\|_2}}.$$

Instead of using the midpoint rule, we will use as update rule $\alpha_+ := (3\alpha_+ + 1)/4$ for the bisection routine, which seemingly gives better results. We will then choose $\alpha_+ := \hat{\alpha}_+$, which is the last value at which (4.2) holds. As seen in the previous subsection, as long as (4.2) is fulfilled, we can and do choose $\rho = 1$.

- by taking $\hat{\alpha}_1 := (3\hat{\alpha}_+ + 1)/4$, $\hat{\alpha}_2 := (\hat{\alpha}_+ + 1)/2$, and $\hat{\alpha}_3 := (\hat{\alpha}_+ + 3)/4$, which, when $\hat{\alpha}_+$ is obtained as above, all violate (4.2). The corresponding relaxation parameters will be denoted by $\rho(\hat{\alpha}_1)$, $\rho(\hat{\alpha}_2)$ and $\rho(\hat{\alpha}_3)$, respectively, and chosen to satisfy (4.6). Another value of α_+ which violates (4.2) is 1, which we will also use in the experiments in combination with a relaxation parameter $\rho(1)$ fulfilling (4.6) as well.

Stopping criteria. For $A \in \mathbb{R}^{n \times n}$, we will run each of the algorithms at most 10000 iterations if $n < 100$ and 50000 otherwise. We count the algorithms ModMAP and SpFeasDC as “success” if the stopping criterion

$$\min\{(BQ_k)_{i,j}\} \geq -\text{To1}_{\text{fea}} \quad (4.7)$$

is reached before the maximal number of iterations is attained. This is nothing else than the stopping criterion used in [33, 23]. For SpFeasDC, we will set $\text{To1}_{\text{fea}} := 10^{-16}$ if the matrix A belongs to $\text{int}(\mathcal{CP}_n)$, and $\text{To1}_{\text{fea}} := 10^{-7}$ otherwise. For ModMAP we will take as threshold $10 \times \text{To1}_{\text{fea}}$.

For all instances of Algorithm 1 we will use as stopping criterion the relative error condition

$$\frac{\|A - X_k X_k^T\|_F^2}{\|A\|_F^2} < \text{To1}_{\text{val}}. \quad (4.8)$$

Also here, we will set $\text{To1}_{\text{val}} := 10^{-16}$ if A belongs to $\text{int}(\mathcal{CP}_n)$, and $\text{To1}_{\text{val}} := 10^{-7}$ otherwise.

Tables. In the tables with numerical results, we report the (rounded) successful rate over the total number of trials (**Rate**), the average CPU time in seconds for both successful (**Time (s)**) and failed (**Time (f)**) trials, and the average number of iterations (**Iter.**) needed to reach the stopping criteria for the successful trials. We also use boldfaces to highlight the best results among all methods that have successful rate 1.

Plots. In the figures 1 - 2 and 9 - 12 we plot for some particular instances of the matrix A the sequences of function values $\{\mathcal{E}(Z_k) - \mathcal{E}_{\min}\}_{k \geq 2}$ and of distances $\{\frac{1}{2} \|X_k - X_{\text{sol}}\|_F^2\}_{k \geq 0}$ in logarithmic scale, where \mathcal{E}_{\min} denotes the smallest objective function value over all methods and X_{sol} is the last iterate X_k for each method. With the plots we want to emphasize that the sequences of both function values and iterates have linear rates of convergence.

In the figures 3 - 8 we emphasize to what extent the performances of the algorithms are sensitive to the number of columns r of the factor.

Algorithms. We summarize here the different variants of Algorithm 1 with corresponding parameter choices we will use in the numerical experiments:

- (i) **PG:** the classical projected gradient algorithm formulated in Example 5 in case $\rho = 1$;
- (ii) **FISTA:** the Nesterov/FISTA algorithm from [47, 12];
- (iii) **IPG-const:** the inertial projected gradient algorithm formulated in Example 6 (for $\rho = 1$) with constant inertial parameters $\alpha_k = \alpha_+$ for any $k \geq 1$ and $\hat{\alpha}_+$ chosen to satisfy (4.2);
- (iv) **IPG-sFISTA:** the inertial projected gradient algorithm formulated in Example 7 (for $\rho = 1$) with inertial parameters fulfilling (4.4) for $\kappa := \hat{\alpha}_+$;
- (v) **IPG-mod:** the modification of Nesterov's scheme from [37] discussed in Example 8 with $\kappa := \hat{\alpha}_+$ and step size $\mu := 1/L_F$. The setting goes beyond the one in which convergence was proved in [37], but it is within the one for which our convergence result holds.
- (vi) **RIPG-const, RIPG-sFISTA and RIPG-mod:** the relaxed versions of **IPG-const**, **IPG-sFISTA** and **IPG-mod**, respectively, for different values of α_+ that violate (4.2), as in Example 9, and with corresponding relaxation parameters ρ satisfying (4.6).

Numerical experiment 1. In our first experiment, we use randomly generated completely positive matrices as in [33, Section 7.8]. Precisely, in each test we generate a random $n \times 2n$ matrix B_0 and then we set $A := |B_0| |B_0|^T$; here the absolute value operator $|\cdot|$ is understood entrywise. We test the algorithms on 50 randomly generated 40×40 matrices, 10 randomly generated 100×100 matrices, and 10 randomly generated 500×500 matrices, all via the approach described above. For the nonnegative factorization we choose in each case $r := 1.5n + 1$ and $r := 3n + 1$, which have been used also in [23]. Notice that the choice $r := 1.5n + 1$ may not be sufficient since the test instances are generated using matrices of order $n \times 2n$. Nevertheless, we obtain satisfactory results for these choices of r . The performances of the different numerical methods on the for the different instances are captured in the Tables 1 - 6.

One can notice that SpFeasDC outperforms the other methods with respect to the number of iterations, which is due the fact that SpFeasDC uses a linesearch routine to improve the step size, while the other methods have quite conservative step size rules. However, some of the instances of Algorithm 1 can compete with SpFeasDC in terms of computational time. This is due to the fact that the latter runs in every iteration a SVD routine, which is much more time expensive than the simple projection step made by Algorithm 1. In particular with growing dimensions our algorithm becomes faster than SpFeasDC.

Method	Rate	Time (s)	Time (f)	Iter.
ModMAP	0.80	2.5137×10^0	7.0416×10^0	3467.08
SpFeasDC	1.00	4.1259×10^{-2}	—/—	38.51
PG	0.00	—/—	4.5239×10^{-1}	—/—
IPG-const: $\alpha = \hat{\alpha}_+$	1.00	1.3017×10^{-1}	—/—	2554.45
IPG-sFISTA: $\alpha = \hat{\alpha}_+$	1.00	1.2994×10^{-1}	—/—	2561.51
IPG-mod: $\alpha = \hat{\alpha}_+$	1.00	1.3122×10^{-1}	—/—	2562.88
RIPG-const: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	2.8331×10^{-1}	—/—	5490.14
RIPG-const: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	2.8589×10^{-1}	—/—	5532.32
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	8.8411×10^{-2}	—/—	1752.14
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	1.4610×10^{-1}	—/—	2906.58
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	8.9617×10^{-2}	—/—	1751.66
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	1.4798×10^{-1}	—/—	2904.48

Table 1: The nonnegative factorization of random completely positive matrices for $n = 40$ and $r = 61$.

Method	Rate	Time (s)	Time (f)	Iter.
ModMAP	0.90	8.3492×10^0	2.1794×10^1	3883.03
SpFeasDC	1.00	6.3118×10^{-2}	—/—	19.22
PG	0.00	—/—	8.4875×10^{-1}	—/—
IPG-const: $\alpha = \hat{\alpha}_+$	1.00	1.9973×10^{-1}	—/—	2020.26
IPG-sFISTA: $\alpha = \hat{\alpha}_+$	1.00	2.5665×10^{-1}	—/—	2589.74
IPG-mod: $\alpha = \hat{\alpha}_+$	1.00	2.6477×10^{-1}	—/—	2591.06
RIPG-const: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	5.0055×10^{-1}	—/—	4964.26
RIPG-const: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	5.0620×10^{-1}	—/—	5014.23
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	1.6188×10^{-1}	—/—	1634.78
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	2.7420×10^{-1}	—/—	2760.50
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	1.6681×10^{-1}	—/—	1633.88
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	2.8115×10^{-1}	—/—	2756.80

Table 2: The nonnegative factorization of random completely positive matrices for $n = 40$ and $r = 121$.

Method	Rate	Time (s)	Time (f)	Iter.
ModMAP	0.62	6.4857×10^1	1.3183×10^2	24245.13
SpFeasDC	1.00	5.3558×10^{-1}	—/—	109.72
PG	0.68	1.0220×10^1	1.0925×10^1	47216.68
IPG-const: $\alpha = \hat{\alpha}_+$	1.00	1.9569×10^0	—/—	7948.22
IPG-sFISTA: $\alpha = \hat{\alpha}_+$	1.00	1.6213×10^0	—/—	6606.02
IPG-mod: $\alpha = \hat{\alpha}_+$	1.00	1.6379×10^0	—/—	6607.08
RIPG-const: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	3.4802×10^0	—/—	14271.40
RIPG-const: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	3.5571×10^0	—/—	14465.50
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	8.3203×10^{-1}	—/—	3160.96
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	8.1442×10^{-1}	—/—	3216.90
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	8.2046×10^{-1}	—/—	3163.08
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	7.9077×10^{-1}	—/—	3215.90

Table 3: The nonnegative factorization of random completely positive matrices for $n = 100$ and $r = 151$.

Method	Rate	Time (s)	Time (f)	Iter.
ModMAP	0.16	6.1287×10^2	9.1004×10^2	34943.88
SpFeasDC	1.00	2.1906×10^0	—//—	96.08
PG	0.80	2.4696×10^1	2.3458×10^1	47725.30
IPG-const: $\alpha = \hat{\alpha}_+$	1.00	1.9569×10^0	—//—	7948.22
IPG-sFISTA: $\alpha = \hat{\alpha}_+$	1.00	1.6213×10^0	—//—	6606.02
IPG-mod: $\alpha = \hat{\alpha}_+$	1.00	1.6379×10^0	—//—	6607.08
RIPG-const: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	3.8786×10^0	—//—	13377.24
RIPG-const: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	3.7777×10^0	—//—	13551.98
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	2.0073×10^0	—//—	3232.04
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	1.7938×10^0	—//—	3021.04
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_2, \rho(\hat{\alpha}_2))$	1.00	1.9433×10^0	—//—	3234.30
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	1.7880×10^0	—//—	3018.80

Table 4: The nonnegative factorization of random completely positive matrices for $n = 100$ and $r = 301$.

Method	Rate	Time (s)	Time (f)	Iter.
SpFeasDC	1.00	$1.6557e \times 10^2$	—//—	929.38
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	1.4526×10^2	—//—	7919.40
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	1.4861×10^2	—//—	7921.64

Table 5: The nonnegative factorization of random completely positive matrices for $n = 500$ and $r = 751$.

Method	Rate	Time (s)	Time (f)	Iter.
SpFeasDC	1.00	1.3813×10^3	—//—	914.15
RIPG-sFISTA: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	2.2975×10^2	—//—	7776.30
RIPG-mod: $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$	1.00	2.3037×10^2	—//—	7779.60

Table 6: The nonnegative factorization of random completely positive matrices for $n = 500$ and $r = 1501$.

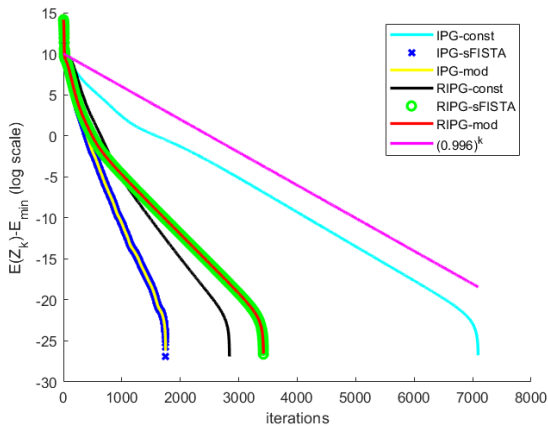


Figure 1: The sequence $\mathcal{E}(Z_k) - \mathcal{E}_{\min}$ in logarithmic scale for a particular instance of A in case $n = 40$ and $r = 61$.

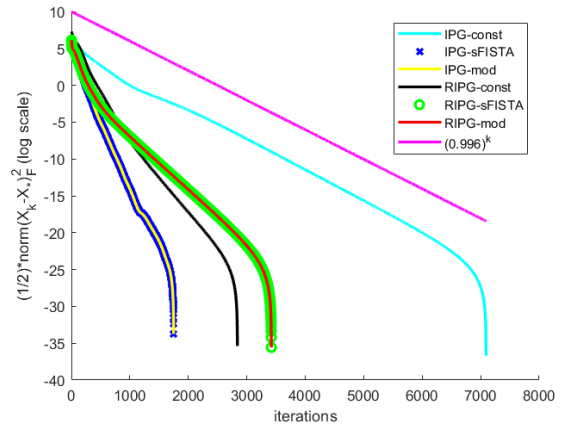


Figure 2: The sequence $\frac{1}{2} \|X_k - X_{\text{sol}}\|_F^2$ in logarithmic scale for a particular instance of A in case $n = 40$ and $r = 61$.

Numerical experiment 2. In the second numerical experiment we examine the efficiency of the factorization algorithms when the number of columns r of the factor varies.

We first consider the factorization of a matrix of the form

$$A_n := \begin{pmatrix} 0 & \mathbf{j}_{n-1}^T \\ \mathbf{j}_{n-1} & \mathbb{I}_{n-1} \end{pmatrix}^T \begin{pmatrix} 0 & \mathbf{j}_{n-1}^T \\ \mathbf{j}_{n-1} & \mathbb{I}_{n-1} \end{pmatrix} \in \mathbb{R}^{n \times n}, \quad (4.9)$$

and recall that \mathbb{I}_n and \mathbf{j}_n denote the $n \times n$ identity matrix and the all-ones-vector in \mathbb{R}^n , respectively. It has been observed in [33] that for such matrices the rate of success of ModMAP, when applied with random initial points, increases with higher values for r . We notice that $A_n \in \text{int}(\mathcal{CP}_n)$ for any $n \geq 2$ ([55]).

A similar behaviour can be noticed for various instances of Algorithm 1, as it can be seen in Figure 3. Here we plot the rate of success with which the algorithms ModMAP, PG and IPG-sFISTA with $\alpha = \hat{\alpha}_+$ and RIPG-sFISTA with $(\alpha, \rho) = (\hat{\alpha}_3, \rho(\hat{\alpha}_3))$ provided a factorization of the matrix A_{40} for $r \in \{40, 51, 61, 71, 81, 101, 121\}$ and 100 random initial points. The number of required iterations is plotted in Figure 4. For the variants of Algorithm 1 similar results can be reported.

We repeat the experiment for a completely positive matrix $A := |B_0| |B_0|^T$ constructed as in the previous numerical experiment from a randomly generated 100×200 matrix B_0 for random initial points and various $r \in \{151, 176, 201, 251, 301\}$. As it can be seen in Figure 5, the rate of success for different variants of Algorithm 1 increases with higher values for r , however, this is not anymore the case for ModMAP. Moreover, according to Figure 4, the numbers of iterations required by the first provide a factorization that is more stable than the one required by ModMAP.

With the figures 6 and 8 we want to underline that, while IPG-sFISTA requires for all instances of r less iterations than RIPG-sFISTA when factorizing A_{40} given by (4.9), the situation changes to the opposite when it comes to the factorization of the randomly generated matrix $A \in \mathcal{CP}_{100}$.

Numerical experiment 3. In this numerical experiment we address the factorization of the matrix from [56, Example 2.7]

$$A := \begin{pmatrix} 41 & 43 & 80 & 56 & 50 \\ 43 & 62 & 89 & 78 & 51 \\ 80 & 89 & 162 & 120 & 93 \\ 56 & 78 & 120 & 104 & 62 \\ 50 & 51 & 93 & 62 & 65 \end{pmatrix}, \quad (4.10)$$

which is known to be completely positive with $\text{cpr}(A) = \text{rank}(A) = 3$ (see [56, Theorem 2.5]). However, at the time this matrix was introduced no completely positive factorization of it was known. A completely positive factorization of this matrix with two zero columns was obtained for the first time in [33] and it is given by

$$A = \tilde{X} \tilde{X}^T, \quad \text{where} \quad \tilde{X} = \begin{pmatrix} 0.0000 & 3.3148 & 4.3615 & 3.3150 & 0.0000 \\ 0.0000 & 0.7261 & 4.3485 & 6.5241 & 0.0000 \\ 0.0000 & 4.5242 & 9.9675 & 6.4947 & 0.0000 \\ 0.0000 & 0.1361 & 7.4192 & 6.9955 & 0.0000 \\ 0.0000 & 5.3301 & 3.8960 & 4.6272 & 0.0000 \end{pmatrix},$$

for the generation of which the spectral decomposition of A has been used.

With Algorithm 1 we obtain several other factorizations of A . We present exemplary the following factors, all having two zero columns,

$$\tilde{X}_1 = \begin{pmatrix} 4.4017 & 0 & 2.7669 & 0 & 3.7376 \\ 4.1001 & 0 & 6.4472 & 0 & 1.9034 \\ 6.9385 & 0 & 7.0193 & 0 & 8.0366 \\ 3.7388 & 0 & 8.4422 & 0 & 4.3302 \\ 6.8248 & 0 & 2.5512 & 0 & 3.4515 \end{pmatrix},$$

$$\tilde{X}_2 = \begin{pmatrix} 2.6507 & 0 & 5.1505 & 0 & 2.7287 \\ 6.3431 & 0 & 3.3813 & 0 & 3.2144 \\ 5.6648 & 0 & 8.7429 & 0 & 7.3124 \\ 7.0264 & 0 & 3.9453 & 0 & 6.2502 \\ 3.4789 & 0 & 7.1126 & 0 & 1.5191 \end{pmatrix}, \quad \tilde{X}_3 = \begin{pmatrix} 0 & 0 & 3.9911 & 3.2352 & 3.8216 \\ 0 & 0 & 2.3524 & 1.7597 & 7.3054 \\ 0 & 0 & 5.8924 & 7.4202 & 8.4981 \\ 0 & 0 & 1.8483 & 4.3608 & 9.0315 \\ 0 & 0 & 6.2922 & 2.5714 & 4.3355 \end{pmatrix},$$

and notice that the matrix \tilde{X}_1 is obtained with IPG-const, \tilde{X}_2 with IPG-sFISTA, and \tilde{X}_3 with RIPG-mod.

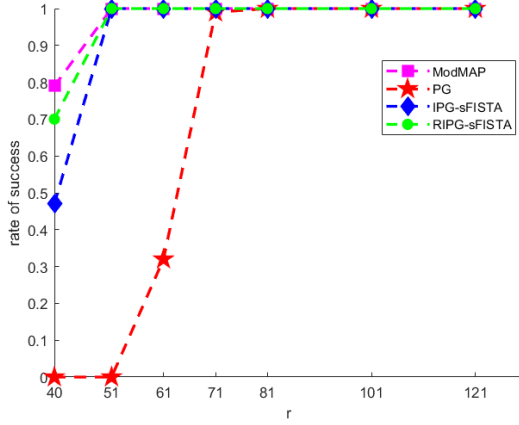


Figure 3: The rate of success for the factorization of A_{40} given by (4.9) for different values of r and random initial points.

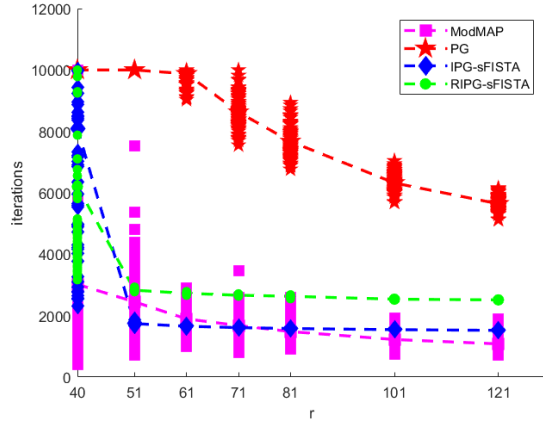


Figure 4: The number of iterations required for the random factorization of A_{40} given by (4.9) for different values of r and random initial points.

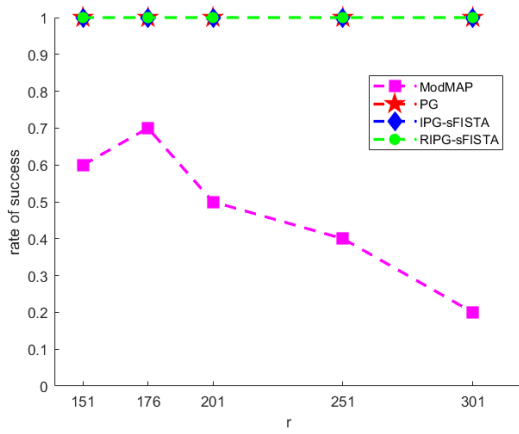


Figure 5: The rate of success for the factorization of a randomly generated matrix $A \in \mathcal{CP}_{100}$ for different values of r and random initial points.

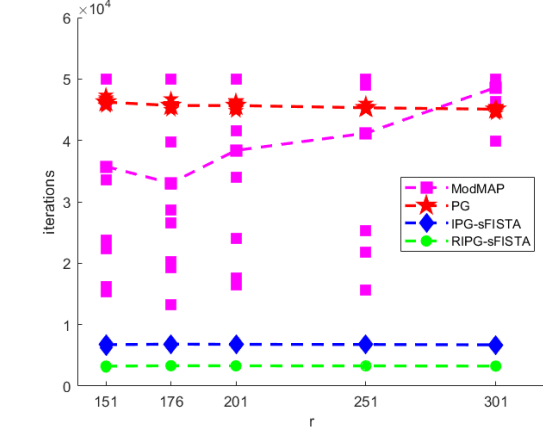


Figure 6: The number of iterations required for the factorization of a randomly generated matrix $A \in \mathcal{CP}_{100}$ for different values of r and random initial points.

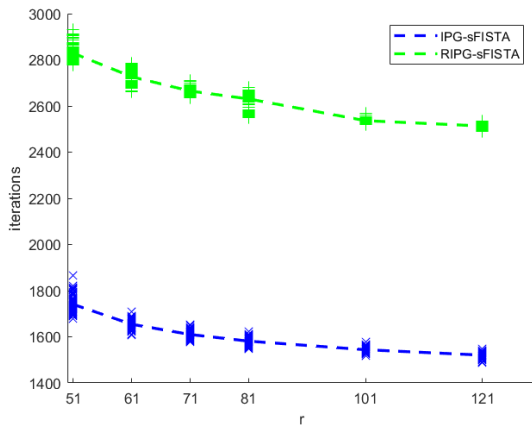


Figure 7: Comparison of the number of iterates required by IPG-sFISTA and RIPG-sFISTA for the factorization of A_{40} given by (4.9) for different values of r and random initial points.

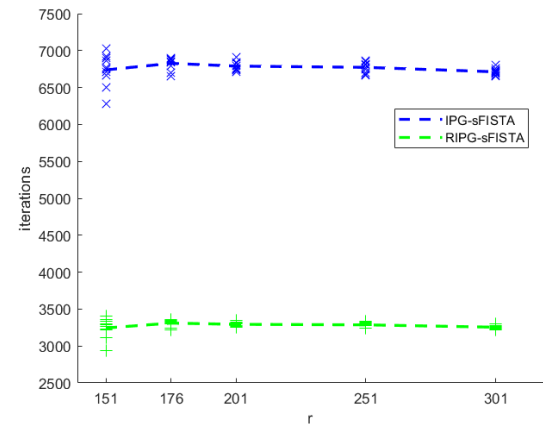


Figure 8: Comparison of the number of iterates required by IPG-sFISTA and RIPG-sFISTA for the factorization of a randomly generated matrix $A \in \mathcal{CP}_{100}$ for different values of r and random initial points.

Numerical experiment 4. In this numerical experiment, we consider the perturbed matrix A_ω defined by

$$A_\omega := \omega A + (1 - \omega) P, \quad \text{for } \omega \in [0, 1], \quad (4.11)$$

where

$$A := \begin{pmatrix} 8 & 5 & 1 & 1 & 5 \\ 5 & 8 & 5 & 1 & 1 \\ 1 & 5 & 8 & 5 & 1 \\ 1 & 1 & 5 & 8 & 5 \\ 5 & 1 & 1 & 5 & 8 \end{pmatrix} \quad \text{and} \quad P := \begin{pmatrix} 2 & 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 & 1 \\ 1 & 1 & 2 & 1 & 1 \\ 1 & 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 & 2 \end{pmatrix}. \quad (4.12)$$

Both A and A_ω belong to \mathcal{CP}_5 for all $\omega \in [0, 1]$. Furthermore, $A_\omega \in \text{int}(\mathcal{CP}_5)$ whenever $0 \leq \omega < 1$, since $P = [\mathbf{j}_5 | \mathbb{I}_5][\mathbf{j}_5 | \mathbb{I}_5]^T \in \text{int}(\mathcal{CP}_5)$, while $A \in \mathcal{CP}_5 \setminus \text{int}(\mathcal{CP}_5)$. It has been observed in [33, 23] that it is much more difficult to perform a nonnegative factorization of A than of A_ω when $\omega < 1$. In particular, the rate of success for ModMAP and SpFeasDC decreases to zero when ω to 1, that is, when A_ω becomes nearly identical to A . For this experiment, we set, according to the lower bounds for the cp-rank derived in [17], $r := 11$ for $\omega := 1$ and $r := 12$ otherwise. We present in Table 7 and in Table 8 the numerical performances of the algorithms applied to the nonnegative factorization of the matrices $A_{0.99}$ and $A_{1.00} = A$, respectively. One can see that both ModMAP and SpFeasDC practically fail to factorize the two matrices, a fact which was noticed in [33, 23]. In what concerns the inertial methods IPG-const, IPG-sFISTA and IPG-mod, they also seem to face some difficulties in solving these matrices, as the rate of success is not for every initial matrix equal to 1. On the other hand, the methods RIPG-sFISTA and RIPG-mod combining inertial and relaxation parameters always return nonnegative factorizations for α_+ taken equal to $\hat{\alpha}_3$ and equal to 1. This emphasizes the importance of the interplay between the inertial and relaxation parameters, as mentioned in Example 9, and provides a strong motivation for the approach proposed in this paper.

Numerical experiment 5. Let \mathbb{I}_n and \mathbf{J}_n denote the identity matrix and the all-ones-matrix in $\mathbb{R}^{n \times n}$, respectively, and define

$$A_{2n} := \begin{pmatrix} n\mathbb{I}_n & \mathbf{J}_n \\ \mathbf{J}_n & n\mathbb{I}_n \end{pmatrix}. \quad (4.13)$$

This family of matrices, that lie on the boundary of \mathcal{CP}_{2n} , has been also considered in [33]. The authors report that the algorithms they propose fail to factorize matrices in this family, which is also the case with SpFeasDC, as we have seen in our experiments. We exemplify this in Table 9 for $n = 15$ and $r = 30$. On the other hand, the methods RIPG-sFISTA and RIPG-mod combining inertial and relaxation parameters provide a factorization in reasonable time, as it is also the case for $n = 50$ and $r = 100$ on which we report in Table 10. It is also interesting to notice that, for this family of matrices, FISTA outperforms all the other methods, despite of the fact that the parameter choice for this method does not fail into the setting for which convergence was proved.

5 Further perspectives

Numerical evidence (see the figures 1 - 2 and 9 - 12) suggests that the convergence rates of our model are linear, which at its turn suggests that the Lojasiewicz exponent of the function Ψ_τ is at most 1/2. Even though the Lojasiewicz exponent has played an important role in the derivation of many convergence rates results, to little is known about the calculation of its exact values for functions with complex structure. Some calculus rules for the Lojasiewicz exponent have been provided in [39] and in [41] for some simple models, however, it is not yet clear how to calculate it for Ψ_τ . This is an interesting topic of future research.

The empirical evidence on the benefit of the use of linesearch techniques gives rise to the interesting question of studying the theoretical convergence guarantees of the iterates generated by a Algorithm 1 enhanced with such a procedure. Another topic of further research is related to the extension of the convergence analysis beyond the current setting, in order to cover the parameter choice of the FISTA method, which, for the numerical experiments 4 and 5, proves to have excellent numerical performances.

Further, one can replace in the formulation of the optimization problem (P_{mod}) the closed ball with radius $\sqrt{\text{trace}(A)}$ by the sphere of the same radius, formulate a projected gradient algorithm with relaxation and inertial parameters (by using the formula of the projection on the intersection of a cone and a sphere from [9]), determine a parameter setting for which convergence can be guaranteed and

Method	Rate	Time (s)	Time (f)	Iter.
ModMAP	0.00	—//—	4.7649×10^{-1}	—//—
SpFeasDC	0.02	7.0223×10^{-1}	7.5259×10^{-1}	9220.50
PG	0.27	1.8571×10^{-2}	2.7675×10^{-2}	7069.00
FISTA	1.00	2.1624×10^{-3}	—//—	728.32
IPG-const: $\alpha_+ = 0.9814$	1.00	7.2203×10^{-3}	—//—	2385.20
IPG-sFISTA: $\alpha_+ = 0.9814$	1.00	7.9190×10^{-3}	—//—	2474.65
IPG-mod: $\alpha_+ = 0.9814$	1.00	7.7214×10^{-3}	—//—	2473.84
RIPG-const: $(\alpha, \rho) = (0.9954, 0.9705)$	0.93	1.3141×10^{-2}	3.1291×10^{-2}	4383.86
RIPG-const: $(\alpha, \rho) = (1.0000, 0.9661)$	0.94	1.3217×10^{-2}	3.2318×10^{-2}	4446.59
RIPG-sFISTA: $(\alpha, \rho) = (0.9954, 0.9705)$	1.00	3.5561×10^{-3}	—//—	1050.93
RIPG-sFISTA: $(\alpha, \rho) = (1.0000, 0.9661)$	1.00	2.5225×10^{-3}	—//—	742.12
RIPG-mod: $(\alpha, \rho) = (0.9954, 0.9705)$	1.00	3.5350×10^{-3}	—//—	1056.10
RIPG-mod: $(\alpha, \rho) = (1.0000, 0.9661)$	1.00	2.4953×10^{-3}	—//—	744.37

Table 7: The nonnegative factortization of $A_{0.99}$ given by (4.11) - (4.12) for $r = 12$.

Method	Rate	Time (s)	Time (f)	Iter.
ModMAP	0.00	—//—	5.0659×10^{-1}	—//—
SpFeasDC	0.00	—//—	9.1030×10^{-1}	—//—
PG	0.01	1.7454×10^{-2}	2.7524×10^{-2}	7531.00
FISTA	1.00	3.1237×10^{-3}	—//—	1067.09
IPG-const: $\alpha_+ = 0.9814$	0.99	1.1232×10^{-2}	2.9201×10^{-2}	3785.31
IPG-sFISTA: $\alpha_+ = 0.9814$	0.95	1.2694×10^{-2}	3.3234×10^{-2}	4052.98
IPG-mod: $\alpha_+ = 0.9814$	0.95	1.2337×10^{-2}	3.0064×10^{-2}	4041.04
RIPG-const: $(\alpha, \rho) = (0.9954, 0.9705)$	0.76	1.7583×10^{-2}	2.9249×10^{-2}	5882.72
RIPG-const: $(\alpha, \rho) = (1.0000, 0.9661)$	0.76	1.7549×10^{-2}	2.9381×10^{-2}	5908.16
RIPG-sFISTA: $(\alpha, \rho) = (0.9954, 0.9705)$	1.00	6.0671×10^{-3}	—//—	1835.64
RIPG-sFISTA: $(\alpha, \rho) = (1.0000, 0.9661)$	1.00	3.6109×10^{-3}	—//—	1083.75
RIPG-mod: $(\alpha, \rho) = (0.9954, 0.9705)$	1.00	6.0041×10^{-3}	—//—	1850.06
RIPG-mod: $(\alpha, \rho) = (1.0000, 0.9661)$	1.00	3.6073×10^{-3}	—//—	1084.20

Table 8: The nonnegative factortization of $A_1 = A$ given by (4.11) - (4.12) for $r = 11$.

Method	Rate	Time (s)	Time (f)	Iter.
ModMAP	0.00	—//—	3.4746×10^2	—//—
SpFeasDC	0.00	—//—	5.8390×10^2	—//—
PG	0.00	—//—	1.3049×10^0	—//—
FISTA	1.00	9.9557×10^{-1}	—//—	6959.95
IPG-const: $\alpha_+ = 0.9861$	0.00	—//—	1.5734×10^0	—//—
IPG-sFISTA: $\alpha_+ = 0.9861$	0.00	—//—	1.5584×10^0	—//—
IPG-mod: $\alpha_+ = 0.9861$	0.00	—//—	1.5747×10^0	—//—
RIPG-const: $(\alpha, \rho) = (0.9965, 0.9730)$	0.00	—//—	1.6052×10^0	—//—
RIPG-const: $(\alpha, \rho) = (1.0000, 0.9697)$	0.00	—//—	1.6032×10^0	—//—
RIPG-sFISTA: $(\alpha, \rho) = (0.9965, 0.9730)$	1.00	1.4735×10^0	—//—	7719.29
RIPG-sFISTA: $(\alpha, \rho) = (1.0000, 0.9697)$	1.00	1.4564×10^0	—//—	7037.52
RIPG-mod: $(\alpha, \rho) = (0.9965, 0.9730)$	1.00	1.4998×10^0	—//—	7728.84
RIPG-mod: $(\alpha, \rho) = (1.0000, 0.9697)$	1.00	1.4641×10^0	—//—	7036.06

Table 9: The nonnegative factorization of A_{30} given by (4.13) for $r = 30$.

Method	Rate	Time (s)	Time (f)	Iter.
FISTA	1.00	1.9818×10^2	—//—	22246.50
RIPG-sFISTA: $(\alpha, \rho) = (0.9998, 0.9796)$	1.00	2.3743×10^2	—//—	23125.20
RIPG-sFISTA: $(\alpha, \rho) = (1.0000, 0.9794)$	1.00	2.3330×10^2	—//—	22467.40
RIPG-mod: $(\alpha, \rho) = (0.9998, 0.9794)$	1.00	2.3752×10^2	—//—	23130.90
RIPG-mod: $(\alpha, \rho) = (1.0000, 0.9794)$	1.00	2.3290×10^2	—//—	22463.90

Table 10: The nonnegative factorization of A_{100} given by (4.13) for $r = 100$.

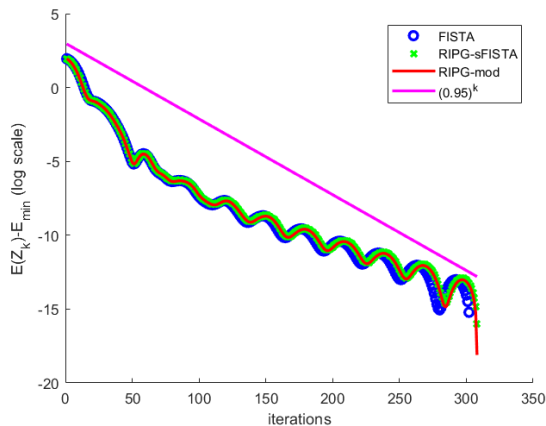


Figure 9: The sequence $\mathcal{E}(Z_k) - \mathcal{E}_{\min}$ for the factorization of $A_{0.99}$ given by (4.11) - (4.12).

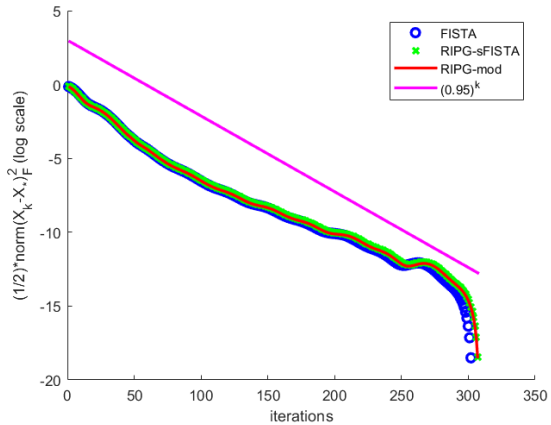


Figure 10: The sequence $\frac{1}{2} \|X_k - X_{\text{sol}}\|_F^2$ for the factorization of $A_{0.99}$ given by (4.11) - (4.12).

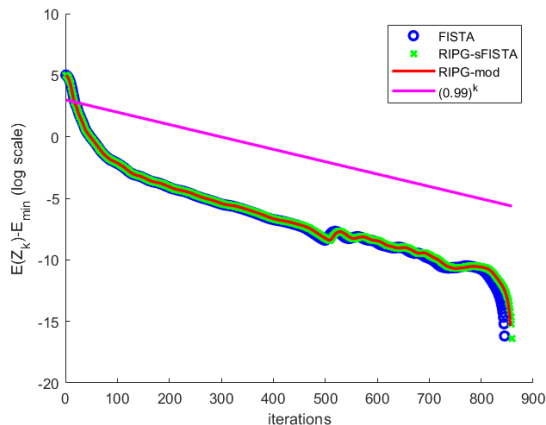


Figure 11: The sequence $\mathcal{E}(Z_k) - \mathcal{E}_{\min}$ for the factorization of $A_1 = A$ given by (4.11) - (4.12).

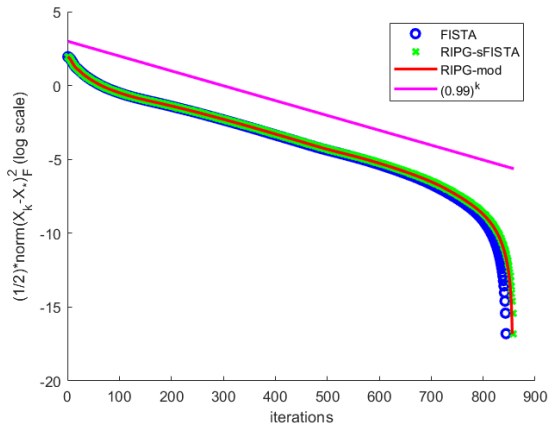


Figure 12: The sequence $\frac{1}{2} \|X_k - X_{\text{sol}}\|_F^2$ for the factorization of $A_1 = A$ given by (4.11) - (4.12).

convergence rates can be derived (in the spirit of the analysis for inertial proximal gradient algorithms in the fully nonconvex setting from [20]), and, of course, investigate its numerical performances.

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