Projection, Degeneracy, and Singularity Degree for Spectrahedra

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Abstract

Facial reduction, **FR**, is a regularization technique for convex programs where the strict feasibility constraint qualification, **CQ**, fails. Though this **CQ** holds generically, failure is pervasive in applications such as semidefinite relaxations of hard discrete optimization problems. In this paper we relate **FR** to the analysis of the convergence behaviour of a semismooth Newton root finding method for the projection onto a spectrahedron, i.e., onto the intersection of a linear manifold and the semidefinite cone. We examine the effect of failure of strict feasibility on the projection problem. In the process, we derive an elegant formula for the projection onto a face of the semidefinite cone obtained via regularization and discuss pathologies that arise in the absence of strict feasibility. We show further that the ill-conditioning of the Jacobian of the Newton method near optimality characterizes the degeneracy of the nearest point in the spectrahedron. We apply the results, both theoretically and empirically, to the problem of finding nearest points to the sets of: (i) correlation matrices or the *elliptope*; and (ii) semidefinite relaxations of permutation matrices or the *vontope*, i.e., the feasible sets for the semidefinite relaxations of the max-cut and quadratic assignment problems, respectively.

Key Words: facial reduction, spectrahedra, degeneracy, Jacobian, singularity degree, elliptope, vontope.

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1 Introduction

Facial reduction, **FR**, is a finite step process that regularizes convex programs where the strict feasibility constraint qualification, **CQ**, fails. This **CQ** holds generically for linear conic programs, see e.g., [19]. However, failure is pervasive in applications such as semidefinite programming, SDP, relaxations of hard discrete optimization problems, e.g., [18]. The minimum number of **FR** steps is denoted as the *singularity degree of* $\mathcal{F}$, $\operatorname{sd}(\mathcal{F})$, of the program with feasible set $\mathcal{F}$. It has been shown to be related to stability, error analysis, and convergence rates, see e.g., [16, 17, 50, 51]. Further generalized notions of singularity degree such as the maximum number of **FR** steps are studied in [30, 33] and shown to also relate to stability and convergence rates. In this paper we study $\operatorname{sd}(\mathcal{F})$ and relations to the projection problem, or best approximation problem (**BAP**), onto a *spectrahedron*, the intersection of a linear manifold and the positive semidefinite cone in symmetric matrix space.

Our main purpose is to examine the effect of failure of strict feasibility on the projection problem. In the absence of strict feasibility, we find surprising relationships between the eigenpairs of small eigenvalues of the Jacobian in a newly proposed Newton method for the projection problem and finding exposing vectors for **FR**. Furthermore, we provide a characterization that links the degeneracy of a point $\bar{X}$ in the spectrahedron, which pertains solely to the feasible set, to the singularity of the Jacobian computed in the course of the Newton method applied to the **BAP**, where $\bar{X}$ is the projected point. This establishes a connection between the degeneracy and the behaviour of the Newton method. We apply the results, both theoretically and empirically, to the problem of finding nearest points to the sets of: (i) correlation matrices or the elliptope; and (ii) semidefinite relaxations of permutation matrices or the vontope, i.e., the feasible sets for the semidefinite relaxations of the max-cut and quadratic assignment problems, respectively.

1.1 Projection Problem

We work with the Euclidean space of $n \times n$ real symmetric matrices, $\mathbb{S}^n$, equipped with the trace inner product. Let the *data,* $W \in \mathbb{S}^n$, be given. The projection, or basic *best approximation problem,* **BAP**, is

$$X^* = \begin{array}{ll} \arg\min & \frac{1}{2}\|X - W\|^2, \\ \text{s.t.} & X \in \mathcal{F} := \mathcal{L} \cap \mathbb{S}^n_+, \end{array} \qquad p^* = \frac{1}{2}\|X^* - W\|^2, \tag{1.1}$$

where $\mathbb{S}^n_+ \subseteq \mathbb{S}^n$ is the closed convex cone of positive semidefinite matrices in the vector space of real symmetric matrices of order n, equipped with the trace inner product. Given a convex cone $\mathcal{X}$, we let $X \succeq_{\mathcal{X}} 0$ denote $X \in \mathcal{X}$; and we often use $X \succeq 0$ for $X \succeq_{\mathbb{S}^n_+} 0$ when the meaning is clear. Here $\mathcal{L} \subseteq \mathbb{S}^n$ is a linear manifold; and, p^*, X^* are the optimal value and optimum, respectively. The representation of the linear manifold is essential in algorithms and different representations can result in different stability properties for the problem, e.g., [55]. We let $\mathcal{L} = \{X \in \mathbb{S}^n : \mathcal{A}X = b\}$, where $\mathcal{A} : \mathbb{S}^n \to \mathbb{R}^m$ is a given surjective (without loss of generality) linear transformation; $\mathcal{A}X = (\operatorname{tr} A_i X) \in \mathbb{R}^m$ for given fixed linearly independent $A_i \in \mathbb{S}^n, i = 1, \ldots, m$. We assume that $\mathcal{F}$ is a nonempty feasible set; it is called a *spectrahedron*. Here the data of **BAP** is $W, \mathcal{A}, b$.

Nearest point problems are pervasive in the literature and are often the essential step in feasiblity seeking problems, e.g., [4, 12, 39]. We study these problems and show that they reveal hidden structure and information about the stability and conditioning of feasible sets and the degeneracy of optimal points. Related convergence analysis and new types of singularity degree are given in [17,33]. Recall that a *correlation matrix* is a positive semidefinite matrix with diagonal all one. The set of correlation matrices is often called the *elliptope*. Finding the nearest correlation matrix is one application [7,27,28] that arises in many areas, e.g., finance. In addition, we specifically look at the feasible set of the SDP relaxation of the quadratic assignment problems **QAP**, which we call the *vontope*. We characterize degeneracy of nearest points and the resulting effects on stability of the nearest point algorithm for these two special instances.

1.1.1 Related Results

The **BAP** for the polyhedral case is studied in [11] with application to linear programming. (In the linear programming, LP, case, $\mathbb{S}^n \leftarrow \mathbb{R}^n, \mathbb{S}^n_+ \leftarrow \mathbb{R}^n_+$.) Generalized Jacobians play a critical role, though the relation to stability is not studied. The SDP case is studied in e.g., [26,37]. They use a quasi-Newton method to solve a dual problem similar to our dual problem; though we use a regularized semismooth Newton method with a generalized Jacobian and illustrate fast quadratic convergence for well-posed problems. Further related results on spectral functions, projections, and Jacobians, appear in [38].

In [31] it is shown that *any* conic program that fails strict feasibility has implicit redundancies and every point is degenerate. Relationships with the Barvinok-Pataki bound and strengthened bound [3,32,46] for conic programs is discussed. Further discussions on degeneracy related to loss of strict complementarity appear in [15].

The paper [17] provides a sublinear upper bound based on the singularity degree for the convergence rate of the method of alternating projections applied to spectrahedra. The paper [42] (preprint was published as we were finishing the preparation of this manuscript) furnishes analytic formulas for the sequence generated by alternative projection that reveal that this upper bound can fail to be tight. Although this work is not restricted to the singleton case, much of the analysis is developed with emphasis on the singleton setting. Further results on accuracy and differentiability appear in [24,38].

1.2 Outline

We continue in Section 2 with the background of projections and an overview of **FR** focused on the connections to degeneracy and strict feasibility. Section 3 presents the equation to be solved using the semismooth Newton root finding method, which is derived through a detailed examination of the optimality conditions along with notions on facial structure. We also derive an useful formula for the projection onto a *face* of the semidefinite cone. In Section 4 we introduce the semismooth Newton method for the **BAP** and derive Jacobians associated with the Newton method. In Section 5, we investigate various phenomena arising in the absence of strict feasibility. This includes the relationships between the eigenpairs of small eigenvalues of the Jacobian in the Newton method and identification of exposing vectors for **FR** (Section 5.1); the singularity of the Jacobian and its link to degeneracy (Section 5.2); and applications to the set of correlation matrices and the feasible set of the SDP relaxations of the **QAP** (Section 5.3). We present numerical experiments in Section 6 with results and observations discussed in Section 5. Our concluding remarks are in Section 7.

2 Background

We first present some background on projections and related spectral functions, and then include the notions of facial reduction for regularization, singularity, and degeneracy.

2.1 Derivatives of Projection Operators

We follow the work and notation in [22, 35, 38, 45, 56]. We work with $f : \mathbb{S}^n \to \mathbb{R} \cup \{+\infty\}$, a closed proper extended valued convex function on $\mathbb{S}^n$. We denote P_S, *projection onto a nonempty closed convex set* S, i.e.,

$$P_S(W) = \arg\min_{X \in S} \frac{1}{2}\|W - X\|^2.$$

And for a convex set S, we denote the *indicator function,* ι_S. The *Moreau regularization of* $\iota_{\mathbb{S}^n_-}$, $\mathbb{S}^n_- := -\mathbb{S}^n_+$, (see [45]) is given by

$$\Delta(X) = \min_{Z \in \mathbb{S}^n} \left\{ \frac{1}{2}\|X - Z\|^2 + \iota_{\mathbb{S}^n_-}(Z) \right\}. \tag{2.1}$$

A *spectral function* $g : \mathbb{S}^n \to \mathbb{R} \cup \{+\infty\}$ is one that is invariant under orthogonal conjugation (congruence)

$$g(X) = g(U^T X U),\ \forall\, X \in \mathbb{S}^n, \forall\, U \in \mathcal{O}^n,$$

where $\mathcal{O}^n$ is the set of orthogonal matrices of order n. In [38, Lemmas 2.3-4], it is shown that the Moreau regularization, $\Delta(X)$, of $\iota_{\mathbb{S}^n_-}$ is a *spectral function* with its gradient given as $\nabla\Delta(X) = P_{\mathbb{S}^n_+}(X)$. See Lemma 2.2 below. Let $\lambda : \mathbb{S}^n \to \mathbb{R}^n$ denote the eigenvalue function, i.e., $\lambda(X)$ is the vector of eigenvalues of $X \in \mathbb{S}^n$ in nonincreasing order.

Lemma 2.1 ([38, Lemma 2.3])**.** *The function* Δ *in* (2.1) *is the spectral function* $\Delta = \delta \circ \lambda$, *where the function* δ *on* $x \in \mathbb{R}^n$ *is:*

$$\delta(x) = \frac{1}{2}\sum_{i=1}^{n} \max\{0, x_i\}^2.$$

Proof. We include the proof from [38, Lemma 2.3] for completeness. For any $X \in \mathbb{S}^n$ we have

$$\begin{array}{rcl}\Delta(X) & = & \frac{1}{2}\|X - P_{\mathbb{S}^n_-}(X)\|^2 \\ & = & \frac{1}{2}\|P_{\mathbb{S}^n_+}(X)\|^2 \\ & = & \frac{1}{2}\sum_{i=1}^n \max\{0, \lambda_i(X)\}^2 \\ & = & \delta(\lambda(X)).\end{array}$$

■

Lemma 2.2 ([38, Lemma 2.4]). *The function* Δ *in* (2.1) *is convex and differentiable. Moreover, its gradient at* $X \in \mathbb{S}^n$ *is* $P_{\mathbb{S}^n_+}(X)$*, i.e.,*

$$\Delta(X)'(dX) = \langle \nabla\Delta(X), dX\rangle = \langle P_{\mathbb{S}^n_+}(X), dX\rangle = \operatorname{tr} P_{\mathbb{S}^n_+}(X)dX.$$

From spectral function theory e.g., [22,35,38], we know that the differentiability in Lemma 2.2 follows from the differentiability of $\delta \circ \lambda$. The formula for the derivative follows from the spectral function formula with $X = U \operatorname{Diag}(\lambda(X))U^T$:

$$\nabla(\delta \circ \lambda)(X) = U\left(\operatorname{Diag} \nabla\delta(\lambda(X))\right)U^T, \ U \in \mathcal{O}^n.$$

The derivative (Jacobian) of the projection can be found from the Hessian of the regularization function

$$P'_{\mathbb{S}^n_+}(X) = \nabla^2\Delta(X).$$

2.2 Facial Reduction

The facial structure of cones plays an essential role when analyzing various stability concepts. In this section we study various properties that arise from the absence of strict feasibility. Section 2.2.1 presents the basics of the facial structure of $\mathbb{S}^n_+$ and the facial reduction process for $\mathcal{F}$. In Section 2.2.2 we revisit known notions of singularities and the length of the facial reduction process that connects to the dimension of the solution set of our problem (1.1).

2.2.1 Facial Reduction Process

We first review the basic facial structure of $\mathbb{S}^n_+$. Recall that the convex cone $f \subseteq K$ is a face of a convex cone $K \subseteq \mathbb{S}^n$, denoted by $f \trianglelefteq K$, if

$$x, y \in K, z = x + y, z \in f \implies x, y \in f.$$

The cone f is a proper face if $\{0\} \subsetneq f \subsetneq K$. Here we denote f^Δ, *conjugate face of* f, defined as the intersection of the nonnegative polar cone with the orthogonal complement, $f^\Delta = f^\perp \cap K^+$, where $K^+ := \{\phi : \langle \phi, k\rangle \geqslant 0, \forall k \in K\}$ is the *nonnegative polar cone* of K. The facial structure of $\mathbb{S}^n_+$ is well-studied and has an intuitive characterization. For any convex set $C \subseteq \mathbb{S}^n_+$, the minimal face of $\mathbb{S}^n_+$ containing C, i.e., the intersection of all faces of $\mathbb{S}^n_+$ containing C, is denoted $\operatorname{face}(C, \mathbb{S}^n_+)$. For the singleton $C = \{X\} \subseteq \mathbb{S}^n_+$, we get

$$\operatorname{face}(X, \mathbb{S}^n_+) = \{Y \in \mathbb{S}^n_+ : \operatorname{range}(Y) \subseteq \operatorname{range}(X)\}.$$

Facial reduction (**FR**) for $\mathcal{F}$, the constraint system in (1.1), is the process of identifying the minimal face of $\mathbb{S}^n_+$ containing $\mathcal{F}$. It is known that a point $\hat{X}$ in the relative interior of $\mathcal{F}$, $\operatorname{relint}(\mathcal{F})$, provides the following characterization

$$\operatorname{face}(\hat{X}, \mathbb{S}^n_+) = \operatorname{face}(\mathcal{F}, \mathbb{S}^n_+).$$

Furthermore, $\operatorname{face}(\hat{X}, \mathbb{S}^n_+) = V\mathbb{S}^r_+V^T$ for some rank-r matrix V satisfying $\operatorname{range}(V) = \operatorname{range}(\hat{X})$. Such a matrix V is called a *facial range vector* for $\operatorname{face}(\hat{X}, \mathbb{S}^n_+)$.

Finding $\mathrm{face}(\mathcal{F}, \mathbb{S}^n_+)$ for an arbitrary $\mathcal{F}$ analytically is a challenging task. An alternative approach that is often used is to find the minimal face numerically. Proposition 2.3 below provides a tool for the **FR** process. Below, $\mathcal{A}^*$ refers to the *adjoint* of $\mathcal{A}$.

Proposition 2.3 (theorem of the alternative)**.** *For the feasible constraint system $\mathcal{F}$ defined in* (1.1)*, exactly one of the following statements holds:*

(i) there exists $X \succ 0$ such that $X \in \mathcal{L}$;

(ii) there exists $\lambda \in \mathbb{R}^m$ that satisfies the auxiliary system

$$0 \neq Z = \mathcal{A}^* \lambda \succeq 0, \ \langle b, \lambda \rangle = 0. \tag{2.2}$$

The vector Z in (2.2) is called an *exposing vector* for the face $(Z^\perp \cap \mathbb{S}^n_+) \supseteq \mathcal{F}$, as $X \in \mathcal{F}$ implies

$$0 = \langle b, \lambda \rangle = \langle \mathcal{A}X, \lambda \rangle = \langle X, \mathcal{A}^* \lambda \rangle = \langle X, Z \rangle.$$

Here the face $(Z^\perp \cap \mathbb{S}^n_+)$ is exposed by the hyperplane $Z^\perp = \{Z\}^\perp$, and this allows for a simplified expression of feasible points. This restriction results in an equivalent strictly smaller dimensional problem. Finding a solution to (2.2) does not necessarily lead directly to the minimal face, i.e., we can have $(Z^\perp \cap \mathbb{S}^n_+) \supsetneq \mathrm{face}(\mathcal{F}, \mathbb{S}^n_+)$. For such a case, the process is reapplied until $\mathrm{face}(\mathcal{F}, \mathbb{S}^n_+)$ is found. The number of times the system (2.2) needs to be solved varies, though it is at most $\min\{m, n\}$, see Section 2.2.2 below. A reader may refer to Example 3.5 for a brief illustration of how the theorem of the alternative is used for the **FR** process.

2.2.2 Three Notions of Singularity Degree

We now exhibit some properties that originate from the number of **FR** iterations.

Definition 2.4. *The* singularity degree *of $\mathcal{F}$, denoted* $\mathrm{sd}(\mathcal{F})$*, is the* <u>*minimum*</u> *number of* ***FR*** *iterations for finding* $\mathrm{face}(\mathcal{F}, \mathbb{S}^n_+)$*. The* maximum singularity degree *of $\mathcal{F}$, denoted* $\mathrm{maxsd}(\mathcal{F})$*, is the* <u>*maximum*</u> *number of nontrivial* ***FR*** *iterations for finding* $\mathrm{face}(\mathcal{F}, \mathbb{S}^n_+)$*.*

The singularity degree is often used to relate error bounds to explain the difficulty of solving problems numerically; see [50, 51]. It is known that a high singularity degree results in a worse *forward error bound* relative to the backward errors. The maximum singularity degree is a relatively new notion, and this motivates the idea of *implicit problem singularity,* $\mathrm{ips}(\mathcal{F})$. Every nontrivial step of **FR** results in redundant linear constraints. More specifically, **FR** reveals redundant equalities in $\mathcal{A}(\cdot) = b$; see [30]. The total number of these implicitly redundant constraints is called $\mathrm{ips}(\mathcal{F})$ and a short argument shows that $\mathrm{ips}(\mathcal{F}) \geqslant \mathrm{maxsd}(\mathcal{F})$. Proposition 2.5 below uses $\mathrm{maxsd}(\mathcal{F})$ to extend the result in [49, Lemma 3.5.2] and shows an interesting property that a **FR** sequence generates.[1]

Proposition 2.5. *[36, Theorem 1], [49, Lemma 3.5.2] Let the exposing vector obtained in the i-th* ***FR*** *iteration be nontrivial, $Z^i = \mathcal{A}^*(\lambda^i) \neq 0, i = 1, \ldots, k \leqslant \mathrm{maxsd}(\mathcal{F})$. Then the vectors, $\lambda^1, \lambda^2, \ldots, \lambda^k$, are linearly independent.*

We relate Proposition 2.5 to the dimension of the set of the roots that arise in the algorithm for solving the **BAP**, e.g., see Theorem 3.4.

[1] We note that the concepts of $\mathrm{maxsd}(\mathcal{F}), \mathrm{ips}(\mathcal{F})$ did not yet exist in [49]. Moreover, it is shown empirically in [30] that ips is directly related to the forward error for LPs.

2.3 Degeneracy and Relations to Strict Feasibility

Many of the concepts of degeneracy arise from the early work with the simplex method for linear programs. The *stalling* phenomenon of the simplex method is a well-known subject of research [6,13,40] and many methods are proposed to overcome this difficulty. In this section we use a generalized definition of degeneracy proposed by Pataki [47] to extend the discussion to spectrahedra. We then examine a connection between the *Slater constraint qualification* (strict feasibility), and degeneracy of feasible points. We identify a type of degeneracy that inevitably arises in the absence of strict feasibility.

Definition 2.6. *[47, Definition 3.3.1] A point $X \in \mathcal{F}$ is called nondegenerate if*

$$\mathrm{lin}(\mathrm{face}(X, \mathbb{S}^n_+)^\Delta) \cap \mathrm{range}(\mathcal{A}^*) = \{0\}.$$

Definition 2.6 immediately yields Lemma 2.7.

Lemma 2.7. *[47, Corollary 3.3.2] Let $X \in \mathcal{F}$ and let*

$$X = \begin{bmatrix} V & \bar{V} \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V & \bar{V} \end{bmatrix}^T, \, D \succ 0, \tag{2.3}$$

be a spectral decomposition of X. Then

$$\begin{array}{c} X \text{ is a nondegenerate point of } \mathcal{F} \\ \text{if, and only if,} \\ \left\{ \begin{bmatrix} V^T A_i V & V^T A_i \bar{V} \\ \bar{V}^T A_i V & 0 \end{bmatrix} \right\}_{i=1}^m \text{ is a set of linearly independent matrices in } \mathbb{S}^n. \end{array} \tag{2.4}$$

Remark 2.8. *The degeneracy of a point $X \in \mathcal{F}$ can be identified by constructing a matrix using the characterization (2.4). We let $W_i := \begin{bmatrix} V^T A_i V & V^T A_i \bar{V} \\ \bar{V}^T A_i V & 0 \end{bmatrix}$, $i = 1, \ldots, m$ and denote $t(n) = n(n+1)/2$, triangular number. We let vec denote the vectorization of a matrix by column; and $\mathrm{svec} : \mathbb{S}^k \to \mathbb{R}^{t(k)}$ denotes the isometry that vectorizes a symmetric matrix using the upper triangular part after multiplying the strict upper-triangular part by $\sqrt{2}$. We construct the following matrix $L \in \mathbb{R}^{t(n) \times m}$ with an appropriate permutation matrix Π and the i-th column:*

$$Le_i = \Pi \, \mathrm{svec} \, W_i = \begin{pmatrix} \mathrm{svec} \, V^T A_i V \\ \sqrt{2} \, \mathrm{vec} \, V^T A_i \bar{V} \\ \mathrm{svec} \, 0 \end{pmatrix}, \; \forall i \in \{1, \ldots, m\},$$

where V and $\bar{V}$ are given in Lemma 2.7. Consider the matrix $\bar{L}$, with the i-th column $\bar{L}e_i = \begin{pmatrix} \mathrm{svec} \, V^T A_i V \\ \sqrt{2} \, \mathrm{vec} \, V^T A_i \bar{V} \\ \mathrm{svec} \, \bar{V}^T A_i \bar{V} \end{pmatrix}$. Note that $\bar{L}$ is full-column rank given $\mathcal{A}$ is surjective. The matrix L is obtained after zeroing out the last $t(\mathrm{nullity}(X))$ rows of $\bar{L}$. We note that $\mathrm{rank}(L) < \mathrm{rank}(\bar{L})$ (i.e., degeneracy holds) if, and only if, the orthogonal complement of the span of the first $t(n) - t(\mathrm{nullity}(X))$ rows of $\bar{L}$ has nonzero intersection with the span of the remaining rows that are then changed to 0. Therefore, if $t(n) > m + t(\mathrm{nullity}(X))$, then generically nondegeneracy holds.

Theorem 2.9. *Suppose that $\mathcal{F}$ fails strict feasibility and let $X = VDV^T \in \mathcal{F}$ be found using (2.3). Then the set $\{A_iV\}_{i=1}^m$ is linearly dependent. In particular, any solution λ to (2.2) certifies the linear dependence of the set $\{A_iV\}_{i=1}^m$. Thus every point in $\mathcal{F}$ is degenerate.*

Proof. Suppose that $\mathcal{F}$ fails strict feasibility. Let $X = VDV^T \in \mathcal{F}$ and let λ be a solution to the *auxiliary system* (2.2). Then $\mathcal{A}^*(\lambda)$ is an exposing vector and hence the inner product $\langle \mathcal{A}^*(\lambda), X\rangle = 0$ which yields

$$0 = \mathcal{A}^*(\lambda)X = (\mathcal{A}^*(\lambda)V)\, DV^T \implies 0 = \mathcal{A}^*(\lambda)V = \sum_{i=1}^m \lambda_i\,(A_iV)\,. \tag{2.5}$$

Since λ is a nonzero vector, (2.5) shows the linear dependence.

The linear dependence of the set $\{A_iV\}_{i=1}^m$ shown above allows for verifying *total* degeneracy that occurs in the absence of strict feasibility of $\mathcal{F}$. Then the above provides $\sum_{i=1}^m \lambda_i A_i V = 0, \lambda \neq 0$. We observe that

$$\begin{array}{rcccl} 0 & = & V^T\left(\sum_{i=1}^m \lambda_i A_i V\right) & = & \sum_{i=1}^m \lambda_i V^T A_i V, \\ 0 & = & \bar{V}^T\left(\sum_{i=1}^m \lambda_i A_i V\right) & = & \sum_{i=1}^m \lambda_i \bar{V}^T A_i V. \end{array}$$

This immediately implies that the matrices in (2.4) are linearly dependent and hence X is degenerate.

■

In Corollary 2.10 we now connect nondegeneracy to strict feasibility.

Corollary 2.10. *Let $\mathcal{F}$ be given. Then the following holds:*

(i) If $\mathcal{F}$ contains a nondegenerate point, then strict feasibility holds.

(ii) Every $X \in \mathcal{F} \cap \mathbb{S}^n_{++}$ is nondegenerate.

Proof. Item (i) is the contrapositive of Theorem 2.9. Item (ii) is immediate from the definition of nondegeneracy, Definition 2.6, since $\operatorname{face}(X, \mathbb{S}^n_+)^\Delta = 0$, for all $X \succ 0$.

■

Propositions 2.11 and 2.12 below provide sufficient conditions for the nondegeneracy of certain points of spectrahedra. They enable identifying nearest points where the semismooth Newton method for the **BAP** performs effectively.

Proposition 2.11. *Let $X_1, X_2 \in \mathcal{F}$ and let X_1 be a nondegenerate point. Then, $\gamma X_1 + (1-\gamma)X_2$ is a nondegenerate point of $\mathcal{F}$, for all $\gamma \in (0, 1]$.*

Proof. Let $X_1, X_2 \in \mathcal{F}$ and let X_1 be a nondegenerate point. Let $\gamma \in (0,1]$ and $X' = \gamma X_1 + (1-\gamma) X_2$. We observe that

$$\begin{array}{rrcl} & \text{face}(X_1, \mathbb{S}^n_+) & \subseteq & \text{face}(X', \mathbb{S}^n_+) \\ \Longrightarrow & \text{face}(X_1, \mathbb{S}^n_+)^\Delta & \supseteq & \text{face}(X', \mathbb{S}^n_+)^\Delta \\ \Longrightarrow & \text{lin}\left(\text{face}(X_1, \mathbb{S}^n_+)^\Delta\right) & \supseteq & \text{lin}\left(\text{face}(X', \mathbb{S}^n_+)^\Delta\right) \\ \Longrightarrow & \text{lin}\left(\text{face}(X_1, \mathbb{S}^n_+)^\Delta\right) \cap \text{range}(\mathcal{A}^*) & \supseteq & \text{lin}\left(\text{face}(X', \mathbb{S}^n_+)^\Delta\right) \cap \text{range}(\mathcal{A}^*). \end{array}$$

Since X_1 is a nondegenerate point, we have $\text{lin}\left(\text{face}(X_1, \mathbb{S}^n_+)^\Delta\right) \cap \text{range}(\mathcal{A}^*) = \{0\}$. Thus, X' is a nondegenerate point.

■

Proposition 2.12. *Let f be a face of $\mathcal{F}$ containing a nondegenerate point. Then every point in* relint(f) *is nondegenerate.*

Proof. Let $X_1 \in f$ be a nondegenerate point. For any $X \in \text{relint}(f)$ there exists X_2 such that X belongs to the segment (X_1, X_2). The nondegeneracy of X then follows from Proposition 2.11.

■

3 Characterization of Optimality for the BAP

We now study the optimality conditions of the **BAP** (1.1) and present several properties, including an equation for the application of Newton's method.

Theorem 3.1. *Consider the projection problem* (1.1). *Then the following hold:*

(i) p^* is finite and the optimum X^* exists and is unique.

(ii) There is a zero duality gap between the primal and the dual problem of (1.1), *where the Lagrangian dual is the maximization of the dual functional, $\phi(y, Z)$, i.e.,*

$$p^* = d^* \quad = \quad \max_{Z \succeq 0, y \in \mathbb{R}^m} -\tfrac{1}{2}\|Z + \mathcal{A}^* y\|^2 + \langle y, b - \mathcal{A}W \rangle - \langle Z, W \rangle. \tag{3.1}$$

(iii) Strong duality (zero duality gap and dual attainment) holds in (1.1) *if, and only if, there exists a root $\bar{y}, F(\bar{y}) = 0$, of the function*

$$F(y) := \mathcal{A} P_{\mathbb{S}^n_+}(W + \mathcal{A}^* y) - b. \tag{3.2}$$

Moreover, in this case the solution to the primal problem is given by

$$X^* = P_{\mathbb{S}^n_+}(W + \mathcal{A}^* \bar{y}).$$

Proof. Item (i): The primal problem (1.1) is the minimization of a strongly convex function over a nonempty closed convex set. This yields that the optimal value is finite and is attained at a unique point.

Item (ii): Since the primal objective function is coercive, there is a zero duality gap, see e.g., [2, Theorem 5.4.1]. Let $Z \succeq 0$. The Lagrangian function of problem (1.1) and its gradient are given by

$$L(X, y, Z) = \frac{1}{2}\|X - W\|^2 + \langle y, b - \mathcal{A}X\rangle - \langle Z, X\rangle, \quad \nabla_X L(X, y, Z) = X - W - \mathcal{A}^* y - Z.$$

It follows that X is a stationary point of the Lagrangian if

$$X = W + \mathcal{A}^* y + Z. \tag{3.3}$$

By means of this equality, we can eliminate X and write the Lagrangian dual as the following maximization problem in Z, y.

$$\begin{aligned}
d^* &= \max_{Z \succeq 0, y} \min_X L(X, y, Z) \\
&= \max_{Z \succeq 0, y} \min_X \frac{1}{2}\|X - W\|^2 + \langle y, b - \mathcal{A}X\rangle - \langle Z, X\rangle \\
&= \max_{Z \succeq 0, y, X} \left\{ \frac{1}{2}\|X - W\|^2 + \langle y, b - \mathcal{A}X\rangle - \langle Z, X\rangle : \nabla_X L(X, y, Z) = 0 \right\} \\
&= \max_{Z \succeq 0, y} -\frac{1}{2}\|Z + \mathcal{A}^* y\|^2 + \langle y, b - \mathcal{A}W\rangle - \langle Z, W\rangle.
\end{aligned}$$

Item (iii): Let $\bar{X}$ be the unique optimal solution, as found by the above. Then strong duality holds if, and only if, there exists $(\bar{y}, \bar{Z})$ such that the following *Karush-Kuhn-Tucker,* ***KKT*** conditions hold:

$$\begin{array}{lll}
\bar{X} - W - \mathcal{A}^* \bar{y} - \bar{Z} = 0, & \bar{Z} \succeq 0, & \text{(dual feasibility)}, \\
\mathcal{A}\bar{X} - b = 0, & \bar{X} \succeq 0, & \text{(primal feasibility)}, \\
\langle \bar{Z}, \bar{X}\rangle = 0, & & \text{(complementary slackness)}.
\end{array} \tag{3.4}$$

Note that the complementary slackness condition and the fact that $\bar{X}, \bar{Z} \succeq 0$ yield

$$P_{\mathbb{S}^n_+}(W + \mathcal{A}^* \bar{y}) = \bar{X} \text{ and } P_{\mathbb{S}^n_-}(W + \mathcal{A}^* \bar{y}) = -\bar{Z}, \tag{3.5}$$

due to $\bar{X} + (-\bar{Z}) = W + \mathcal{A}^* \bar{y}$ being the Moreau decomposition. Finally, substituting $\bar{X} = P_{\mathbb{S}^n_+}(W + \mathcal{A}^* \bar{y})$ in the primal feasibility condition, we conclude that the **KKT** conditions imply $F(\bar{y}) = \mathcal{A}P_{\mathbb{S}^n_+}(W + \mathcal{A}^* \bar{y}) - b = 0$.

Conversely, directly from the Moreau decomposition theorem, if we are given some $\bar{y} \in Y$ satisfying $F(\bar{y}) = 0$, then the tuple $(\bar{X}, \bar{y}, \bar{Z})$, with $\bar{X}$ and $\bar{Z}$ defined as in (3.5), satisfies the above **KKT** conditions.

■

Theorem 3.1 (iii) shows how to obtain a solution to the primal problem (1.1) from a root of F. In addition, the pair $(\bar{y}, \bar{Z})$, with

$$\bar{Z} = -P_{\mathbb{S}^n_-}(W + \mathcal{A}^* \bar{y}),$$

is a dual optimal solution of the dual problem (3.1). This fact immediately follows from the proof of Theorem 3.1 (iii), where we showed that the tuple $(\bar{X}, \bar{y}, \bar{Z})$ satisfies the **KKT** conditions of problem (1.1).

3.1 Regularization for Strong Duality

The projection problem (1.1) always admits a solution given that the feasible set $\mathcal{F}$ is nonempty. If the dual (3.1) of (1.1) has an optimal solution, one can verify that the system given by the function in (3.2), i.e.,

$$F(y) = \mathcal{A}\left(P_{\mathbb{S}^n_+}(W + \mathcal{A}^* y)\right) - b$$

has a root $y \in \mathbb{R}^m$. However, when (3.2) does not have a root, then strong duality fails. We elaborate on this pathology further in Section 5.1. One way to guarantee that dual optimal set is nonempty is to *regularize* (1.1) using **FR**. In Theorem 3.2 below, we list some properties induced by **FR** properties that guarantee strong duality.

Theorem 3.2. *Consider the projection problem (1.1) with data $W, \mathcal{A}, b$. Denote $f := \operatorname{face}(\mathcal{F}, \mathbb{S}^n_+)$, the minimal face of $\mathbb{S}^n_+$ containing $\mathcal{F}$. Let $\hat{X} \in \operatorname{relint} f$ and let V be a full column rank facial range vector with orthonormal columns with $\operatorname{range} V = \operatorname{range} \hat{X}$, $\operatorname{rank}(V) = r$. Let $\overline{W} = V^T W V \in \mathbb{S}^r$. Define the linear transformation*

$$\mathcal{V}(R) := V R V^T, \; R \in \mathbb{S}^r.$$

Let $\bar{\mathcal{A}}, \bar{b}$ define the affine constraints obtained from $(\mathcal{A} \circ \mathcal{V})(\cdot), b$ after deleting redundant constraints. Then the following hold:

(i) A facially reduced problem of (1.1) in the original space $\mathbb{S}^n$ is

$$\begin{array}{rll} X^*(W) := & \arg\min & \frac{1}{2}\|X - W\|^2 \\ & s.t. & \mathcal{A}X = b, \; X \in f \qquad (X \succeq_f 0, \; f \trianglelefteq \mathbb{S}^n_+). \end{array} \tag{3.6}$$

*The **KKT** conditions hold at $X^*(W)$ with optimal dual pair $y^* \in \mathbb{R}^m, Z^* \in f^+$.*

(ii) A facially reduced problem of (1.1) in the smaller space $\mathbb{S}^r$ with surjective constraint $\bar{\mathcal{A}} : \mathbb{S}^r_+ \to \mathbb{R}^{\bar{m}}$ is

$$\mathcal{V}^\dagger(X^*(W)) = R^*(\overline{W}) := \arg\min \left\{ \tfrac{1}{2}\|R - \overline{W}\|^2 \; : \; \bar{\mathcal{A}}R = \bar{b}, \; R \in \mathbb{S}^r_+ \right\}, \tag{3.7}$$

*where we denote $\mathcal{V}^\dagger$ for the Moore-Penrose generalized inverse of $\mathcal{V}$.[2] The **KKT** conditions hold at $R^*(\overline{W})$ with optimal dual pair $y^* \in \mathbb{R}^{\bar{m}}, Z^* \in \mathbb{S}^r_+$.*

*(iii) Strong duality holds for the **FR** problems (3.6) and (3.7). Moreover:*

$$X^* = \mathcal{V}(R^*(\overline{W})) \textit{ solves the original problem (1.1);}$$

*and, $\bar{R} = R^*(\overline{W})$ is a solution to the **FR** primal problem (3.7) if, and only if,*

$$\bar{R} = P_{\mathbb{S}^r_+}(\overline{W} + \bar{\mathcal{A}}^* \bar{y}),$$

[2] The Moore-Penrose generalized inverse of a linear transformation $\mathcal{V}$ is the unique linear transformation satisfying the four Penrose equations, e.g., [5].

where $\bar{y}$ is a root of the function

$$\bar{F}(y) := \bar{\mathcal{A}} P_{\mathbb{S}^r_+}(\overline{W} + \bar{\mathcal{A}}^* y) - \bar{b}. \tag{3.8}$$

Equivalently, $X^*(W)$ is a solution to the original primal problem (1.1) if, and only if, there exists $\hat{y}$ such that

$$0 = F_f(\hat{y}) := \mathcal{A} P_f(W + \mathcal{A}^* \hat{y}) - b, \quad X^*(W) = P_f(W + \mathcal{A}^* \hat{y}), \tag{3.9}$$

where P_f stands for the projection onto $f := \mathrm{face}(\mathcal{F}, \mathbb{S}^n_+)$ given by:

$$P_f(u) = V\left(P_{\mathbb{S}^r_+}(V^T(u)V)\right)V^T \quad \left(= \mathcal{V}\left(P_{\mathbb{S}^r_+}\mathcal{V}^*(u)\right), \quad \mathcal{V}^*\mathcal{V} = I\right). \tag{3.10}$$

Proof. The proof for Items (i) and (ii) follows from the regularization in [8] with the substitution $X \leftarrow VRV^T$. We note that the number of variables in the objective function reduces since V has orthonormal columns and the norm is orthogonally invariant. The details follow from the proof of Theorem 3.1 using the **KKT** conditions after **FR**. Note that the first-order optimality conditions for the facially reduced problem are:

$$\begin{array}{rll} X - W - \mathcal{A}^* y - Z = 0, & Z \succeq_{f^+} 0, & \text{(dual feasibility)}, \\ \mathcal{A}X - b = 0, & X \succeq_f 0, & \text{(primal feasibility)}, \\ \langle Z, X \rangle = 0, & & \text{(complementary slackness)}. \end{array} \tag{3.11}$$

Item (iii): We first show the *elegant* projection formula (3.10). To show that the expression for $P_f(u)$ solves the nearest point problem defined as $P_f(u) = \arg\min_{v \in f} \frac{1}{2}\|v - u\|^2$, we now verify the optimality conditions [29, Theorem 3.1.1.]:

$$\mathrm{tr}\left\{(P_f(u) - u)(x - P_f(u))\right\} \geqslant 0, \ \forall x \in f,$$

i.e., for each $x \in f$, there is $R \in \mathbb{S}^r_+$ such that $x = VRV^T$ and thus,

$$\begin{array}{rl} & \mathrm{tr}\left\{(V(P_{\mathbb{S}^r_+}(V^T(u)V))V^T - u)(x - V(P_{\mathbb{S}^r_+}(V^T(u)V))V^T)\right\} \\ = & \mathrm{tr}\left\{(V(P_{\mathbb{S}^r_+}(V^T(u)V))V^T - u)(VRV^T - V(P_{\mathbb{S}^r_+}(V^T(u)V))V^T)\right\} \\ = & \mathrm{tr}\left\{V(P_{\mathbb{S}^r_+}(V^T(u)V))V^TVRV^T + uV(P_{\mathbb{S}^r_+}(V^T(u)V))V^T \right. \\ & \left. -V(P_{\mathbb{S}^r_+}(V^T(u)V))V^TV(P_{\mathbb{S}^r_+}(V^T(u)V))V^T - uVRV^T\right\} \\ = & \mathrm{tr}\left\{(P_{\mathbb{S}^r_+}(V^T(u)V))(V^TVRV^TV) + (V^TuV)(P_{\mathbb{S}^r_+}(V^T(u)V)) \right. \\ & \left. -(P_{\mathbb{S}^r_+}(V^T(u)V))(P_{\mathbb{S}^r_+}(V^T(u)V)) - uVRV^T\right\} \\ = & \mathrm{tr}\left\{(P_{\mathbb{S}^r_+}(V^T(u)V))(R) + (V^TuV)(P_{\mathbb{S}^r_+}(V^T(u)V)) \right. \\ & \left. -(P_{\mathbb{S}^r_+}(V^T(u)V))(P_{\mathbb{S}^r_+}(V^T(u)V)) - V^TuVR\right\} \\ = & \mathrm{tr}\left\{(P_{\mathbb{S}^r_+}(V^TuV) - (V^TuV))(R - P_{\mathbb{S}^r_+}(V^TuV))\right\} \geqslant 0, \end{array}$$

where the last inequality comes from the projection. This completes the proof of (3.10) and establishes the formula for the projection onto the face.

We continue to study the case where the **CQ** (strict feasibility) fails. With P being the projection that makes the linear transformation onto, we get (3.8) is equivalent to:

$$\begin{array}{rcl}\bar{F}(y) & = & \bar{\mathcal{A}} P_{\mathbb{S}^r_+}(\overline{W} + \bar{\mathcal{A}}^* y) - \bar{b} \\ & = & (P\mathcal{A} \circ \mathcal{V}) P_{\mathbb{S}^r_+}(V^T W V + (P\mathcal{A} \circ \mathcal{V})^* y) - Pb, \text{ for given data } W \\ & = & (P\mathcal{A} \circ \mathcal{V}) P_{\mathbb{S}^r_+}(V^T W V + (\mathcal{V}^* \circ \mathcal{A}^* P^T)(y)) - Pb \\ & = & (P\mathcal{A}) \left(V \left[P_{\mathbb{S}^r_+}(V^T (W + \mathcal{A}^* P^T y) V) \right] V^T \right) - Pb \\ & = & (P\mathcal{A}) \left(P_f (W + \mathcal{A}^* P^T y) \right) - Pb \\ & = & (P\mathcal{A}) \left(P_f (W + (P\mathcal{A})^* y) \right) - Pb,\end{array}$$

where we have used the elegant formula (3.10).

This shows that we can work in the original space if we have done facial reduction. Moreover,

$$P_f(W + \mathcal{A}^* P^T y) = \mathcal{V} \left[P_{\mathbb{S}^r_+}(\mathcal{V}^*(W + \mathcal{A}^* P^T y)) \right].$$

Recall that $V^T V = I$. In summary, necessity of (3.8) is clear. Therefore necessity of (3.9) follows from

$$\begin{array}{rcl} 0 & = & \bar{\mathcal{A}} P_{\mathbb{S}^r_+}(\overline{W} + \bar{\mathcal{A}}^* y) - \bar{b} \\ & = & (P\mathcal{A}) \mathcal{V} P_{\mathbb{S}^r_+}(\mathcal{V}^*(W + \mathcal{A}^* P^T y)) - Pb \\ & = & (P\mathcal{A}) P_f (W + \mathcal{A}^* P^T y) - Pb. \end{array}$$

We can remove P in the last line and ignore the redundant constraints.

■

We emphasize that strong duality holds in Theorem 3.1, Item (iii), only when there is a dual optimal solution that attains the dual optimal value d^*. However, strong duality is *guaranteed* to hold in Theorem 3.2, Item (iii), as a result of the regularization.

Remark 3.3. *The proof of Theorem 3.2 above provides the following elegant formula for the projection of $u \in \mathbb{S}^n$ onto the face $f = V \mathbb{S}^r_+ V^T, V^T V = I$,*

$$\boxed{P_f(u) = V \left(P_{\mathbb{S}^r_+}(V^T (u) V) \right) V^T = \mathcal{V} \left(P_{\mathbb{S}^r_+} \mathcal{V}^*(u) \right), \quad \mathcal{V}^* \mathcal{V} = I,} \tag{3.12}$$

i.e., the work of finding the projection onto the face f is reduced to the well-known projection onto the smaller dimensional proper cone $\mathbb{S}^r_+$.

We now consider dual optimal sets

$$\mathcal{S} := \{ y \in \mathbb{R}^m : F(y) = 0 \} \text{ and } \mathcal{S}_f := \{ y \in \mathbb{R}^m : F_f(y) = 0 \}, \tag{3.13}$$

where F is defined in (3.2) and F_f is defined in (3.9). In fact, when strict feasibility fails, $\mathcal{S}$ is unbounded given that $\mathcal{S} \neq \emptyset$ (see Theorem 5.4 (i) below). Moreover, $\mathcal{S}$ and $\mathcal{S}_f$ are convex and $\mathcal{S} \subseteq \mathcal{S}_f$.

Theorem 3.4. *The facially reduced problem* (3.9) *admits at least* $\operatorname{maxsd}(\mathcal{F})$ *number of affinely independent dual solutions y.*

Proof. Let $(\bar{X}, \bar{y}, \bar{Z})$ be a triple satisfying (3.4). Let $\lambda^1, \lambda^2, \ldots, \lambda^{\text{maxsd}(\mathcal{F})}$ be vectors generated by **FR** iterations. By (2.2), each λ^i satisfies $\mathcal{A}^*(\lambda^i) \succeq 0$ and $\langle \bar{X}, \mathcal{A}^*(\lambda^i)\rangle = 0$. Since $\bar{y}$ satisfies $\bar{X} - W - \mathcal{A}^*\bar{y} - \bar{Z} = 0$, it follows that $\bar{X} - W - \mathcal{A}^*(\bar{y} - \lambda^i) - (\bar{Z} + \mathcal{A}^*(\lambda^i)) = 0$. Moreover, $\bar{Z} + \mathcal{A}^*(\lambda^i) \succeq 0$ and $\langle \bar{X}, \bar{Z} + \mathcal{A}^*(\lambda^i)\rangle = 0$. Thus the vectors in the following set

$$\mathcal{S}_\lambda := \bar{y} - \{\lambda^1, \ldots, \lambda^{\text{maxsd}(\mathcal{F})}\} = \{\bar{y} - \lambda^1, \ldots, \bar{y} - \lambda^{\text{maxsd}(\mathcal{F})}\}$$

are solutions to (3.9) as well. Consequently, the result follows from the linear independence in Proposition 2.5.

■

We show in Example 3.5 that $\mathcal{S}$ and $\mathcal{S}_f$ can differ, i.e., the containment $\mathcal{S} \subseteq \mathcal{S}_f$ can be strict.

Example 3.5 ($\mathcal{S} \subsetneq \mathcal{S}_f$). *Consider the instance $\mathcal{F}$ given by the data:*

$$A_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, A_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, A_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \text{ and } b = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

*The singularity degree of $\mathcal{F}$ is 2, $\text{sd}(\mathcal{F}) = 2$. The first **FR** iteration yields a face that strictly contains the minimal face and corresponds to $\lambda^1 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ with the facial range vector $V_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}$; and the second **FR** iteration yields $\lambda^2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ with the facial range vector $V_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. Thus, the minimal facial range vector V for $\mathcal{F}$ is $V = V_1 V_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$. The facially reduced system is $\{R \in \mathbb{S}^1_+ : \begin{bmatrix} 1 \end{bmatrix} R = 1\}$. We note that $\mathcal{F}$ contains a unique point $e_1 e_1^T$.*

We now consider the **BAP** *(1.1) with $W = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & -1 & 0 \end{bmatrix}$. We consider the triple $(\bar{X}, \bar{Z}, \bar{y})$ where*

$$\bar{X} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \bar{Z} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 2 \end{bmatrix}, \text{ and } \bar{y} = \begin{pmatrix} 1 \\ 0 \\ -2 \end{pmatrix}.$$

The triple $(\bar{X}, \bar{Z}, \bar{y})$ satisfies the first-order optimality conditions.

We note that $\bar{y} - \lambda^1$ and $\bar{y} - \lambda^2$ are solutions to (3.9). However, $\bar{y} - \lambda^2$ is not a solution to (3.2) since

$$W + \mathcal{A}^*(\bar{y} - \lambda^2) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & -1 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & -2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & -2 & -1 \\ -1 & -1 & -2 \end{bmatrix},$$

and $\bar{X} - W - \mathcal{A}^*(\bar{y} - \lambda^2)$ has a negative eigenvalue.

It is of interest that the containment relation $\mathcal{S} \subsetneq \mathcal{S}_f$ in Example 3.5 stems from the solutions to (2.2). This can also be seen from the optimality characterization (3.4) with $Z \succeq 0$ and the regularized characterization (3.11) with $Z \succeq_{f^+} 0$, where the failure of strict feasibility implies $f \subsetneq \mathbb{S}^n_+, f^+ \supsetneq \mathbb{S}^n_+$.

4 A Basic Newton Method

We design a Newton-like method that solves for a root $\bar{y}$, $F(\bar{y}) = 0$, where

$$F(y) = \mathcal{A} P_{\mathbb{S}^n_+}(W + \mathcal{A}^* y) - b.$$

Rather than applying an optimization algorithm to solve the dual as in [37], we highlight that we solve a system of equations of the form $F(y) = 0$ to find points satisfying the first-order optimality conditions as is done in [9, 11, 41]. Given that $F(\bar{y}) = 0$, it follows that the optimum of the **BAP** (1.1) is $\bar{X} = P_{\mathbb{S}^n_+}(W + \mathcal{A}^* \bar{y})$. We note that $P_{\mathbb{S}^n_+}$ is found using the Eckart-Young Theorem [20], i.e., we use a spectral decomposition and set the negative eigenvalues to 0. Primal feasibility is immediate from the definitions and the projection. An application of the Moreau theorem yields the dual feasibility and complementarity.

We now present the pseudo-code of our Semi-Smooth Newton Method for the **BAP** (1.1) in Algorithm 4.1. The algorithm proceeds as follows: at each iteration, the search direction is computed by forming a (Clarke generalized) Jacobian J_k of F at the current iterate y_k, and the triple (X_k, Z_k, y_k) is then updated using this search direction. We resort to evaluations of unit vectors to construct J_k, the computational steps are discussed in Section 4.1

Algorithm 4.1 Semi-Smooth Newton Method for **BAP** for Spectrahedra

Require: $(W \in \mathbb{S}^n, \mathcal{A} : \mathbb{S}^n \to \mathbb{R}^m, b \in \mathbb{R}^m)$, $(y_0 \in \mathbb{R}^m, \varepsilon > 0,$ maxiter $\in \mathbb{N})$

Initialization: $k \leftarrow 0$, $F_0 \leftarrow \mathcal{A}(X_0) - b$, stopcrit $\leftarrow \|F_0\|/(1 + \|b\|)$,
$X_0 \leftarrow P_{\mathbb{S}^n_+}(W + \mathcal{A}^* y_0)$, $Z_0 \leftarrow (X_0 - W - \mathcal{A}^* y_0)$
while (stopcrit $> \varepsilon$) & ($k \leqslant$ maxiter) **do**
  construct Jacobian J_k by evaluating at unit vectors $J_k(e_i)$
  choose a regularization parameter $\sigma \geqslant 0$ for positive definite $\bar{J} = (J_k + \sigma I_m)$
  solve system $\bar{J} d = -F_k$ ▷ (Obtain Newton direction d)
  update:
    $y_{k+1} \leftarrow y_k + d$
    $X_{k+1} \leftarrow P_{\mathbb{S}^n_+}(W + \mathcal{A}^* y_{k+1})$
    $Z_{k+1} \leftarrow X_{k+1} - (W + \mathcal{A}^* y_{k+1})$
    $F_{k+1} \leftarrow \mathcal{A}(X_{k+1}) - b$
    stopcrit $\leftarrow \|F_{k+1}\|/(1 + \|b\|)$
    $k \leftarrow k + 1$
end while
Output: Primal-dual near optimum: $X_k, (y_k, Z_k)$

Remark 4.1 (On the convergence of Algorithm 4.1)**.** *Convergence guarantees for Algorithm 4.1 are derived from the so-called* inexact Semismooth Newton's Algorithm *in Facchinei and Pang's book;*

see [21, Algorithm 7.5.4]. Specifically, Facchinei and Pang consider an inexact Newton's method for obtaining a zero of a semismooth operator $F : \mathbb{R}^m \to \mathbb{R}^m$, with search direction d^k defined by

$$F(x^k) + J_k d^k = r^k, \quad \forall k,$$

where J_k is an element of the Clarke generalized Jacobian of F at x^k, and the error r^k satisfies

$$\|r^k\| \leqslant \eta_k \|F(x^k)\|$$

for some nonnegative sequence $\{\eta_k\}$. According to [21, Theorem 7.5.5], if the generalized Jacobian is nonsingular at a point x^* satisfying $F(x^*) = 0$, and if there exists a constant $\bar{\eta} > 0$ such that $\eta_k \leqslant \bar{\eta}$ for all k, then the method converges locally to x^*.

Our algorithm can be regarded as a realization of this inexact Semismooth Algorithm where $r^k = -\sigma d^k$, with $\sigma > 0$, and therefore $d^k = -(J_k + \sigma I_m)^{-1} F(x^k)$. Hence, we may choose η_k as

$$\eta_k = \frac{\|r^k\|}{\|F(x^k)\|} = \frac{\|(J_k + \sigma I_m)^{-1} F(x^k)\|}{\|F(x^k)\|} \sigma \leqslant \frac{\sigma}{\lambda_{\min}(J_k) + \sigma} \leqslant 1, \quad \forall k,$$

where $\lambda_{min}(J_k)$ stands for the smallest eigenvalue of J_k. Therefore, [21, Theorem 7.5.5] provides local convergence guarantees for Algorithm 4.1.

4.1 Alternative Directional Derivative Formulation

We now outline the computation of the Jacobian J_k at line 4 in Algorithm 4.1. In principle, obtaining a Clarke generalized Jacobian of F in our semismooth Newton method would require computing an element in the Clarke generalized Jacobian of $P_{\mathbb{S}^n_+}$. Every element in the generalized Jacobian is a 4-*tensor* on $\mathbb{R}^n$, whose complete formulation can be found in [38]. In matrix form this would be expressed as a square matrix of order n^4. The memory requirements for storing a matrix of such dimension can be too demanding even for moderate values of n. In particular, MATLAB software would have problems with size $n \geqslant 150$.

In order to overcome the memory deficiency, we make use of an elegant formula for evaluating Clarke generalized Jacobians of $P_{\mathbb{S}^n_+}$ derived by Sun in [52], which builds upon earlier developments in [44, 53]. In what follows we show this formula can be leveraged to efficiently compute a Clarke generalized Jacobian of F through evaluations involving only the unit vectors $e_i \in \mathbb{R}^m$. We begin by introducing the following notation.

Let $S = U \Lambda U^T \in \mathbb{S}^n$ be the spectral decomposition with vector of eigenvalues λ given as above. We partition the index sets of the eigenvalues based on their signs:

$$\alpha = \{i : \lambda_i > 0\},\ \beta = \{i : \lambda_i = 0\},\ \gamma = \{i : \lambda_i < 0\}.$$

Accordingly, the eigenvalue and eigenvector matrices can be block-partitioned as

$$\Lambda = \text{blkdiag}(\Lambda_\alpha, 0, \Lambda_\gamma), \quad \text{and} \quad U = [U_\alpha \, U_\beta \, U_\gamma].$$

Next, we define $\Omega \in \mathbb{S}^n$ entry-wise by

$$\Omega_{ij} = \frac{\max(\lambda_i, 0) + \max(\lambda_j, 0)}{|\lambda_i| + |\lambda_j|}, \ \forall i, j, \tag{4.1}$$

where the convention $\frac{0}{0} := 1$ is adopted. By [52, Proposition 2.2], for any matrix $S = U\Lambda U^T$, a linear map G_1 belongs to the Clarke generalized Jacobian $\partial_C P_{\mathbb{S}^n_+}(S)$ if and only if there exists $G_2 \in \partial_C P_{\mathbb{S}^{|\beta|}_+}(0)$ such that for all $H \in \mathbb{S}^n$,

$$G_1(H) = U \begin{bmatrix} \tilde{H}_{\alpha\alpha} & \tilde{H}_{\alpha\beta} & \Omega_{\alpha\gamma} \circ \tilde{H}_{\alpha\gamma} \\ \tilde{H}^T_{\alpha\beta} & G_2(\tilde{H}_{\beta\beta}) & 0 \\ \tilde{H}^T_{\alpha\gamma} \circ \Omega^T_{\alpha\gamma} & 0 & 0 \end{bmatrix} U^T, \tag{4.2}$$

where $\tilde{H} = U^T H U$. Equation (4.2) indicates that any element of the Clarke generalized Jacobian $\partial_C P_{\mathbb{S}^n_+}(S)$ is determined by a Clarke generalized Jacobian in $G_2 \in \partial_C P_{\mathbb{S}^{|\beta|}_+}(0)$. Consequently, the problem reduces to finding an element in $\partial_C P_{\mathbb{S}^{|\beta|}_+}(0)$.

In particular, by [38, Example 3.8], the Clarke subdifferential of $P_{\mathbb{S}^{|\beta|}_+}$ at 0 is characterized by the set of 4-tensors on $\mathbb{R}^{|\beta|}$ given by

$$\partial_C P_{\mathbb{S}^{|\beta|}_+}(0) = \operatorname{conv}\left(\mathcal{O}^{|\beta|} \cdot (\operatorname{Diag}^{(12)} \mathcal{D}_{\{01\}}(|\beta|))\right),$$

where $\operatorname{conv}(S)$ stands for the convex hull of a set S and

(i) $\mathcal{D}_{\{01\}}(|\beta|)$ is the set of $|\beta| \times |\beta|$ symmetric matrices with entries in $\{0, 1\}$ such that the entries in each row (from left to right) or column (from top to bottom) form a noincreasing sequence;

(ii) for any matrix M in $\mathbb{R}^{|\beta| \times |\beta|}$, $\operatorname{Diag}^{(12)} M$ is defined as the 4-tensor on $\mathbb{R}^{|\beta|}$ whose components are given by

$$(\operatorname{Diag}^{(12)} M)_{\substack{i_1 i_2 \\ j_1 j_2}} = \begin{cases} M_{i_1 i_2}, & \text{if } i_1 = j_2 \text{ and } i_2 = j_1, \\ 0, & \text{otherwise.} \end{cases}$$

We note that, since the zero matrix of size $|\beta| \times |\beta|$ belongs to $D_{\{01\}}(|\beta|)$, the zero tensor from $\mathbb{R}^{|\beta| \times |\beta|}$ to $\mathbb{R}^{|\beta| \times |\beta|}$ belongs to $\partial_C P_{\mathbb{S}^{|\beta|}_+}(0)$.

Hence, in Algorithm 4.1, we can always choose the generalized Jacobian $G_1 \in \partial_C P_{\mathbb{S}^n_+}(S)$ associated with $G_2 = 0$. Under this choice, the evaluation of G_1 at any $H \in \mathbb{S}^n$ simplifies to

$$G_1(H) = U \begin{bmatrix} \tilde{H}_{\alpha\alpha} & \tilde{H}_{\alpha\beta} & \Omega_{\alpha\gamma} \circ \tilde{H}_{\alpha\gamma} \\ \tilde{H}^T_{\alpha\beta} & 0 & 0 \\ \tilde{H}^T_{\alpha\gamma} \circ \Omega^T_{\alpha\gamma} & 0 & 0 \end{bmatrix} U^T, \quad \forall H \in \mathbb{S}^n, \tag{4.3}$$

where $\tilde{H} = U^T H U$. Finally, observe that a Clarke Jacobian for our function F is a matrix that can be explicitly constructed by evaluating this operator along the standard basis vectors.

The following lemma provides an explicit expression for evaluating this particular Jacobian $J \in \partial_C F(y)$ for any $y \in \mathbb{R}^n$ along any direction.

Lemma 4.2. *Let $y \in \mathbb{R}^m$ be such that $Y := W + \mathcal{A}^* y \in \mathbb{S}^n$. Let $Y := U \operatorname{Diag}(\lambda(Y)) U^T$ be a spectral decomposition of Y such that the eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$ are sorted in nonincreasing order, and denote with α, β and γ the sets of indices associated with positive, zero and negative eigenvalues, respectively, i.e., $\alpha := \{i : \lambda_i > 0\}$, $\beta := \{i : \lambda_i = 0\}$ and $\gamma = \{i : \lambda_i < 0\}$. Then* *there exists a Clarke generalized Jacobian J in $\partial_C F$ at y such that its evaluation at any direction $\Delta y \in \mathbb{R}^m$ is given by*

$$J(\Delta y) = \mathcal{A}\left(U \begin{bmatrix} \tilde{H}_{\alpha\alpha} & \tilde{H}_{\alpha\beta} & \Omega_{\alpha\gamma} \circ \tilde{H}_{\alpha\gamma} \\ \tilde{H}_{\alpha\beta}^T & 0 & 0 \\ \tilde{H}_{\alpha\gamma}^T \circ \Omega_{\alpha\gamma}^T & 0 & 0 \end{bmatrix} U^T\right), \tag{4.4}$$

where $\tilde{H} := U^T \left(\mathcal{A}^* \Delta y\right) U$.

Proof. It suffices to recall that the chain rule for Clarke subdifferential applied to F yields

$$\partial_C F(y) = \mathcal{A} \partial_C P_{\mathbb{S}^n_+}(W + \mathcal{A}^* y) \mathcal{A}^*,$$

where the equality above is by [14, Theorem 2.3.10], since semismooth implies Clarke regular. Hence, by taking $G_1 \in \partial_C P_{\mathbb{S}^n_+}(S)$ given above for $S = W + \mathcal{A}^* y$, the equation in (4.3) provides (4.4). ■

We now outline the steps for computing the Clarke generalized Jacobian J_k at line 4 in Algorithm 4.1. Specifically, by Lemma 4.2, the Jacobian of F evaluated at $y \in \mathbb{R}^m$, $J(y)$, is computed following the steps below.

(i) Let $Y = W + \mathcal{A}^* y \in \mathbb{S}^n$. Consider the spectral decomposition of Y given by

$$Y = \begin{bmatrix} V_\alpha & V_\beta & V_\gamma \end{bmatrix} \operatorname{Diag}(\lambda(Y)) \begin{bmatrix} V_\alpha & V_\beta & V_\gamma \end{bmatrix}^T,$$

where V_α, V_β and V_γ are the matrices of eigenvectors associated with the positive, zero and negative eigenvalues of Y, respectively.

(ii) Define the rotation $\mathcal{R}_Y : \mathbb{S}^n \to \mathbb{S}^n$, by

$$\mathcal{R}_Y(\rho) := \begin{bmatrix} V_\alpha & V_\beta & V_\gamma \end{bmatrix} \rho \begin{bmatrix} V_\alpha & V_\beta & V_\gamma \end{bmatrix}^T; \tag{4.5}$$

(iii) For each $j = 1, \dots, m$, compute

$$T_j := \begin{bmatrix} V_\alpha^T A_j V_\alpha & V_\alpha^T A_j V_\beta & \Omega_{\alpha\gamma} \circ V_\alpha^T A_j V_\gamma \\ (V_\alpha^T A_j V_\beta)^T & 0 & 0 \\ \left(\Omega_{\alpha\gamma} \circ V_\alpha^T A_j V_\gamma^T\right)^T & 0 & 0 \end{bmatrix} \in \mathbb{S}^n; \tag{4.6}$$

(iv) The j-th column of the Jacobian at y, $J(y)$, is

$$\mathcal{A}(\mathcal{R}_Y(T_j)) =: A \operatorname{svec}\left(\mathcal{R}_Y(T_j)\right). \tag{4.7}$$

5 Failure of Regularity and Degeneracy

This section examines various aspects of Algorithm 4.1 that result from the failure of strict feasibility. The failure of regularity is known to result in pathologies in conic programs, both on theoretical and practical aspects. We show that Algorithm 4.1 is not an exception to this phenomenon.

This section is organized in three parts. In Section 5.1 we discuss two types of pathologies. One well-known pathology is the possibility of failure of strong duality. Since the primal and dual optimal values agree (Theorem 3.1 (ii)), the only difficulty left is that the dual optimal value may not be attained by any dual feasible point. We identify a condition where this occurs (see Lemma 5.2) and show how to construct instances where strong duality fails. Another well-known consequence of the absence of strict feasibility is that the dual optimal set is unbounded [23]. We explain why Algorithm 4.1 experiences difficulties in this case in Section 5.1.2. The second part in Section 5.2 is devoted to understanding the properties of the Jacobian of F computed near the optimal point as seen through the lens of degeneracy. We recall the discussions from Section 2.3 to help explain the behaviour of Algorithm 4.1. In particular, we rely on the fact that *every point in $\mathcal{F}$ is degenerate in the absence of strict feasibility.* We conclude in Section 5.3 with the application of degeneracy identification to two real-world examples: the elliptope and the vontope.

5.1 Pathologies Arise in the Absence of Strict Feasibility

In this section we discuss pathologies that arise as a result of the absence of strict feasibility. We provide a method of constructing instances where the dual optimal value is not attained. In addition, assuming that the dual optimal value is attained, we provide members that certify the unbounded dual optimal set; and we examine the behaviour of Algorithm 4.1.

5.1.1 Unattained Dual Optimal Value

Theorem 3.1 states that there is always a *zero duality gap*, $p^* = d^*$ and the solution value of the primal problem, p^*, is attained. However, in the absence of strict feasibility, the dual attainment does not necessarily hold. Example 5.1 below illustrates that strong duality can fail for (1.1) when strict feasibility fails.

Example 5.1 (Failure of strong duality)**.** *Consider the following instance of* **BAP** (1.1) *given by*

$$\min_X \left\{ \frac{1}{2} \left\| X - \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \right\|^2 \ : \ X_{11} = 0, \ X \succeq_{\mathbb{S}^2_+} 0 \right\}. \tag{5.1}$$

The set of feasible solutions of (5.1) *is* $\{X \in \mathbb{S}^2 : X_{11} = X_{12} = X_{21} = 0, X_{22} \geqslant 0\}$*. Therefore, the optimal value of the problem is*

$$1 = \min_{X_{22} \geqslant 0} \frac{1}{2} \left\| \begin{bmatrix} 0 & 1 \\ 1 & X_{22} \end{bmatrix} \right\|^2 = \frac{1}{2} \left(2 + X_{22}^2\right),$$

which is attained when $X_{22} = 0$. In other words, the optimal solution of the best approximation problem is attained at $\bar{X} = 0$.

Now, note that the primal constraint in (5.1) *is given by* $\operatorname{tr}(E_{11}X) = \mathcal{A}X = 0$*, and therefore* $\mathcal{A}^*y = yE_{11}$ *for all* $y \in \mathbb{R}$*. Thus, dual feasibility of the optimality conditions (see* (3.4)*) implies*

$$-\begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} - \bar{y}E_{11} = \begin{bmatrix} -\bar{y} & 1 \\ 1 & 0 \end{bmatrix} \in \mathbb{S}^2_+, \text{ for some } \bar{y} \in \mathbb{R}.$$

However this does not hold for any $\bar{y} \in \mathbb{R}$*. Thus attainment fails for the dual.*

Example 5.1 above illustrates that strong duality may fail in the absence of strict feasibility; the linear manifold defined by $X_{11} = 0$ entirely consists of singular matrices. We note that strong duality can hold even in the absence of strict feasibility. Remark 5.3 presents a constructive approach for generating instances that fail strong duality. We first recall the following.

Lemma 5.2 ([48, Lemma 2.2])**.** *Suppose that* $0 \neq K \trianglelefteq \mathbb{S}^n_+$*, is a proper face of* $\mathbb{S}^n_+$*. Then*

$$\mathbb{S}^n_+ + K^\perp = \overline{\mathbb{S}^n_+ + \operatorname{span} K^\Delta}.$$

Furthermore,

$$\mathbb{S}^n_+ + \operatorname{span} K \text{ is not closed.} \tag{5.2}$$

Remark 5.3 (Constructing instances that fail strong duality)**.** *The dual feasibility of the first-order optimality conditions* (3.4) *states:*

$$\bar{X} - W \in \operatorname{range}(\mathcal{A}^*) + \mathbb{S}^n_+.$$

From (5.2)*, we can choose any proper face* $K \trianglelefteq \mathbb{S}^n_+$ *and construct a linear map* $\mathcal{A}$ *to satisfy* $\operatorname{range}(\mathcal{A}^*) = \operatorname{span} K$*. Therefore,*

$$\bar{X} - W \in \overline{\operatorname{range}(\mathcal{A}^*) + \mathbb{S}^n_+} \setminus \left(\operatorname{range}(\mathcal{A}^*) + \mathbb{S}^n_+\right), \ \bar{X} \succeq 0,$$

results in the failure of (3.4)*. Example 5.1 indeed falls into this category. Note that we can always choose* $b = \mathcal{A}\bar{X}$ *so that we still have a zero duality gap.*

5.1.2 Unbounded Dual Optimal Set and Singular Jacobian

We now discuss a property of the dual optimal set that, if it exists, results in a poor behaviour of Algorithm 4.1. Recall that the absence of strict feasibility of $\mathcal{F}$ implies the existence of a solution λ of the auxiliary system (2.2). We use the solution λ of (2.2) to derive two properties of the dual solution set $\mathcal{S} = \{y \in \mathbb{R}^m : F(y) = 0\}$ defined in (3.13):

$$\text{Slater fails, } \mathcal{S} \neq \emptyset \implies \begin{cases} \text{(i): solution set } \mathcal{S} \text{ is unbounded;} \\ \text{(ii) Jacobian at any solution } \bar{y} \in \mathcal{S} \text{ is singular.} \end{cases} \tag{5.3}$$

Theorem 5.4 below clarifies the conditions that result in the unbounded dual solution set in (5.3)(i); it then explains why we get an ill-conditioned Jacobian and thus provides a rationale for regularization of the search direction at line 4 in Algorithm 4.1.

Theorem 5.4. *Suppose that strict feasibility fails for the (primal) spectrahedron* (1.1) but *strong duality holds. Let* $\bar{y} \in \mathcal{S}$ *and let* λ *be any solution to* (2.2)*. Then the following hold:*

(i) *The solution set* $\mathcal{S}$ *is unbounded. Moreover,* λ *provides a recession direction,* $F(\bar{y} - t\lambda) = 0, \forall t \in \mathbb{R}_+$.

(ii) *The directional derivative of* F *at* $\bar{y}$ *along* λ *exists and is equal to zero.*

(iii) *In addition suppose that* F *is differentiable at* $\bar{y} \in \mathcal{S}$*. Then the Jacobian* $F'(\bar{y})$ *is singular. Moreover,* $\lambda \in \operatorname{null} F'(\bar{y})$.

Proof. Item (i): Let $(\bar{X}, \bar{y}, \bar{Z})$ be a triple that satisfies the optimality conditions in (3.4). We now let λ be a solution to the auxiliary system (2.2) and $Z := \mathcal{A}^*\lambda \succeq 0$. We aim to show that, for any $t > 0$, the triple $(\bar{X}, \bar{y} - t\lambda, \bar{Z} + tZ)$ also satisfies the optimality conditions. Indeed, for all $t > 0$, we have $\bar{Z} + tZ \succeq 0$ and

$$\begin{array}{rcl} 0 & = & \bar{X} - W - \mathcal{A}^*\bar{y} - \bar{Z} \\ & = & \bar{X} - W - \mathcal{A}^*(\bar{y} - t\lambda) - (\bar{Z} + tZ). \end{array}$$

The verification of primal feasibility is trivial. Finally complementarity follows:

$$\langle \bar{Z} + tZ, \bar{X} \rangle = t\langle Z, \bar{X} \rangle = t\langle \lambda, \mathcal{A}\bar{X} \rangle = t\langle \lambda, b \rangle = 0, \quad \forall t > 0,$$

where the last equality follows from (2.2). Finally, by the proof of Theorem 3.1 (iii) we conclude that $\bar{y} - t\lambda$ is a root of F for all $t > 0$, or equivalently,

$$\{\bar{y} - t\lambda : t \in \mathbb{R}_+\} \subseteq \mathcal{S}.$$

Item (ii): This directly follows from the fact that $F(\bar{y}) = F(\bar{y} - t\lambda)$ for all $y \in \mathcal{S}$ and $t \in \mathbb{R}_+$.

Item (iii): Suppose F is differentiable at a point $\bar{y} \in \mathcal{S}$. Then the partial derivative of F at $\bar{y}$ in the direction of λ is given by

$$F'(\bar{y})\lambda = 0,$$

where $F'(\bar{y})$ denotes the Jacobian of F at $\bar{y}$.

■

We note that the system (2.2) may contain multiple linearly independent solutions. Let $\{\lambda^1, \ldots, \lambda^k\}$ be a set of linearly independent solutions to (2.2). Hence by Theorem 5.4 we deduce that the solution set $\mathcal{S}$ contains a k-dimensional recession cone. Moreover, if the differentiability of F at $\bar{y}$ is further assumed, $\operatorname{null} F'(\bar{y})$ contains at least k zero singular values. Another interesting consequence of Theorem 5.4 is that if $F'(\bar{y})$ is nonsingular, then strict feasibility holds for $\mathcal{F}$.

The unboundedness of the set $\mathcal{S}$ immediately translates into the unboundedness of the set of optimal solutions of the dual problem (3.1). The proof of Theorem 5.4 Item (i) shows that the triple $(\bar{X}, \bar{y} - t\lambda, \bar{Z} + t\mathcal{A}^*\lambda)$ satisfies the optimality conditions (3.4) for all $t \in \mathbb{R}_+$. Therefore, the unbounded set

$$\{(\bar{y}, \bar{Z}) + t(-\lambda, \mathcal{A}^*\lambda) \, : \, t \in \mathbb{R}_+\}$$

constitutes recession directions of the set of dual solutions.

Furthermore, as stated in [23] (and related papers), the dual optimal set is unbounded when Mangasarian-Fromovitz type constraint qualifications fail. Here this means that the dual optimal set is unbounded when strict feasibility fails for the primal (1.1), since we assume that $\mathcal{A}$ is surjective. Our dual Algorithm 4.1 can encounter numerical difficulties in this setting. We now provide the details why the norms of the dual variables typically diverge.

Let $\bar{y} \in \mathcal{S}$. Suppose that we are at a point $\hat{y}$ such that $0 \neq \epsilon = F(\hat{y})$, $\hat{y} = \bar{y} + \Delta y$. We note that

$$\epsilon = F(\bar{y} + \Delta y) - F(\bar{y}) \approx F'(\bar{y})\Delta y.$$

When $||\epsilon||$ is small, Δy is close to being in $\text{null}(F'(\bar{y}))$. We have shown in Theorem 5.4 that a solution λ to (2.2) always satisfies

$$F(\bar{y} + \lambda) = 0 \text{ and } F'(\bar{y})\lambda = 0.$$

Therefore, *large* choices for Δy that include a large component from the nullspace is possible. This is in particular true when the Jacobian is singular at the optimum and the regularization parameter is converging to zero.

A typical behaviour of Algorithm 4.1 in the absence of strict feasibility is illustrated in Figure 5.1, i.e., we see the growth of the norms of the dual variables.

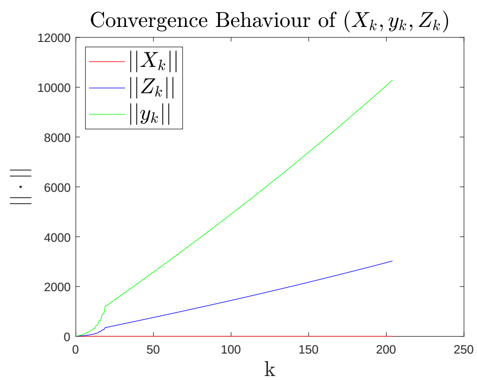

Figure 5.1: Typical behaviour of $\{(X_k, y_k, Z_k)\}$ from Algorithm 4.1 in the absence of strict feasibility.

5.2 Jacobian Behaviour Near-Optimum and Degeneracy

In this section we study properties of the Jacobian of F computed near the optimal point and relate its behaviour to the degeneracy status of the optimal point. We show that the degeneracy status of the optimal point *characterizes* the singularity of the Jacobian matrix.

We extend the discussion of computing the Jacobian presented in Lemma 4.2 and elaborate the computational steps. Let $(\bar{X}, \bar{y}, \bar{Z})$ be an optimal triple that solves (3.4). We further assume that $\bar{X}$ and $\bar{Z}$ satisfy *strict complementarity*. Since $\bar{X}$ and $\bar{Z}$ are mutually orthogonally diagonalizable, we obtain

$$\bar{X} - \bar{Z} = W + \mathcal{A}^*(\bar{y}) = \begin{bmatrix} V & \bar{V} \end{bmatrix} \begin{bmatrix} R & 0 \\ 0 & -S \end{bmatrix} \begin{bmatrix} V & \bar{V} \end{bmatrix}^T, \quad R \succ 0,\, S \succ 0,$$

where $\bar{X} = VRV^T$ and $\bar{Z} = \bar{V}S\bar{V}^T$.

Recall the steps for computing the Jacobian in Section 4.1 and the rotation operator in (4.5). Since we are now assuming that the matrix $\bar{X} - \bar{Z} = W + \mathcal{A}^*(\bar{y})$ is nonsingular, then the matrices of eigenvectors in (4.5) are given by $V_\alpha = V$, $V_\beta = 0$ and $V_\gamma = \bar{V}$. Hence, the rotation operator we are interested in now is $\mathcal{R}_{\bar{X}-\bar{Z}}(\cdot) = \begin{bmatrix} V & \bar{V} \end{bmatrix} (\cdot) \begin{bmatrix} V & \bar{V} \end{bmatrix}^T$. We now closely observe how the (i,j)-th element of the Jacobian in (4.7) is evaluated. Let T_j be the matrix defined in (4.6). Then

$$\begin{array}{rl} & \operatorname{tr}(A_i \mathcal{R}_{\bar{X}-\bar{Z}}(T_j)) \\ = & \left\langle A_i, \begin{bmatrix} V & \bar{V} \end{bmatrix} T_j \begin{bmatrix} V & \bar{V} \end{bmatrix}^T \right\rangle \\ = & \left\langle \begin{bmatrix} V & \bar{V} \end{bmatrix}^T A_i \begin{bmatrix} V & \bar{V} \end{bmatrix}, T_j \right\rangle \\ = & \left\langle \begin{bmatrix} V^T A_i V & V^T A_i \bar{V} \\ \bar{V}^T A_i V & \bar{V}^T A_i \bar{V} \end{bmatrix}, \begin{bmatrix} V^T A_j V & \Omega_{\alpha\gamma} \circ V^T A_j \bar{V} \\ \left(\Omega_{\alpha\gamma} \circ V^T A_j \bar{V}\right)^T & 0 \end{bmatrix} \right\rangle \\ = & \left\langle \begin{bmatrix} V^T A_i V & V^T A_i \bar{V} \\ \bar{V}^T A_i V & 0 \end{bmatrix}, \begin{bmatrix} V^T A_j V & \Omega_{\alpha\gamma} \circ V^T A_j \bar{V} \\ \left(\Omega_{\alpha\gamma} \circ V^T A_j \bar{V}\right)^T & 0 \end{bmatrix} \right\rangle . \end{array} \tag{5.4}$$

Note that the two arguments in the last trace inner product in (5.4) share the analogous block structure, with the difference arising from both the use of A_i versus A_j and an element-wise (Hadamard) scaling applied to the off-diagonal block. Lemma 5.5 below links the degeneracy of the optimal point $\bar{X}$ to the invertibility of the Jacobian of F at $\bar{y}$.

Lemma 5.5. *Let $D \in \mathbb{S}^n_{++}$ be a diagonal matrix, and let $\{x_1, \ldots, x_m\} \subseteq \mathbb{R}^n$ be given. Let $U = \begin{bmatrix} x_1 & x_2 & \cdots & x_m \end{bmatrix}$. Then $\operatorname{rank}(U) = \operatorname{rank}(U^T U) = \operatorname{rank}(U^T D U)$.*

Now we use (5.4), Lemma 5.5, and Lemma 2.7 to characterize the singularity of the Jacobian of F evaluated at an optimal solution. We note that [1, Theorem 3.1] addresses nonsingularity of Jacobians of linear SDPs under nondegeneracy assumptions.

Theorem 5.6. *Let $(\bar{X}, \bar{y}, \bar{Z})$ satisfy the optimality condition (3.4) and the strict complementarity condition. Then $\bar{X}$ is degenerate if, and only if, the Jacobian of F at $\bar{y}$ is singular.*

Proof. Let $\bar{X}$ be the optimal point of (1.1). Let

$$D = \operatorname{Diag}\left(\operatorname{svec}\left(\begin{bmatrix} M & \frac{1}{\sqrt{2}} \Omega_{\alpha\gamma}(\bar{X}) \\ \frac{1}{\sqrt{2}} \Omega_{\alpha\gamma}(\bar{X})^T & M \end{bmatrix} \right) \right) \in \mathbb{S}^{t(n)}_{++},$$

where $M = \frac{1}{\sqrt{2}} E + \left(1 - \frac{1}{\sqrt{2}}\right) I$ and where we include the dependence on $\bar{X}$ of Ω given as in (4.1). Let $X_i := \begin{bmatrix} V^T A_i V & V^T A_i \bar{V} \\ \bar{V}^T A_i V & 0 \end{bmatrix}$, and let $x_i := \operatorname{svec}(X_i)$. We recall the definition of T_j in (4.6) and note that

$$\operatorname{svec}(T_j) = D x_j.$$

We then observe the last inner product in (5.4):

$$\langle X_i, T_j \rangle = \langle \operatorname{svec}(X_i), \operatorname{svec}(T_j) \rangle = \langle x_i, D x_j \rangle.$$

Now we form $U := \begin{bmatrix} x_1 & x_2 & \cdots & x_m \end{bmatrix} \in \mathbb{R}^{t(n) \times m}$. Then, $\forall i, j$, we have

$$(U^T D U)_{i,j} = \left(\begin{bmatrix} x_1^T \\ \vdots \\ x_m^T \end{bmatrix} \begin{bmatrix} D x_1 \cdots D x_m \end{bmatrix} \right)_{i,j} = x_i^T D x_j = \operatorname{tr}(A_i \mathcal{R}_{\bar{X}}(T_j)).$$

Therefore we conclude

$$\begin{array}{llll} \bar{X} \text{ is degenerate} & \iff & \operatorname{rank}(U) < m, & \text{by (2.4)}, \\ & \iff & U^T D U \text{ is singular}, & \text{by Lemma 5.5}, \\ & \iff & \text{Jacobian of } F \text{ at } \bar{X} \text{ is singular.} & \end{array}$$

■

Recall the sufficient conditions for producing a nondegenerate solution given in Propositions 2.11 and 2.12. Therefore, any projection point $\bar{X}$ that satisfies the conditions in Propositions 2.11 and 2.12 yields a nonsingular Jacobian.

5.3 Nondegeneracy of the Elliptope and Degeneracy of the Vontope

We study degeneracies of two classes of spectrahedra; the elliptope (the set of correlation matrices), and the vontope (feasible region of the SDP relaxation of the quadratic assignment problem, **QAP**). We introduce these sets to illustrate how degeneracy interacts with the performance of Algorithm 4.1 in Section 6.2. We exhibit the result from [47] that the elliptope has only nondegenerate points; however all vertices of the vontope are degenerate before **FR**, and some vertices of the vontope are degenerate even after **FR**.

Example 5.7 (Elliptope, [47, Thm 3.4.2])**.** *We consider the problem of finding the nearest correlation matrix:*

$$\min \left\{ \frac{1}{2}\|X - W\|_F^2 \,:\, \operatorname{diag}(X) = e,\, X \succeq 0 \right\},$$

where e is the vector of all ones. The feasible region of the above problem is called the elliptope. Note that the elliptope is the feasible region of the SDP relaxation of the max-cut problem. Every point in the elliptope is nondegenerate.

Example 5.8 (Vontope, [57])**.** *Let Π_n be the set of n-by-n permutation matrices. For $X \in \Pi_n$, let*

$$Y_X = y_X y_X^T, \text{ where } y_X = \begin{pmatrix} 1 \\ \operatorname{vec} X \end{pmatrix} \in \mathbb{R}^{n^2+1},$$

be the lifted matrix. Here we index the rows and columns of a matrix starting from 0. The lifting process gives rise to the following feasible region for the SDP relaxation:

$$\mathcal{F}_{\boldsymbol{QAP}} := \left\{ Y \in \mathbb{S}_+^{n^2+1} : \begin{array}{l} G_J(Y) = e_0, \mathrm{b}^0\operatorname{diag}(Y) = I_n, \mathrm{o}^0\operatorname{diag}(Y) = I_n, \\ Y_{0,j} = Y_{j,j}, \forall j = 1, \ldots, n^2+1 \end{array} \right\}. \tag{5.5}$$

Here, $G_J : \mathbb{S}^{n^2+1} \to \mathbb{R}^{|J|}$ is a linear map that chooses the elements in the index set J that correspond to the $(0,0)$-element of Y, the off-diagonal elements of the n-by-n diagonal blocks, and the diagonal elements of the n-by-n off-diagonal blocks; $\mathrm{b}^0\operatorname{diag} : \mathbb{S}^{n^2+1} \to \mathbb{S}^n$ is the linear map that sums the n-by-n diagonal blocks; and $\mathrm{o}^0\operatorname{diag} : \mathbb{S}^{n^2+1} \to \mathbb{S}^n$ is the linear map defined by $\mathrm{o}^0\operatorname{diag}(Y) = \left(\operatorname{tr}(\hat{Y}^{i,j})\right)_{i,j}$, where $\hat{Y}^{i,j}$ is the (i,j)-th n-by-n block submatrix in Y; see [57] for details on the construction of $G_J, \mathrm{b}^0\operatorname{diag}$ and $\mathrm{o}^0\operatorname{diag}$.

We remark that the expression in (5.5) *contains redundant linear constraints. It is well-known that the SDP relaxation of the* ***QAP*** *fails strict feasibility* [57] *and so we employ* ***FR*** *and work in a smaller space. Let*

$$H = \begin{bmatrix} e^T \otimes I_n \\ I_n \otimes e^T \end{bmatrix} \in \mathbb{R}^{2n \times n^2}, \; K = \begin{bmatrix} -e & H \end{bmatrix} \in \mathbb{R}^{2n \times (n^2+1)},$$

and let $\hat{V} \in \mathbb{R}^{(n^2+1)\times((n-1)^2+1)}$ *be the matrix with orthonormal columns that spans* $\mathrm{null}(K)$.[3] ***FR*** *leads to the following constraints:*

$$\mathcal{F}^{\boldsymbol{FR}}_{\boldsymbol{QAP}} := \{R \in \mathbb{S}^{(n-1)^2+1} : G_{\hat{J}}(\hat{V}R\hat{V}^T) = e_0, \, R \succeq 0\}, \tag{5.6}$$

where $G_{\hat{J}} : \mathbb{S}^{n^2+1} \to \mathbb{R}^{|\hat{J}|}$ *a newly defined surjective linear map that chooses indices in* $\hat{J}$ *such that* $\hat{J} \subsetneq J$*. This aligns with the fact that* ***FR*** *reveals implicit redundant constraints. It is known that the number of equality constraints reduces to* $n^3 - 2n^2 + 1$ *after* ***FR****; see* [57].[4]

We now discuss the degeneracy of each lifted matrix $Y_X = y_X y_X^T = \hat{V} R_X \hat{V}^T$*, where* $X \in \Pi_n$*. Due to the orthonormality of* $\hat{V}$*, we get*

$$R_X = \hat{V}^T Y_X \hat{V} \in \mathbb{S}^{(n-1)^2+1}.$$

We note that $\mathrm{rank}(R_X) = 1$*. We let* $\{A_i\}_{i=1}^{n^3-2n^2+1} \subseteq \mathbb{S}^{(n-1)^2+1}$ *be the set of matrices defining data matrices for the affine constraints. Hence the linear dependence of the matrices of the set* (2.4) *can be analyzed by considering their first columns. For* $n \geqslant 3$*, we observe that the vectors*

$$\left\{ \begin{pmatrix} V_X^T A_i V_X \\ \bar{V}_X^T A_i V_X \end{pmatrix} \right\}_{i=1}^{n^3-2n^2+1} \subseteq \mathbb{R}^{(n-1)^2+1}, \quad n^3 - 2n^2 + 1 > (n-1)^2 + 1, \; n \geqslant 3,$$

are linearly dependent. This proves that the rank-one vertices that arise from Π_n *remains degenerate after* ***FR****.*

Remark 5.9. *If we replace* $\mathbb{S}^n_+$ *with* $\mathbb{R}^n_+$*, the set* $\mathcal{F}$ *reduces to a polyhedron and the discussion on the degeneracy simplifies. The degeneracy status of a point* x *in a polyhedron can be confirmed by evaluating the rank of* $A(:, \mathrm{supp}(x))$*, where* $\mathrm{supp}(x) = \{i : x_i \neq 0\}$ *denotes the support of* x*; see* [47]*. The performance of the proposed algorithm in* [11] *is also affected by the degeneracy of the optimal point. Moreover every point of* $\mathcal{F}$ *as a polyhedron is degenerate in the absence of strict feasibility.*

6 Numerical Experiments

To illustrate the effects on convergence and degeneracy, we now present multiple experiments using diverse spectrahedra $\mathcal{F}$ with various ranges of values for the *singularity degree,* $\mathrm{sd}(\mathcal{F})$, and for the *implicit problem singularity,* $\mathrm{ips}(\mathcal{F})$. In our algorithm, dual feasibility and complementary slackness

[3] Note that the last row of K is linearly dependent and, for efficiency and accuracy, is best ignored when finding the nullspace.

[4] The last column of off-diagonal blocks and the $(n-2, n-1)$ off-diagonal block are linearly dependent and are ignored, see [25, 57].

are satisfied exactly. Therefore, we use the following $\varepsilon^k \in \mathbb{R}_+$ to denote the relative residual of the optimality conditions at iteration k:

$$\varepsilon^k := \min\left\{1, \frac{\|F(y^k)\|}{1+\|b\|}\right\} =: \alpha_k 10^{-t_k},\ 1 \leqslant \alpha_k < 10.$$

We denote the condition number of the Jacobian of F at y^k as $\operatorname{cond}(J_k)$, and let

$$\operatorname{cond}(J_k) = \beta_k 10^{s_k},\ 1 \leqslant \beta_k < 10.$$

We stop Algorithm (4.1) once

$$(i)\quad \varepsilon^k \leqslant 10^{-13} \text{ or } (ii)\quad s_k + t_k > 16 \text{ or } (iii)\quad k > 2000.$$

If condition (i) holds, then the we consider the **BAP** problem is solved. If condition (ii) holds, then we consider the optimal solution of the **BAP** problem as being degenerate. In our algorithm, if (ii) or (iii) hold, then we conclude that a small eigenvalue for the Jacobian exists and we assume that strict feasibility fails.[5] And, by looking at the nonzero elements of an eigenvector associated to the *smallest eigenvalue* we get information on an exposing vector; and we identify constraints that give rise to the failure of strict feasibility. This solves an auxiliary system for a **FR** step, see Proposition 2.3. Using the information on the exposing vector, we then solve a *reduced auxiliary system*, using a *Gauss–Newton* approach[6]. This results in a **FR** step. Following this, we remove the redundant constraints that arise from the **FR** step. We repeat until strict feasibility holds.

Numerical experiments are conducted with MATLAB R2023b on a Windows 11 PC with Intel(R) Core(TM) i5-10210U CPU @ 1.60GHz, RAM 16.0GB.

6.1 Comparison With(out) Strict Feasibility

As expected, our tests in Table 6.1, show that Algorithm 4.1 performs exceptionally well for instances with strict feasibility but struggles when strict feasibility fails. In fact, we observe that Algorithm 4.1 achieves the relative precision of 10^{-7} in under 7 iterations when strict feasibility holds. In contrast, when strict feasibility fails and Algorithm 4.1 converges, hundreds of iterations are needed to reach the desired precision. In Table 6.2, we repeat the same experiment setting a relative precision tolerance of 10^{-13} and allowing 2000 iteration limit. In this case, Algorithm 4.1 never reached the desired relative precision within the maximum number of iterations.

n	10	20	50	100
Slater	100%	100%	100%	100%
No Slater	55%	50%	50%	25%

Table 6.1: 20 randomly generated problems (1.1); % converged $\varepsilon^k \leqslant 10^{-8}, k \leqslant 1000$.

We now look at the case where the singularity degree $\operatorname{sd}(\mathcal{F}) = 1$, while the implicit singularity $\operatorname{ips}(\mathcal{F})$ varies.

[5] Note that by Remark 2.8, nondegeneracy holds for our problem generically.
[6] https://github.com/j5im/FacialReductionSpectrahedron

n	10	20	50	100
Slater	100%	100%	100%	100%
No Slater	0%	0%	0%	0%

Table 6.2: 20 randomly generated problems (1.1); % converged $\varepsilon^k \leqslant 10^{-13}, k \leqslant 2000$.

6.1.1 $\operatorname{ips}(\mathcal{F}) = 1$

We use a spectrahedra with singularity degree 1 and $n = 15, m = 7$. The singularity degree is obtained by constructing an exposing vector as a linear combination of 5 out of the 7 constraints of the problem. Algorithm 4.1 is used to monitor the eigenvalues of the Jacobian of F at every iteration k, see Figure 6.1. We observe that only one of the eigenvalues tends to 0. After 452 iterations the method reaches a relative residual of 9.9567×10^{-8}, while the condition number of the Jacobian is 7.0236×10^{12}. Therefore the algorithm stops and indicates which of the constraints are causing strict feasibility to fail. After applying **FR** and removing the single (implicit) redundant constraint found, the algorithm now succeeds and converges to a point with a relative residual of 1.0231×10^{-15} in only 8 iterations, see Table 6.3.

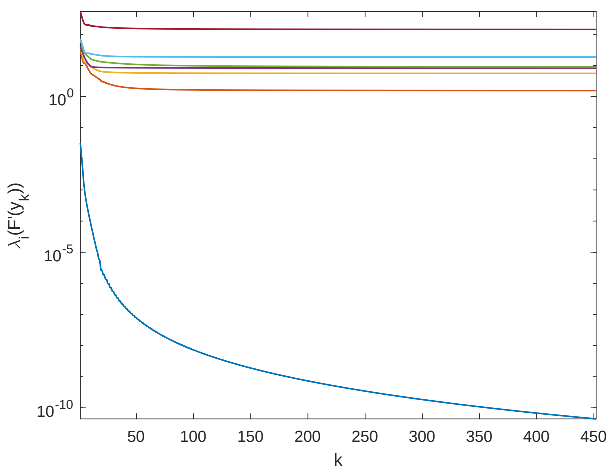

Figure 6.1: Changes in eigenvalues of Jacobian of F for spectrahedron in Section 6.1.1.

	n	m	ε^k(rel. res.)	cond$(F'(y_k))$	$\lambda_n(y_k)$	k
Before **FR**	15	7	9.9567e-08	7.0236e+12	-1.7238e-16	452
After **FR**	15	6	1.0231e-15	198.08	2.5515e-17	8

Table 6.3: Spectrahedron in Section 6.1.1; at final iteration k; before and after **FR** iters

6.1.2 ips($\mathcal{F}$) > 1

In our second experiment, see Table 6.4, we work with data obtained from a SDP relaxation of the protein side-chain positioning problems, e.g., [10]. The spectrahedron we are considering has singularity degree 1, but the implicit problem singularity is greater than 1, i.e., there are more than 1 redundant constraints after applying **FR** . In particular, the dimension of the space is $n = 35$ and the number of constraints is $m = 75$. By running our algorithm, we observe that a large number of eigenvalues of the Jacobian tend to 0 along the iterations (see Figure 6.2). After applying **FR** , we reduced the dimension of the problem to $n = 10$ and the number of constraints to $m = 22$. In the next run of the algorithm, only one eigenvalue of the Jacobian tends to 0, but we detect that a second iteration of **FR** is needed. This time, we reduce n to 9 and we remove 6 more redundant constraints, resulting in $m = 16$. The next time we apply our algorithm, the method converges to the solution in 18 iterations, see Table 6.4.

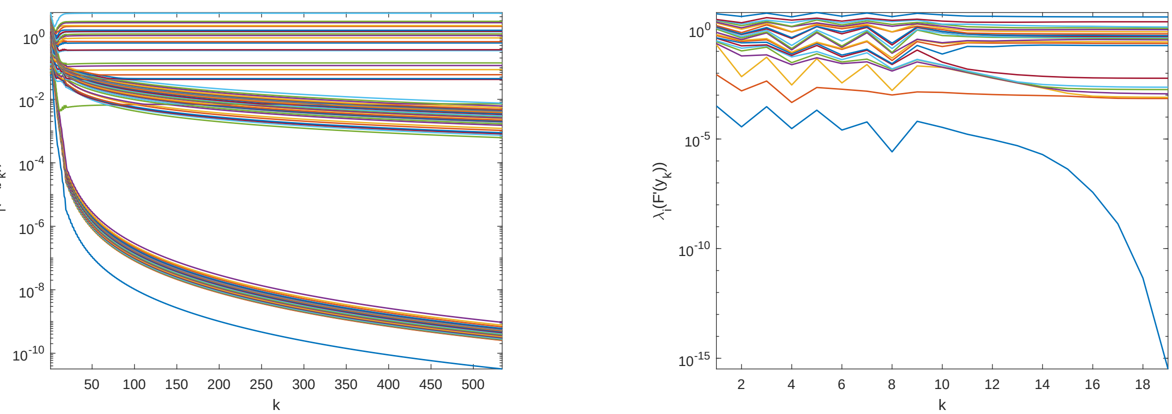

Figure 6.2: Iterations k vs eigenvalues; spectrahedron in Section 6.1.2; before and after one **FR** iteration

	n	m	ε^k(rel. res.)	cond($F'(y_k)$)	$\lambda_n(y_k)$	k
Before **FR**	35	76	8.5351e-08	1.0060e+12	-1.6941e-15	534
After **FR** 1	10	22	7.6363e-04	1.8739e+16	-5.2097e-16	19
After **FR** 2	9	16	8.7202e-14	16103.37	-5.6900e-16	18

Table 6.4: Spectrahedron in Section 6.1.2; at final iteration k; before and after **FR** iters

6.2 Experiments with Elliptope and Vontope

In this section we address the importance of strict feasibility and degeneracy on the performance of Algorithm 4.1. We consider the elliptope and vontope cases. Furthermore we compare the performance of Algorithm 4.1 with the interior point solver SDPT3[7].

From Section 5.3 we recall that the **MC** problem satisfies strict feasibility and every point of the elliptope, the feasible set, is nondegenerate; see Example 5.7. The results from the **MC** problem are displayed in the line labelled 'Elliptope' in Table 6.5. As for the **QAP**, without **FR**, the SDP relaxation of **QAP** fails strict feasibility and all the feasible points are degenerate. Hence in our tests, we consider two models of the same set of instances: $\mathcal{F}_{\boldsymbol{QAP}}$ obtained directly by the lifting of the variables (see (5.5)); and $\mathcal{F}^{\boldsymbol{FR}}_{\boldsymbol{QAP}}$ obtained after **FR** is applied to $\mathcal{F}_{\mathbf{QAP}}$ (see (5.6)). In Table 6.5, **QAP** ($\mathbf{QAP_{FR}}$, resp.) indicates the results obtained from $\mathcal{F}_{\mathbf{QAP}}$ ($\mathcal{F}^{\mathbf{FR}}_{\mathbf{QAP}}$, resp.).

We used two settings for the choice of W in the objective function. The first setting for W forces the optimal solution $\bar{X}$ to be rank 1. Recall that rank-one optimal solutions for **QAP** are degenerate and thus lead to ill-conditioned Jacobians as can be seen by the huge condition numbers demonstrated later in Table 6.5. The second setting chooses a random W. Followed by the discussions in Remark 2.8 and Proposition 2.11, $\bar{X}$ is generically nondegenerate when strict feasibility holds.

For SDPT3 we provided the following second-order cone formulation of (1.1):

$$\min_{X,y,t} \{ \ t \ : \mathrm{svec}(X) + y = \mathrm{svec}(W), \ ||y||_2 \leqslant t, \ X \in \mathcal{F} \ \} .$$

The default settings for SDPT3 were used for the tests.

Each line of Table 6.5 reports on the average of 10 instances, problem order $n = 10$. The meaning of the header names used in Table 6.5 is as follows:

(i) The headers 'pf', 'df' and 'cs' under Semi-Smooth Newton refer to the average of the primal feasibility, dual feasibility and complementarity, respectively, introduced in (3.11). The df includes both the linear dual feasibility and the violation of semidefiniteness. Both are essentially zero up to roundoff error of the arithmetic. Note that the values 10^{-15} and smaller for pf and df are essentially zero (machine precision). The headers pf, df and cs under SPDT3 refer to the solver outputs, pinfeas, dinfeas and gap, respectively.

(ii) k is the average number of iterations.

(iii) time is the average run time in cpu-seconds.

(iv) $\mathrm{cond}(F'(y^k))$ is the average condition number of the Jacobian $(F'(y^k))$; we only have this metric for the semismooth Newton method.

W Generation	Problem	Semi-Smooth Newton						SDPT3				
		pf	df	cs	k	time	$\mathrm{cond}(F'(y^k))$	pf	df	cs	k	time
W, $\mathrm{rank}(\bar{X}) = 1$	Elliptope	9e-13	9e-16	2e-16	6.8	4e-02	3e+00	4e-12	6e-12	2e-07	15.5	2e-01
	$\mathbf{QAP_{FR}}$	4e-07	2e-15	1e-16	7.5	7e+00	4e+15	5e-10	1e-09	9e-06	17.9	7e+01
	QAP	8e-09	3e-15	1e-16	8.6	2e+01	4e+14	5e-10	5e-09	1e-05	18.9	6e+01
random W	Elliptope	3e-12	1e-15	6e-17	6.3	1e-02	2e+00	1e-11	6e-12	3e-08	11.5	9e-02
	$\mathbf{QAP_{FR}}$	2e-12	3e-15	7e-17	20.6	2e+01	3e+05	5e-10	5e-10	7e-07	13.9	5e+01
	QAP	1e-07	5e-13	3e-16	537.9	1e+03	6e+11	1e-08	2e-09	1e-06	17.3	7e+01

Table 6.5: Algorithm 4.1 and SDPT3 on: Elliptope and Vontope; $n = 10$;

We now discuss the results in Table 6.5. We start with the Semi-Smooth Newton, Algorithm 4.1. The 'pf' column clearly indicates that the degeneracy of the optimal point $\bar{X}$ plays a significant

[7] https://www.math.cmu.edu/~reha/sdpt3.html, version SDPT3 4.0 [54].

role. Except for random W with $\mathbf{QAP_{FR}}$, the 'pf' values for the **QAP** are poor. This correlates with the condition number values; see also the discussion in Section 5. The condition numbers of the Jacobian near optimal points, $\mathrm{cond}(F'(y^k))$, become ill-conditioned when strict feasibility fails and the optimal solution is degenerate. The good measures for 'df' and 'cs' of Semi-Smooth Newton method is attributed to the construction of Algorithm 4.1. We observe that the average number of iterations for **QAP** is high when a random W is constructed, since the algorithm's difficulty in achieving the stopping tolerance ϵ, set to 10^{-7}.

SDPT3 exhibits overall strong performance on all instances. However, the 'df' and 'cs' values under SDPT3 are weaker compared to the Semi-Smooth Newton. This is due to interior point methods aiming to satisfy the first-optimality condition simultaneously throughout the process. We also observe that the number of iterations is higher when the optimal solutions are set to be degenerate.

Algorithm 4.1 has a superior performance for **MC** problems as all components of the optimality conditions are satisfied with near machine accuracy. This confirms that the status of the optimal solution plays an important role when it comes to the performance of Algorithm 4.1. In addition, preprocessing the instances so that they satisfy strict feasibility is important as seen by problems failing strict feasibility only contain degenerate points; see Theorem 2.9.

7 Conclusions

We presented and analyzed a semismooth Newton method for the best approximation problem, the projection problem, for spectrahedra. We showed that nondegeneracy is needed for the semismooth Newton method to perform well. We used the unbounded dual optimal set in the absence of a regularity condition to explain the lack of good performance. Moreover, we showed that the absence of strict feasibility results in degeneracy and ill-conditioning of the Jacobian at optimality. Our empirics illustrate the importance of strict feasibility. In particular, we studied the degeneracy for the elliptope and vontope.

Though we concentrated on SDP, many current relaxations for hard problems involve the doubly nonnegative, **DNN**, cone, i.e., $\mathbf{DNN} = \mathbb{S}^n_+ \cap \mathbb{R}^{n\times n}_+$. In particular, splitting methods efficiently exploit this intersection of two cones and facial reduction often provides a natural efficient splitting, e.g., [25,34,43]. It seems that the results we obtained from the Newton method for the **BAP** would extend to applying splitting methods to feasible sets of the type $\mathcal{L} \cap \mathbf{DNN}$.

Data Availability Statement

The results and data used in this paper is generated using our Matlab codes. These are publicly available at the link:
https:\www.math.uwaterloo.ca/~hwolkowi/henry/reports/CodesProjDegSingDegJul2024.d/

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