Tight Error Bounds for the Sign-Constrained Stiefel Manifold

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Abstract

The sign-constrained Stiefel manifold in $\mathbb{R}^{n\times r}$ is a segment of the Stiefel manifold with fixed signs (nonnegative or nonpositive) for some entries of the matrices. It includes the nonnegative Stiefel manifold as a special case. We present global and local error bounds that provide an inequality with easily computable residual functions and explicit coefficients to bound the distance from matrices in $\mathbb{R}^{n\times r}$ to the sign-constrained Stiefel manifold. Moreover, we show that the error bounds cannot be improved except for the multiplicative constants under some mild conditions, which explains why two square-root terms are necessary in the bounds when $1 < r < n$ and why the ℓ_1 norm can be used in the bounds when $r = n$ or $r = 1$ for the sign constraints and orthogonality, respectively. The error bounds are applied to derive exact penalty methods for minimizing a Lipschitz continuous function with orthogonality and sign constraints.

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1 Introduction

Let n and r be two integers such that $1 \le r \le n$, and $\mathbb{S}^{n,r} := \{X \in \mathbb{R}^{n\times r} : X^\top X = I_r\}$ be the Stiefel manifold, where I_r is the $r \times r$ identity matrix. Given two disjoint subsets $\mathcal{P}$ and $\mathcal{N}$ of $\{j : 1 \le j \le r\}$, denote

$$\mathbb{R}^{n\times r}_S := \left\{X \in \mathbb{R}^{n\times r} : X_{i,j} \ge 0 \text{ for } j \in \mathcal{P} \text{ and } X_{i,j} \le 0 \text{ for } j \in \mathcal{N},\ 1 \le i \le n\right\},$$

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which is a subset of $\mathbb{R}^{n\times r}$ with column-wise nonnegative or nonpositive constraints on some columns.

In this paper, we consider the *sign-constrained Stiefel manifold* defined as

$$\mathbb{S}^{n,r}_{S} \;:=\; \mathbb{S}^{n,r} \cap \mathbb{R}^{n\times r}_{S}.$$

When $\mathcal{P} = \{j : 1 \le j \le r\}$, $\mathbb{R}^{n\times r}_{S}$ reduces to the nonnegative orthant $\mathbb{R}^{n\times r}_{+}$, and $\mathbb{S}^{n,r}_{S}$ reduces to the *nonnegative Stiefel manifold* $\mathbb{S}^{n,r}_{+} := \{X \in \mathbb{S}^{n,r} : X \ge 0\}$.

If we define the sign matrix $S \in \mathbb{R}^{n\times r}$ as the matrix with

$$S_{i,j} \;=\; \begin{cases} 1, & \text{if } j \in \mathcal{P}, \\ -1, & \text{if } j \in \mathcal{N}, \qquad 1 \le i \le n, \\ 0, & \text{otherwise}, \end{cases} \tag{1.1}$$

then $\mathbb{S}^{n,r}_{S}$ can be formulated as

$$\mathbb{S}^{n,r}_{S} \;=\; \{X \in \mathbb{R}^{n\times r} : S \circ X \ge 0,\; X^{\mathsf{T}} X = I_r\},$$

where $\circ$ signifies the Hadamard product. We will investigate error bounds

$$\operatorname{dist}(X, \mathbb{S}^{n,r}_{S}) \;\le\; \nu \|(S \circ X)_-\|_{\mathrm{F}}^{q} \qquad \text{for} \quad X \in \mathbb{S}^{n,r}, \tag{1.2}$$

$$\operatorname{dist}(X, \mathbb{S}^{n,r}_{S}) \;\le\; \nu \|X^{\mathsf{T}} X - I_r\|_{\mathrm{F}}^{q} \qquad \text{for} \quad X \in \mathbb{R}^{n\times r}_{S}, \tag{1.3}$$

$$\operatorname{dist}(X, \mathbb{S}^{n,r}_{S}) \;\le\; \nu (\|(S \circ X)_-\|_{\mathrm{F}}^{q} + \|X^{\mathsf{T}} X - I_r\|_{\mathrm{F}}^{q}) \qquad \text{for} \quad X \in \mathbb{R}^{n\times r}, \tag{1.4}$$

where ν and q are positive constants, and $Y_- := \max\{-Y, 0\}$ stands for the entry-wise nonnegative part of $-Y$ for any matrix Y. The bounds (1.2)–(1.4) are global error bounds for $\mathbb{S}^{n,r}_{S}$ relative to $\mathbb{S}^{n,r}$, $\mathbb{R}^{n\times r}_{S}$, and $\mathbb{R}^{n\times r}$, respectively, with the first two being special cases of the last one.

According to the error bound of Luo-Pang presented in [19, Theorem 2.2], there exist $\nu > 0$ and $q > 0$ such that the inequalities in (1.2)–(1.4) hold for all X in a compact subset of $\mathbb{R}^{n\times r}$. Moreover, due to the error bound for polynomial systems given in [14, Corollary 3.8], for all X in a compact subset of $\mathbb{R}^{n\times r}$, there exists a ν such that the inequalities in (1.2)–(1.4) hold with a dimension-dependent value of q that is less than 6^{-2nr}. However, to the best of our knowledge, the explicit value of ν and the value of q that is independent of the dimension in (1.2)–(1.4) are still unknown even in the special case of $\mathbb{S}^{n,r}_{S} = \mathbb{S}^{n,r}_{+}$, and it is also unknown whether the error bounds hold in an unbounded set.

Being a fundamental concept in optimization, error bound plays a crucial role in both theory and methods for solving systems of equations and optimization problems [19, 22]. One of its applications is to develop penalty methods for constrained optimization problems. Let $F : \mathbb{R}^{n\times r} \to \mathbb{R}$ be a continuous function. The minimization problem

$$\min \{F(X) : X \in \mathbb{S}^{n,r}_{S}\} \tag{1.5}$$

can be found in a wide range of optimization models in data science, including nonnegative principal component analysis [15, 30], nonnegative Laplacian embedding [18], discriminative nonnegative spectral clustering [28], orthogonal nonnegative matrix factorization [23, 29], and some K-indicators models for data clustering [3, 26].

Even in the special case of $\mathbb{S}_S^{n,r} = \mathbb{S}_+^{n,r}$, the constraints of problem (1.5) are challenging to handle due to their combinatorial nature (note that, for example, $\mathbb{S}_+^{n,n}$ equals the set of all permutation matrices on $\mathbb{R}^n$). To deal with these difficult constraints, the penalty problems

$$\min\left\{F(X) + \mu\|(S \circ X)_-\|_{\mathrm{F}}^q : X \in \mathbb{S}^{n,r}\right\}, \tag{1.6}$$

$$\min\left\{F(X) + \mu\|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^q : X \in \mathbb{R}_S^{n\times r}\right\}, \tag{1.7}$$

$$\min\left\{F(X) + \mu(\|(S \circ X)_-\|_{\mathrm{F}}^q + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^q) : X \in \mathbb{R}^{n\times r}\right\}, \tag{1.8}$$

have been widely used for solving (1.5) with $\mathbb{S}_S^{n,r} = \mathbb{S}_+^{n,r}$, where μ is the penalty parameter. See for example [1, 24, 28, 30] and the references therein. However, the exactness of problems (1.6)–(1.8) regarding global minimizers and local minimizers of problem (1.5) is not well understood.

The main contribution of this paper is to establish the error bounds (1.2)–(1.4) with $\nu = 15r^{\frac{3}{4}}$ and $q = 1/2$ without any additional restriction on X. Moreover, we demonstrate that the error bounds cannot hold for $q > 1/2$ under mild conditions when $1 < r < n$ and $\mathbb{S}_S^{n,r} = \mathbb{S}_+^{n,r}$. In addition, we show that the error bounds (1.2)–(1.4) hold with $q = 1$ and $\nu = 7\sqrt{r}$ when $|\mathcal{P}|+|\mathcal{N}| = 1$, and hold with $q = 1$ and $\nu = 9n$ when $|\mathcal{P}| + |\mathcal{N}| = n$, but they cannot hold with $q > 1$. As an application of error bounds (1.2)–(1.4) with $\nu = 15r^{\frac{3}{4}}$ and $q = 1/2$, we show the exactness of the penalty problems (1.6) and (1.7) under the assumption that F is Lipschitz continuous, taking $\mathbb{S}_S^{n,r} = \mathbb{S}_+^{n,r}$ as an example. Moreover, we show the existence of Lipschitz continuous functions such that penalty problems (1.6) and (1.7) with $q > 1/2$ are not exact for global and local minimizers of the corresponding constrained problems. The values of q in error bounds (1.2)–(1.4) for some special sign matrices $S \in \mathbb{R}^{n\times r}$ defined in (1.1) by $\mathcal{P}$ and $\mathcal{N}$ are summarized in Table 1.

S	hold	fail
$\lvert\mathcal{P}\rvert = r$ or $\lvert\mathcal{N}\rvert = r, \quad 1 < r < n$	$q = 1/2$	$q > 1/2$
$\lvert\mathcal{P}\rvert = 1$ or $\lvert\mathcal{N}\rvert = 1, \quad 1 \le r \le n$	$q = 1$	$q > 1$
$\lvert\mathcal{P}\rvert + \lvert\mathcal{N}\rvert = n, \quad r = n$	$q = 1$	$q > 1$

Table 1: Error bounds (1.2)–(1.4) hold or fail for some special sign matrices $S \in \mathbb{R}^{n\times r}$

Very recently, our error bounds and matrix inequalities have been used to study constant modulus optimization and optimal orthogonal channel selection [2, 16, 17], which have a wide variety of applications in signal processing, communications, and data science.

The rest of the paper is organized as follows. In Section 2, we introduce some notations and preliminaries. Section 3 derives the error bounds (1.2)–(1.4) in the special case of $\mathbb{S}_S^{n,r} = \mathbb{S}_+^{n,r}$. Section 4 extends these bounds to the general case. Section 5 investigates the exactness of the penalty problems (1.6)–(1.8) using the new error bounds. Section 6 considers applications of the theoretical results established in this paper. We conclude the paper in Section 7.

2 Notation and preliminaries

For any matrix $X \in \mathbb{R}^{n\times r}$, $X_+ \coloneqq \max\{X, 0\} = X + X_-$ is the projection of X onto $\mathbb{R}_+^{n\times r}$. In addition, the singular value vector of X is denoted by $\sigma(X) \in \mathbb{R}^r$, the entries of which are in the descent order. Meanwhile, $\Sigma(X) \in \mathbb{R}^{n\times r}$ is the matrix such that $X = U\Sigma(X)V^\mathsf{T}$ is the singular value decomposition of X, the diagonal of $\Sigma(X)$ being $\sigma(X)$. We use $\mathbf{1}$ to denote the vector with all entries being one, and its dimension will be clear from the context.

Unless otherwise specified, $\|\cdot\|$ stands for a general vector norm. For any constant $p \in [1, +\infty)$, we use $\|\cdot\|_p$ to represent either the ℓ_p-norm of vectors or the operator norm induced by this vector norm for matrices. In addition, we use $\|\cdot\|_{\ell_p}$ to denote the *entry-wise* ℓ_p-norm of a matrix, namely the ℓ_p-norm of the vector that contains all the entries of the matrix. Note that $\|\cdot\|_{\ell_2}$ is the Frobenius norm, which is also denoted by $\|\cdot\|_\mathrm{F}$. When $\mathbb{R}^{n\times r}$ is equipped with the Frobenius norm, we use $\mathcal{B}(X,\delta)$ to represent the open ball in $\mathbb{R}^{n\times r}$ centered at a point $X \in \mathbb{R}^{n\times r}$ with a radius $\delta > 0$, and $\operatorname{dist}(X, \mathcal{T})$ to denote the distance from a point $X \in \mathbb{R}^{n\times r}$ to a set $\mathcal{T} \subset \mathbb{R}^{n\times r}$. Finally, given a minimization problem, we use Argmin to denote the set of global minimizers.

Lemma 2.1 is fundamental for the analysis of distances between matrices. This lemma is stated for unitarily invariant norms (see [10, Section 3.5] for this concept), although we are most interested in the case with the Frobenius norm.

Lemma 2.1 (Mirsky)**.** *For any matrices $X \in \mathbb{R}^{n\times r}$ and $Y \in \mathbb{R}^{n\times r}$, we have*

$$\|\Sigma(X) - \Sigma(Y)\| \;\le\; \|X - Y\| \tag{2.1}$$

for any unitarily invariant norm $\|\cdot\|$ on $\mathbb{R}^{n\times r}$. When $\|\cdot\|$ is the Frobenius norm, the equality holds in (2.1) if and only if there exist orthogonal matrices $U \in \mathbb{R}^{n\times n}$ and $V \in \mathbb{R}^{r\times r}$ such that $X = U\Sigma(X)V^\mathsf{T}$ and $Y = U\Sigma(Y)V^\mathsf{T}$.

The square case (i.e., $n = r$) of inequality (2.1) is due to Mirsky [20, Theorem 5], and the general case can be found in [11, Theorem 7.4.9.1]. A direct corollary of Lemma 2.1 is the following Hoffman-Wielandt [9] type bound for singular values, which is equivalent to the von Neumann trace inequality [25, Theorem I] (see also [13, Theorem 2.1]).

Lemma 2.2 (von Neumann)**.** *For any matrices $X \in \mathbb{R}^{n\times r}$ and $Y \in \mathbb{R}^{n\times r}$, we have*

$$\|\sigma(X) - \sigma(Y)\|_2 \;\le\; \|X - Y\|_\mathrm{F},$$

and equivalently, $\operatorname{tr}(X^\mathsf{T}Y) \le \sigma(X)^\mathsf{T}\sigma(Y)$.

The following lemma is another consequence of Lemma 2.1. For this result, recall that each matrix $X \in \mathbb{R}^{n\times r}$ has a polar decomposition in the form of $X = UP$, where U belongs to $\mathbb{S}^{n,r}$ and $P = (X^\mathsf{T}X)^{\frac{1}{2}}$, with U being called a unitary polar factor of X. The square case of this lemma is due to Fan and Hoffman [7, Theorem 1]. For the general case, see [8, Theorem 8.4], which details a proof based on Lemma 2.1.

Lemma 2.3 (Fan-Hoffman)**.** *If $U \in \mathbb{R}^{n\times r}$ is a unitary polar factor of a matrix $X \in \mathbb{R}^{n\times r}$, then*

$$\|X - U\| \;=\; \min\{\|X - V\| : V \in \mathbb{S}^{n,r}\}$$

for any unitarily invariant norm $\|\cdot\|$ on $\mathbb{R}^{n\times r}$.

Lemma 2.4 collects a few basic facts on the distance from a matrix in $\mathbb{R}^{n\times r}$ to $\mathbb{S}^{n,r}$.

Lemma 2.4. *For any matrix $X \in \mathbb{R}^{n\times r}$, we have*

$$\operatorname{dist}(X, \mathbb{S}^{n,r}) \;=\; \|\sigma(X) - \mathbf{1}\|_2 \;\le\; \min\left\{\|X^\mathsf{T}X - I_r\|_\mathrm{F},\; r^{\frac{1}{4}}\|X^\mathsf{T}X - I_r\|_\mathrm{F}^{\frac{1}{2}}\right\}.$$

In addition, $\|X^\mathsf{T}X - I_r\|_\mathrm{F} \le (\|X\|_2 + 1)\|\sigma(X) - \mathbf{1}\|_2$.

Proof. Let $U \in \mathbb{S}^{n,r}$ be a unitary polar factor of X. By Lemma 2.3,

$$\operatorname{dist}(X, \mathbb{S}^{n,r}) = \|X - U\|_\mathrm{F} = \|U^\mathsf{T}(X - U)\|_\mathrm{F} = \|(X^\mathsf{T}X)^{\frac{1}{2}} - I_r\|_\mathrm{F} = \|\sigma(X) - \mathbf{1}\|_2.$$

The entry-wise inequalities $|\sigma(X) - \mathbf{1}| \le |\sigma(X)^2 - \mathbf{1}| \le (\|X\|_2 + 1)|\sigma(X) - \mathbf{1}|$ imply

$$\|\sigma(X) - \mathbf{1}\|_2 \;\le\; \|\sigma(X)^2 - \mathbf{1}\|_2 \;\le\; (\|X\|_2 + 1)\|\sigma(X) - \mathbf{1}\|_2. \tag{2.2}$$

Noting that $\|\sigma(X)^2 - \mathbf{1}\|_2 = \|X^\mathsf{T}X - I_r\|_\mathrm{F}$, we obtain from (2.2) that

$$\|\sigma(X) - \mathbf{1}\|_2 \le \|X^\mathsf{T}X - I_r\|_\mathrm{F} \le (\|X\|_2 + 1)\|\sigma(X) - \mathbf{1}\|_2.$$

Finally, since $|\sigma(X) - \mathbf{1}|^2 \le |\sigma(X)^2 - \mathbf{1}|$, we have

$$\|\sigma(X) - \mathbf{1}\|_2^2 \;\le\; \|\sigma(X)^2 - \mathbf{1}\|_1 \;\le\; \sqrt{r}\|\sigma(X)^2 - \mathbf{1}\|_2 \;=\; \sqrt{r}\|X^\mathsf{T}X - I_r\|_\mathrm{F}.$$

The proof is complete. □

By Lemmas 2.3 and 2.4, $\operatorname{dist}(X, \mathbb{S}_+^{n,r}) = \|\sigma(X) - \mathbf{1}\|_2$ if X has a nonnegative unitary polar factor. It is the case in the following lemma, where this factor is $X(X^\mathsf{T}X)^{-\frac{1}{2}}$.

Lemma 2.5. *For a matrix $X \in \mathbb{R}_+^{n\times r}$, if $X^\mathsf{T}X$ is nonsingular and diagonal, then*

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;=\; \|\sigma(X) - \mathbf{1}\|_2.$$

Lemma 2.6 is an elementary property of $\mathbb{S}_+^{n,r}$. We omit the proof.

Lemma 2.6. *For a matrix $X \in \mathbb{S}_+^{n,r}$, each row of X has at most one nonzero entry.*

3 Error bounds for the nonnegative Stiefel manifold

This section will establish the error bounds (1.2)–(1.4) in the special case of $\mathbb{S}^{n,r}_S = \mathbb{S}^{n,r}_+$, where $S \circ X$ reduces to X. Subsection 3.1 demonstrates (1.2)–(1.4) with $q = 1$ when $r = 1$ or $r = n$, and points out that they cannot hold with $q > 1$ regardless of $r \in \{1, \dots, n\}$. In Subsection 3.2, we derive the bounds (1.2)–(1.4) with $q = 1/2$ for $1 \le r \le n$, and Subsection 3.3 elaborates on the tightness of these bounds when $1 < r < n$. As an application of our results, we briefly discuss the linear regularity of $\mathbb{R}^{n\times r}_+$ and $\mathbb{S}^{n,r}$ in Subsection 3.4.

General discussions on error bounds can be found in [6, Section 6.1]. Here we focus on error bounds for $\mathbb{S}^{n,r}_+$ defined by two special functions

$$\rho_1(X) \coloneqq \|X_-\|_{\mathrm{F}}^{q_1} + \|\sigma(X) - \mathbf{1}\|_2^{q_2},$$
$$\rho_2(X) \coloneqq \|X_-\|_{\mathrm{F}}^{q_1} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{q_2},$$

where q_1 and q_2 are positive constants. These functions are residual functions for $\mathbb{S}^{n,r}_+$ relative to $\mathbb{R}^{n\times r}$, namely nonnegative-valued functions on $\mathbb{R}^{n\times r}$ whose zeros coincide with the elements of $\mathbb{S}^{n,r}_+$. The residual function ρ_2 is easily computable and it reduces to the one in (1.4) when $q_1 = q_2 = q$.

We say that ρ_1 defines a local error bound for $\mathbb{S}^{n,r}_+$ relative to $\mathbb{R}^{n\times r}$ if there exist positive constants ϵ and ν such that

$$\operatorname{dist}(X, \mathbb{S}^{n,r}_+) \;\le\; \nu\rho_1(X) \tag{3.1}$$

for all $X \in \mathbb{R}^{n\times r}$ satisfying $\|X_-\|_{\mathrm{F}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}} \le \epsilon$, and we say it defines a global error bound for $\mathbb{S}^{n,r}_+$ relative to $\mathbb{R}^{n\times r}$ if (3.1) holds for all $X \in \mathbb{R}^{n\times r}$. Likewise, we can use ρ_1 to define error bounds for $\mathbb{S}^{n,r}_+$ relative to any set $\mathcal{S} \subset \mathbb{R}^{n\times r}$ that contains $\mathbb{S}^{n,r}_+$, for example, $\mathcal{S} = \mathbb{R}^{n\times r}_+$, in which case ρ_1 reduces to its second term. Similar things can be said about ρ_2. Theorems 3.5 and 3.12 will specify the precise range of q_1 and q_2 so that ρ_1 and ρ_2 define local or global error bounds for $\mathbb{S}^{n,r}_+$ relative to $\mathbb{R}^{n\times r}$.

3.1 Tight error bounds with $r = 1$ or $r = n$

In this subsection, we show that the error bounds (1.2)–(1.4) hold for $q = 1$ when $r = 1$ or $r = n$. Moreover, we explain why bounds (1.2)–(1.4) cannot hold for $q > 1$ in general.

The bound for $r = 1$ is easy to establish due to the simple fact that

$$\operatorname{dist}(x, \mathbb{S}^{n,1}_+) \;=\; \operatorname{dist}(x, \mathbb{S}^{n,1}) \;=\; \big|\|x\|_2 - 1\big| \quad \text{for all} \quad x \in \mathbb{R}^n_+. \tag{3.2}$$

Indeed, when $x = 0$, this is trivial; when $x \ne 0$, equality (3.2) is true because the projection of x onto $\mathbb{S}^{n,1}_+$ equals its projection onto $\mathbb{S}^{n,1}$, which is $x/\|x\|_2 \ge 0$.

Theorem 3.1. *For any vector $x \in \mathbb{R}^n$,*

$$\operatorname{dist}(x, \mathbb{S}^{n,1}_+) \;\le\; 2\|x_-\|_2 + \big|\|x\|_2 - 1\big|.$$

Proof. As observed above, $\operatorname{dist}(x_+, \mathbb{S}_+^{n,1}) = \big|\|x_+\|_2 - 1\big|$. Meanwhile,

$$\big|\|x_+\|_2 - 1\big| - \big|\|x\|_2 - 1\big| \;\le\; \big|\|x_+\|_2 - \|x\|_2\big| \;\le\; \|x_+ - x\|_2 \;=\; \|x_-\|_2.$$

Thus $\operatorname{dist}(x, \mathbb{S}_+^{n,1}) \le \|x_-\|_2 + \operatorname{dist}(x_+, \mathbb{S}_+^{n,1}) \le 2\|x_-\|_2 + \big|\|x\|_2 - 1\big|$. □

To establish the error bounds for $r = n$, we first prove Proposition 3.2, which is essentially a weakened version of the observation (3.2) in the current situation. Note that the matrix Y defined in the proof below is indeed the rounding matrix proposed in [12, Procedure 3.1].

Proposition 3.2. *For any matrix $X \in \mathbb{R}_+^{n\times n}$, if $\|\sigma(X) - \mathbf{1}\|_2 < 1/(4\sqrt{n})$, then*

$$\operatorname{dist}(X, \mathbb{S}_+^{n,n}) \;\le\; 7\sqrt{n}\|\sigma(X) - \mathbf{1}\|_2. \tag{3.3}$$

Proof. For each $i \in \{1, \ldots, n\}$, take the smallest integer $l_i \in \{1, \ldots, r\}$ so that

$$X_{i,l_i} \;=\; \max\{X_{i,j} : j = 1, \ldots, r\}.$$

Consider the matrix $Y \in \mathbb{R}_+^{n,r}$ defined by

$$Y_{i,j} \;=\; \begin{cases} X_{i,l_i} & \text{if } j = l_i, \\ 0 & \text{otherwise.} \end{cases} \tag{3.4}$$

We will demonstrate (3.3) by establishing bounds for $\|X - Y\|_{\mathrm{F}}$ and $\operatorname{dist}(Y, \mathbb{S}_+^{n,n})$.

Consider $\|X - Y\|_{\mathrm{F}}$ first. Due to the fact that $\|\sigma(X) - \mathbf{1}\|_2 < 1/(4\sqrt{n})$, all the n singular values of X are at least $3/4$. Since $X \ge 0$ and $X_{i,l_i} = \max\{X_{i,j} : j = 1, \ldots, n\}$, we have

$$X_{i,l_i} \;\ge\; \frac{1}{\sqrt{n}}\left(XX^{\mathsf{T}}\right)^{\frac{1}{2}}_{i,i} \;\ge\; \frac{3}{4\sqrt{n}} \quad \text{for each} \quad i \in \{1, \ldots, n\}.$$

Fix an integer $j \in \{1, \ldots, r\}$. For each $l \in \{1, \ldots, r\}$, define

$$\mathbb{1}(j \ne l) \;=\; \mathbb{1}(l \ne j) \;=\; \begin{cases} 1 & \text{if } l \ne j, \\ 0 & \text{if } l = j. \end{cases}$$

With x^j and y^j denoting the jth columns of X and Y, respectively, we have

$$\begin{aligned}
\frac{9}{16n}\|x^j - y^j\|_2^2 \;&=\; \frac{9}{16n}\sum_{i=1}^n X_{i,j}^2\mathbb{1}(j \ne l_i) \\
&\le\; \sum_{i=1}^n X_{i,l_i}^2 X_{i,j}^2 \mathbb{1}(l_i \ne j) \\
&\le\; \sum_{l=1}^n\sum_{i=1}^n X_{i,l}^2 X_{i,j}^2 \mathbb{1}(l \ne j) \\
&\le\; \sum_{l=1}^n\left(\sum_{i=1}^n X_{i,l}X_{i,j}\right)^2 \mathbb{1}(l \ne j) \\
&=\; \sum_{l=1}^n\left(X^{\mathsf{T}}X - I_n\right)^2_{l,j} \mathbb{1}(l \ne j).
\end{aligned}$$

Hence

$$\|X - Y\|_{\mathrm{F}} \;\le\; \frac{4}{3}\sqrt{n}\|X^{\mathsf{T}}X - I_n\|_{\mathrm{F}}.$$

By Lemma 2.4 and the fact that $\|X\|_2 \le 1 + \|\sigma(X) - \mathbf{1}\|_2 \le 5/4$, we have further

$$\|X - Y\|_{\mathrm{F}} \;\le\; \frac{4}{3}\sqrt{n}(\|X\|_2 + 1)\|\sigma(X) - \mathbf{1}\|_2 \;\le\; 3\sqrt{n}\|\sigma(X) - \mathbf{1}\|_2. \tag{3.5}$$

Now we estimate $\operatorname{dist}(Y, \mathbb{S}^{n,n}_{+})$. According to inequality (3.5) and Lemma 2.2,

$$\|\sigma(Y) - \mathbf{1}\|_2 \;\le\; \|X - Y\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2 \;\le\; 4\sqrt{n}\|\sigma(X) - \mathbf{1}\|_2. \tag{3.6}$$

Since $\|\sigma(X) - \mathbf{1}\|_2 < 1/(4\sqrt{n})$, we have $\|\sigma(Y) - \mathbf{1}\|_2 < 1$, which implies that $Y^{\mathsf{T}}Y$ is nonsingular. Since Y has at most one nonzero entry in each row, it is clear that $Y^{\mathsf{T}}Y$ is diagonal. Thus we can invoke Lemma 2.5 and obtain

$$\operatorname{dist}(Y, \mathbb{S}^{n,n}_{+}) \;=\; \|\sigma(Y) - \mathbf{1}\|_2.$$

Therefore, combining inequalities (3.5) and (3.6), we conclude that (3.3) is true. □

Theorem 3.3 presents global and local error bounds for $\mathbb{S}^{n,n}_{+}$ relative to $\mathbb{R}^{n\times n}$.

Theorem 3.3. *For any matrix $X \in \mathbb{R}^{n\times n}$, we have*

$$\operatorname{dist}(X, \mathbb{S}^{n,n}_{+}) \;\le\; 9n\left(\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2\right). \tag{3.7}$$

Moreover, if $\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2 < 1/(4\sqrt{n})$, then

$$\operatorname{dist}(X, \mathbb{S}^{n,n}_{+}) \;\le\; 8\sqrt{n}\left(\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2\right). \tag{3.8}$$

Proof. We first prove (3.8), assuming that $\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2 < 1/(4\sqrt{n})$. By Lemma 2.2, this assumption ensures $\|\sigma(X_{+}) - \mathbf{1}\|_2 < 1/(4\sqrt{n})$. Thus Proposition 3.2 renders

$$\operatorname{dist}(X_{+}, \mathbb{S}^{n,n}_{+}) \;\le\; 7\sqrt{n}\|\sigma(X_{+}) - \mathbf{1}\|_2 \;\le\; 7\sqrt{n}\left(\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2\right),$$

which justifies inequality (3.8) since $\operatorname{dist}(X, \mathbb{S}^{n,n}_{+}) \le \|X_{-}\|_{\mathrm{F}} + \operatorname{dist}(X_{+}, \mathbb{S}^{n,n}_{+})$.

Now we consider inequality (3.7). If $\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2 < 1/(4\sqrt{n})$, then (3.7) holds due to (3.8). When $\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2 \ge 1/(4\sqrt{n})$, inequality (3.7) is justified by

$$\begin{aligned}
\operatorname{dist}(X, \mathbb{S}^{n,n}_{+}) \;&\le\; \operatorname{dist}(X, \mathbb{S}^{n,n}) + 2\sqrt{n} \\
&\le \|\sigma(X) - \mathbf{1}\|_2 + 8n(\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2) \\
&\le 9n\left(\|X_{-}\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2\right),
\end{aligned}$$

where the first inequality holds because the diameter of $\mathbb{S}^{n,n}$ is $2\sqrt{n}$. □

Remark 3.4. Since $\left|\|x\|_2 - 1\right| \le \left|\|x\|_2^2 - 1\right|$ and $\|\sigma(X) - \mathbf{1}\|_2 \le \|X^\mathsf{T} X - I_n\|_\mathrm{F}$, Theorems 3.1 and 3.3 imply the error bounds (1.2)–(1.4) with $q = 1$ for $r \in \{1, n\}$. These bounds cannot be improved except for the multiplicative constants. Indeed, for any matrix $X \in \mathbb{R}^{n\times r}$ with $r \in \{1, \dots, n\}$ and $\|X\|_2 \le 1$, we have

$$\begin{aligned} \operatorname{dist}(X,\, \mathbb{S}_+^{n,r}) &\ge \max\left\{\operatorname{dist}(X,\, \mathbb{R}_+^{n\times r}),\ \operatorname{dist}(X,\, \mathbb{S}^{n,r})\right\} \\ &\ge \frac{1}{2}\left[\operatorname{dist}(X,\, \mathbb{R}_+^{n\times r}) + \operatorname{dist}(X,\, \mathbb{S}^{n,r})\right] \\ &= \frac{1}{2}\left(\|X_-\|_\mathrm{F} + \|\sigma(X) - \mathbf{1}\|_2\right) \\ &\ge \frac{1}{2}\|X_-\|_\mathrm{F} + \frac{1}{4}\|X^\mathsf{T} X - I_r\|_\mathrm{F}, \end{aligned} \tag{3.9}$$

where the last two lines apply Lemma 2.4. This also implies that the bounds (1.2)–(1.4) cannot hold for any $r \in \{1, \dots, n\}$ with $q > 1$.

Theorem 3.5 is an extension of Theorems 3.1 and 3.3. It specifies the possible exponents of $\|X_-\|_\mathrm{F}$ and $\|\sigma(X) - \mathbf{1}\|_2$ or $\|X^\mathsf{T} X - I_r\|_\mathrm{F}$ in local and global error bounds for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ for $r \in \{1, n\}$. As we will see from (b) of this theorem and its proof, when $r = 1$ or $r = n$, the error bound (1.2) can hold if and only if $q \le 1$, whereas (1.3) and (1.4) can hold if and only if $1/2 \le q \le 1$.

Theorem 3.5. *Let q_1 and q_2 be positive constants. Suppose that $r = 1$ or $r = n$.*

(a) *The function $\rho_1(X) := \|X_-\|_\mathrm{F}^{q_1} + \|\sigma(X) - \mathbf{1}\|_2^{q_2}$ defines a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ if and only if $q_1 \le 1$ and $q_2 \le 1$, and it defines a global error bound if and only if $q_1 \le q_2 = 1$.*

(b) *The function $\rho_2(X) := \|X_-\|_\mathrm{F}^{q_1} + \|X^\mathsf{T} X - I_r\|_\mathrm{F}^{q_2}$ defines a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ if and only if $q_1 \le 1$ and $q_2 \le 1$, and it defines a global error bound if and only if $q_1 \le 1$ and $1/2 \le q_2 \le 1$.*

Proof. We consider only the case with $r = n$. The other case is similar.

(a) Based on (3.8) and (3.9), it is easy to check that ρ_1 defines a local error bound for $\mathbb{S}_+^{n,n}$ relative to $\mathbb{R}^{n\times n}$ if and only if $q_1 \le 1$ and $q_2 \le 1$. Hence we only need to consider the global error bound.

Suppose that $q_1 \le q_2 = 1$. Let us show that

$$\operatorname{dist}(X,\, \mathbb{S}_+^{n,n}) \ \le\ 9n\left(\|X_-\|_\mathrm{F}^{q_1} + \|\sigma(X) - \mathbf{1}\|_2\right) \ =\ 9n\rho_1(X) \tag{3.10}$$

for $X \in \mathbb{R}^{n\times n}$. If $\|X_-\|_\mathrm{F} \le 1$, then (3.10) follows from (3.7). When $\|X_-\|_\mathrm{F} > 1$,

$$\operatorname{dist}(X, \mathbb{S}_+^{n,n}) \ \le\ \operatorname{dist}(X, \mathbb{S}^{n,n}) + 2\sqrt{n} \ \le\ \|\sigma(X) - \mathbf{1}\|_2 + 2\sqrt{n}\|X_-\|_\mathrm{F}^{q_1},$$

which validates (3.10) again. Hence ρ_1 defines a global error bound for $\mathbb{S}_+^{n,n}$ relative to $\mathbb{R}^{n\times n}$.

Now suppose that ρ_1 defines a global error bound for $\mathbb{S}_+^{n,n}$ relative to $\mathbb{R}^{n\times n}$. Then it also defines a local error bound, implying $q_1 \le 1$ and $q_2 \le 1$. Consider a sequence $\{X_k\} \subset \mathbb{R}_+^{n\times n}$ such that $X_k^\mathsf{T} X_k = kI_n$ for each $k \ge 1$. Then

$$\operatorname{dist}(X_k, \mathbb{S}_+^{n,n}) \;\ge\; \operatorname{dist}(X_k, \mathbb{S}^{n,n}) \;=\; \|\sigma(X_k) - \mathbf{1}\|_2 \;=\; [\rho_1(X_k)]^{\frac{1}{q_2}} \;\to\; \infty.$$

By assumption, $\operatorname{dist}(X_k, \mathbb{S}_+^{n,n}) \le \nu\rho_1(X_k)$ for each $k \ge 1$ with a constant ν. Hence we know $q_2 \ge 1$. To conclude, we have $q_1 \le q_2 = 1$. The proof for (a) is complete.

(b) Based on (3.8), (3.9), and the fact that $\|\sigma(X) - \mathbf{1}\|_2 \le \|X^\mathsf{T} X - I_n\|_\mathrm{F}$ (Lemma 2.4), it is easy to check that ρ_2 defines a local error bound for $\mathbb{S}_+^{n,n}$ relative to $\mathbb{R}^{n\times n}$ if and only if $q_1 \le 1$ and $q_2 \le 1$. Hence we consider only the global error bound.

Suppose that $q_1 \le 1$ and $1/2 \le q_2 \le 1$. We will show that

$$\operatorname{dist}(X, \mathbb{S}_+^{n,n}) \;\le\; 9n\left(\|X_-\|_\mathrm{F}^{q_1} + \|X^\mathsf{T} X - I_n\|_\mathrm{F}^{q_2}\right) \;=\; 9n\rho_2(X) \tag{3.11}$$

for $X \in \mathbb{R}^{n\times n}$. If $\|X^\mathsf{T} X - I_n\|_\mathrm{F} \le 1$, then (3.11) holds because of (3.10) and the fact that $\|\sigma(X) - \mathbf{1}\|_2 \le \|X^\mathsf{T} X - I_n\|_\mathrm{F}$. When $\|X^\mathsf{T} X - I_n\|_\mathrm{F} > 1$,

$$\begin{aligned}\operatorname{dist}(X, \mathbb{S}_+^{n,n}) &\le \operatorname{dist}(X, \mathbb{S}^{n,n}) + 2\sqrt{n} \\ &\le n^{\frac{1}{4}}\|X^\mathsf{T} X - I_n\|_\mathrm{F}^{\frac{1}{2}} + 2\sqrt{n}\|X^\mathsf{T} X - I_n\|_\mathrm{F}^{q_2} \\ &\le (n^{\frac{1}{4}} + 2\sqrt{n})\|X^\mathsf{T} X - I_n\|_\mathrm{F}^{q_2},\end{aligned}$$

justifying (3.11) again, where the second inequality applies Lemma 2.4. Hence ρ_2 defines a global error bound for $\mathbb{S}_+^{n,n}$ relative to $\mathbb{R}^{n\times n}$.

Now suppose that ρ_2 defines a global error bound for $\mathbb{S}_+^{n,n}$ relative to $\mathbb{R}^{n\times n}$. Then $q_1 \le 1$ and $q_2 \le 1$, as ρ_2 also defines a local error bound. Consider again a sequence $\{X_k\} \subset \mathbb{R}_+^{n\times n}$ such that $X_k^\mathsf{T} X_k = kI_n$ for each $k \ge 1$. Then

$$\begin{aligned}\operatorname{dist}(X_k, \mathbb{S}_+^{n,n}) \ge \|\sigma(X_k) - \mathbf{1}\|_2 = (\sqrt{k} - 1)\sqrt{n}, \\ \rho_2(X_k) = \|X_k^\mathsf{T} X_k - I_n\|_\mathrm{F}^{q_2} = [(k-1)\sqrt{n}]^{q_2}.\end{aligned}$$

By assumption, $\operatorname{dist}(X_k, \mathbb{S}_+^{n,n}) \le \nu\rho_2(X_k)$ for each $k \ge 1$ with a constant ν. Hence we have $q_2 \ge 1/2$. The proof for (b) is complete. □

3.2 Error bounds with $1 \le r \le n$

Now we shift our attention to the general case with $1 \le r \le n$. Given previous bounds for $r \in \{1, n\}$, we are particularly interested in the situation where $1 < r < n$.

We will first prove a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}_+^{n\times r}$ as detailed in Proposition 3.8. This bound will play a role similar to what observation (3.2) and Proposition 3.2 do in the cases of $r = 1$ and $r = n$, respectively. To simplify its proof, we start with the following lemma.

Lemma 3.6. *For any matrix $X \in \mathbb{R}_+^{n\times r}$, there exists a matrix $Y \in \mathbb{R}_+^{n\times r}$ such that $Y^\mathsf{T} Y$ is diagonal and*

$$\max\left\{\|x^j - y^j\|_2,\ \big|\|y^j\|_2 - 1\big|\right\} \ \le\ \|z^j\|_1^{\frac{1}{2}} \quad \text{for each} \quad j \in \{1,\dots,r\}, \tag{3.12}$$

where x^j, y^j, and z^j denote the jth column of X, Y, and $Z = X^\mathsf{T} X - I_r$, respectively.

Proof. Define l_i $(1 \le i \le n)$ and Y as in the proof of Proposition 3.2. Since $Y^\mathsf{T} Y$ is diagonal as mentioned before, it suffices to establish (3.12) for this Y.

Fix an index $j \in \{1,\dots,r\}$. Recalling that $0 \le X_{i,j} \le X_{i,l_i}$ for each $i \in \{1,\dots,n\}$, we have

$$\begin{aligned} \|x^j - y^j\|_2^2 \ &=\ \sum_{i=1}^n X_{i,j}^2 \mathbb{1}(j \ne l_i) \\ &\le\ \sum_{i=1}^n X_{i,l_i} X_{i,j} \mathbb{1}(l_i \ne j) \\ &\le\ \sum_{l=1}^r \left(\sum_{i=1}^n X_{i,l} X_{i,j}\right) \mathbb{1}(l \ne j). \end{aligned} \tag{3.13}$$

Since $X^\mathsf{T} X$ and Z have the same off-diagonal entries, inequality (3.13) yields

$$\|x^j - y^j\|_2^2 \ \le\ \sum_{l=1}^r |Z_{l,j}| \mathbb{1}(l \ne j) \ =\ \|z^j\|_1 - |Z_{j,j}|. \tag{3.14}$$

It remains to prove $\big|\|y^j\|_2 - 1\big|^2 \le \|z^j\|_1$. To this end, note that

$$\big|\|y^j\|_2 - 1\big|^2 \ \le\ \big|\|y^j\|_2^2 - 1\big| \ \le\ \big|\|x^j\|_2^2 - 1\big| + \|x^j - y^j\|_2^2, \tag{3.15}$$

where the first inequality uses the fact that $|t-1|^2 \le |t^2 - 1|$ for any $t \ge 0$, and the second one is because $\|x^j\|_2^2 - \|y^j\|_2^2 = \|x^j - y^j\|_2^2$ due to the special construction (3.4) of Y. Since $\|x^j\|_2^2 - 1 = Z_{j,j}$, we can combine (3.14) and (3.15) to obtain

$$\big|\|y^j\|_2 - 1\big|^2 \ \le\ \big|\|x^j\|_2^2 - 1\big| + \left(\|z^j\|_1 - |Z_{j,j}|\right) \ =\ \|z^j\|_1.$$

The proof is complete. □

Remark 3.7. As mentioned earlier, the matrix Y in the proof of Lemma 3.6 is the rounding matrix in [12, Procedure 3.1]. Inequality (3.13) is essentially the second inequality in Case II of the proof for [12, Lemma 3.2]. The columns of X are assumed to be normalized in [12], but such an assumption has no effect on this inequality.

Proposition 3.8. *For any matrix $X \in \mathbb{R}_+^{n\times r}$, if $\|\sigma(X) - \mathbf{1}\|_2 < 1/(3\sqrt{r})$, then*

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \ \le\ 2\sqrt{\frac{7r}{3}}\|\sigma(X) - \mathbf{1}\|_2^{\frac{1}{2}}. \tag{3.16}$$

Proof. Let Y and Z be the matrices specified in Lemma 3.6. Then (3.12) leads to

$$\|X - Y\|_{\mathrm{F}}^2 \;=\; \sum_{j=1}^{r} \|x^j - y^j\|_2^2 \;\le\; \sum_{j=1}^{r} \|z^j\|_1 \;=\; \|Z\|_{\ell_1}. \tag{3.17}$$

Since $Y^{\mathsf{T}}Y$ is diagonal, the entries of $\sigma(Y)$ are $\|y^1\|_2, \ldots, \|y^r\|_2$. Thus (3.12) also provides

$$\|\sigma(Y) - \mathbf{1}\|_2^2 \;=\; \sum_{j=1}^{r} (\|y^j\|_2 - 1)^2 \;\le\; \sum_{j=1}^{r} \|z^j\|_1 \;=\; \|Z\|_{\ell_1}. \tag{3.18}$$

Comparing (3.16) with (3.17)–(3.18), we only need to prove that $\|\sigma(X) - \mathbf{1}\|_2 < 1/(3\sqrt{r})$ ensures

$$\|Z\|_{\ell_1} \;\le\; \frac{7r}{3}\|\sigma(X) - \mathbf{1}\|_2 \tag{3.19}$$

and

$$\operatorname{dist}(Y, \mathbb{S}_+^{n,r}) \;=\; \|\sigma(Y) - \mathbf{1}\|_2. \tag{3.20}$$

Since $\|Z\|_{\ell_1} = \sum_{i=1}^{n}\sum_{j=1}^{r} |Z_{ij}| \le r\|Z\|_{\mathrm{F}}$, inequality (3.19) is a direct consequence of

$$\|Z\|_{\mathrm{F}} \;=\; \|X^{\mathsf{T}}X - I_r\|_{\mathrm{F}} \;\le\; (\|X\|_2 + 1)\|\sigma(X) - \mathbf{1}\|_2 \;\le\; \frac{7}{3}\|\sigma(X) - \mathbf{1}\|_2, \tag{3.21}$$

where the last inequality is because $\|X\|_2 \le \|\sigma(X) - \mathbf{1}\|_2 + 1 < 4/3$. Meanwhile, inequality (3.21) also leads to

$$\|z^j\|_1 \;\le\; \sqrt{r}\|Z\|_{\mathrm{F}} \;\le\; \frac{7\sqrt{r}}{3}\|\sigma(X) - \mathbf{1}\|_2 \;<\; 1 \quad \text{for each} \quad j \in \{1, \ldots, r\}.$$

Therefore, inequality (3.12) implies that Y does not contain any zero column. Hence the diagonal entries of $Y^{\mathsf{T}}Y$ are all positive, which ensures the nonsingularity of this matrix since it is diagonal. Thus Lemma 2.5 yields (3.20). The proof is complete. □

Now we are ready to establish a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$.

Theorem 3.9. *For any matrix $X \in \mathbb{R}^{n\times r}$, if $\|X_-\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2 < 1/(3\sqrt{r})$, then*

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;\le\; 4\sqrt{r}\left(\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|\sigma(X) - \mathbf{1}\|_2^{\frac{1}{2}}\right). \tag{3.22}$$

Proof. According to Lemma 2.2,

$$\|\sigma(X_+) - \mathbf{1}\|_2 \;\le\; \|X_-\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2.$$

Thus $\|\sigma(X_+) - \mathbf{1}\|_2 < 1/(3\sqrt{r})$ by assumption, and hence Proposition 3.8 implies

$$\operatorname{dist}(X_+, \mathbb{S}_+^{n,r}) \;\le 2\sqrt{\frac{7r}{3}}\left(\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|\sigma(X) - \mathbf{1}\|_2^{\frac{1}{2}}\right). \tag{3.23}$$

On the other hand, since $\|X_-\|_{\mathrm{F}} < 1/(3\sqrt{r})$, it holds that

$$\|X - X_+\|_{\mathrm{F}} \;=\; \|X_-\|_{\mathrm{F}} \;\le\; \frac{1}{\sqrt{3}r^{\frac{1}{4}}}\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} \;\le\; \sqrt{\frac{r}{3}}\|X_-\|_{\mathrm{F}}^{\frac{1}{2}}. \tag{3.24}$$

Inequality (3.22) follows from (3.23) and (3.24) because $2\sqrt{7/3} + 1/\sqrt{3} < 4$. □

Theorem 3.9 presents only a local error bound. Indeed, $\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|\sigma(X) - \mathbf{1}\|_2^{\frac{1}{2}}$ does not define a global error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$, which will be explained later by Theorem 3.12. To have a global error bound, we need to replace the term $\|\sigma(X) - \mathbf{1}\|_2$ with $\|X^\mathsf{T} X - I_r\|_{\mathrm{F}}$ as in the following theorem.

Theorem 3.10. *For any matrix $X \in \mathbb{R}^{n\times r}$, we have*

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;\le\; 5r^{\frac{3}{4}} \left(\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}} \right). \tag{3.25}$$

Moreover, if $\|X_-\|_{\mathrm{F}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}} < 1/(3\sqrt{r})$, then

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;\le\; 4\sqrt{r} \left(\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}} \right). \tag{3.26}$$

Proof. Recall that $\|\sigma(X) - \mathbf{1}\|_2 \le \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}$ (Lemma 2.4). Thus (3.26) is a direct consequence of Theorem 3.9 when $\|X_-\|_{\mathrm{F}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}} < 1/(3\sqrt{r})$.

Now we prove (3.25). Let us assume that

$$\|X_-\|_{\mathrm{F}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}} \;\ge\; \frac{1}{3\sqrt{r}},$$

as (3.25) is already justified by (3.26) when this inequality does not hold. Under this assumption,

$$\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}} \;\ge\; \frac{1}{\sqrt{3}r^{\frac{1}{4}}}. \tag{3.27}$$

Noting that the diameter of $\mathbb{S}^{n,r}$ is $2\sqrt{r}$, we then have

$$\begin{aligned} \operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;&\le\; \operatorname{dist}(X, \mathbb{S}^{n,r}) + 2\sqrt{r} \\ &\le r^{\frac{1}{4}} \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}} + 2\sqrt{3} r^{\frac{3}{4}} \left(\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}} \right) \\ &\le 5r^{\frac{3}{4}} \left(\|X_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}} \right), \end{aligned} \tag{3.28}$$

where the second inequality applies Lemma 2.4 and (3.27). □

Recently, Theorem 3.10 has been used in [16, 17] to establish error bounds for $\operatorname{dist}(X, \mathbb{S}_+^{n,r})$ for X in the unit ball of spectral norm, i.e., $\{X \in \mathbb{R}^{n\times r} : \|X\| \le 1\}$. See (31) in [16].

3.3 Tightness of the error bounds when $1 < r < n$

The following proposition shows that the bounds presented in Theorems 3.9 and 3.10 are tight up to multiplicative constants when $1 < r < n$, no matter whether X belongs to $\mathbb{S}^{n,r}$, $\mathbb{R}_+^{n\times r}$, or neither of them. Consequently, the error bounds (1.2)–(1.4) cannot hold with $q > 1/2$ when $1 < r < n$.

Proposition 3.11. *Suppose that $1 < r < n$.*

(a) *There exists a sequence $\{X_k\} \subset \mathbb{S}^{n,r} \setminus \mathbb{R}^{n\times r}_+$ such that $(X_k)_- \to 0$ and*

$$\operatorname{dist}(X_k, \mathbb{S}^{n,r}_+) \;\ge\; \frac{1}{\sqrt{2}}\|(X_k)_-\|_{\mathrm{F}}^{\frac{1}{2}}. \tag{3.29}$$

(b) *There exists a sequence $\{X_k\} \subset \mathbb{R}^{n\times r}_+ \setminus \mathbb{S}^{n,r}$ such that $X_k^{\mathsf{T}} X_k \to I_r$ and*

$$\operatorname{dist}(X_k, \mathbb{S}^{n,r}_+) \;\ge\; \frac{1}{\sqrt{2}}\|X_k^{\mathsf{T}} X_k - I_r\|_{\mathrm{F}}^{\frac{1}{2}}. \tag{3.30}$$

(c) *There exists a sequence $\{X_k\} \subset \mathbb{R}^{n\times r} \setminus (\mathbb{R}^{n\times r}_+ \cup \mathbb{S}^{n,r})$ such that $(X_k)_- \to 0$, $X_k^{\mathsf{T}} X_k \to I_r$, and*

$$\operatorname{dist}(X_k, \mathbb{S}^{n,r}_+) \;\ge\; \frac{1}{\sqrt{2}+1}\left(\|(X_k)_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X_k^{\mathsf{T}} X_k - I_r\|_{\mathrm{F}}^{\frac{1}{2}}\right). \tag{3.31}$$

Proof. Take a sequence $\{\varepsilon_k\} \subset (0, 1/2)$ that converges to 0. For each $k \ge 1$, let $X_k \in \mathbb{R}^{n\times r}$ be a matrix such that its first 3 rows are

$$\begin{bmatrix} \varepsilon_k & \varepsilon_k & \overbrace{0 \quad \dots \quad 0}^{r-2} \\ a_k & b_k & 0 \quad \dots \quad 0 \\ c_k & d_k & 0 \quad \dots \quad 0 \end{bmatrix}$$

with a_k, b_k, c_k, d_k being specified later, its 4th to $(r+1)$th rows are the last $r-2$ rows of I_r (if $r \ge 3$), and its other rows are zero (if any). In addition, let $\bar{X}_k$ be a projection of X_k onto $\mathbb{S}^{n,r}_+$. Then the first row of $\bar{X}_k$ contains at most one nonzero entry according to Lemma 2.6. Hence

$$\operatorname{dist}(X_k, \mathbb{S}^{n,r}_+) \;=\; \|X_k - \bar{X}_k\|_{\mathrm{F}} \;\ge\; \varepsilon_k. \tag{3.32}$$

Moreover, it is clear that $(X_k)_- \to 0$ and $X_k^{\mathsf{T}} X_k \to I_r$ if

$$a_k \to 1, \quad b_k \to 0, \quad c_k \to 0, \quad \text{and} \quad d_k \to 1. \tag{3.33}$$

In the sequel, we will configure a_k, b_k, c_k, and d_k subject to (3.33) so that $\{X_k\}$ validates (a), (b), and (c) one by one.

(a) Define

$$a_k \;=\; \sqrt{1-\varepsilon_k^2}, \quad b_k = -\frac{\varepsilon_k^2}{a_k}, \quad c_k = 0, \quad \text{and} \quad d_k = \sqrt{1-\varepsilon_k^2 - b_k^2}.$$

Then $X_k \in \mathbb{S}^{n,r} \setminus \mathbb{R}^{n\times r}_+$. Clearly, $\|(X_k)_-\|_{\mathrm{F}} = \varepsilon_k^2/a_k$. Hence (3.29) holds according to (3.32) and the fact that $a_k \ge \sqrt{1-\varepsilon_k^2} > 1/2$ (recall that $\varepsilon_k < 1/2$).

(b) Define $a_k = d_k = 1$ and $b_k = c_k = 0$. Then $X_k \in \mathbb{R}^{n\times r}_+ \setminus \mathbb{S}^{n,r}$. By straightforward calculations,

$$\|X_k^{\mathsf{T}} X_k - I_r\|_{\mathrm{F}} \;=\; 2\varepsilon_k^2.$$

Thus (3.30) holds according to (3.32).

(c) Define $a_k = d_k = 1$, $b_k = -\varepsilon_k^2$, and $c_k = 0$. Then $X_k \in \mathbb{R}^{n\times r} \setminus (\mathbb{R}_+^{n\times r} \cup \mathbb{S}^{n,r})$. In addition, we can calculate that

$$\|X_k^\mathsf{T} X_k - I_r\|_\mathrm{F} \;=\; \sqrt{\varepsilon_k^4 + (\varepsilon_k^2 + \varepsilon_k^4)^2} \;\le\; \sqrt{\varepsilon_k^4 + \left(\varepsilon_k^2 + \frac{\varepsilon_k^2}{4}\right)^2} \;\le\; 2\varepsilon_k^2$$

and $\|(X_k)_-\|_\mathrm{F} = \varepsilon_k^2$. Therefore, (3.31) holds according to (3.32). $\square$

Theorem 3.12 extends Theorems 3.9 and 3.10, allowing $\|X_-\|_\mathrm{F}$ and $\|\sigma(X) - \mathbf{1}\|_2$ or $\|X^\mathsf{T} X - I_r\|_\mathrm{F}$ to have different exponents in the error bounds. It specifies the precise range of these exponents in local and global error bounds for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ when $1 < r < n$. As we will see from (b) of this theorem and its proof, when $1 < r < n$, the error bound (1.2) can hold if and only if $q \le 1/2$, whereas (1.3) and (1.4) can hold if and only if $q = 1/2$.

Theorem 3.12. *Let q_1 and q_2 be positive constants. Suppose that $1 < r < n$.*

(a) *The function $\rho_1(X) := \|X_-\|_\mathrm{F}^{q_1} + \|\sigma(X) - \mathbf{1}\|_2^{q_2}$ defines a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ if and only if $q_1 \le 1/2$ and $q_2 \le 1/2$, but it cannot define a global error bound no matter what values q_1 and q_2 take.*

(b) *The function $\rho_2(X) := \|X_-\|_\mathrm{F}^{q_1} + \|X^\mathsf{T} X - I_r\|_\mathrm{F}^{q_2}$ defines a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ if and only if $q_1 \le 1/2$ and $q_2 \le 1/2$, and it defines a global error bound if and only if $q_1 \le q_2 = 1/2$.*

Proof. (a) Based on (3.22), it is easy to check that ρ_1 defines a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ if $q_1 \le 1/2$ and $q_2 \le 1/2$. Conversely, if ρ_1 defines a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$, then $q_1 \le 1/2$ and $q_2 \le 1/2$ according to (a) and (b) of Proposition 3.11, respectively.

Now we prove that ρ_1 cannot define a global error bound. According to what has been shown above, we assume that $q_2 \le 1/2$, as a global error bound must be a local one. Consider a sequence $\{X_k\} \subset \mathbb{R}_+^{n\times r}$ with $\|X_k\|_\mathrm{F} \to \infty$. Then $\rho_2(X_k) = \|\sigma(X_k) - \mathbf{1}\|_2^{q_2}$, and hence

$$\frac{\operatorname{dist}(X_k, \mathbb{S}_+^{n,r})}{\rho_1(X_k)} \;\ge\; \frac{\|\sigma(X_k) - \mathbf{1}\|_2}{\|\sigma(X_k) - \mathbf{1}\|_2^{q_2}} \;\to\; \infty.$$

Thus ρ_1 cannot define a global error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$.

(b) Similar to (a), we can show that ρ_2 defines a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ if and only if $q_1 \le 1/2$ and $q_2 \le 1/2$. Hence we only need to consider the global error bound.

Suppose that $q_1 \le q_2 = 1/2$. Let us show that

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;\le\; 5r^{\frac{3}{4}}\left(\|X_-\|_\mathrm{F}^{q_1} + \|X^\mathsf{T} X - I_r\|_\mathrm{F}^{\frac{1}{2}}\right) \;=\; 5r^{\frac{3}{4}}\rho_2(X) \tag{3.34}$$

for all $X \in \mathbb{R}^{n\times r}$. If $\|X_-\|_\mathrm{F} \le 1$, then (3.34) follows from (3.25). When $\|X_-\|_\mathrm{F} > 1$,

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;\le\; \operatorname{dist}(X, \mathbb{S}^{n,r}) + 2\sqrt{r} \;\le\; r^{\frac{1}{4}}\|X^\mathsf{T} X - I_r\|_\mathrm{F}^{\frac{1}{2}} + 2\sqrt{r}\|X_-\|_\mathrm{F}^{q_1} \;\le\; 5r^{\frac{3}{4}}\rho_2(X),$$

where the second inequality applies Lemma 2.4. Hence ρ_2 defines a global error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$.

Now suppose that ρ_2 defines a global error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$. Then it defines a local error bound, implying $q_1 \le 1/2$ and $q_2 \le 1/2$. Similar to the proof for (b) of Theorem 3.5, by considering a sequence $\{X_k\} \subset \mathbb{R}_+^{n\times r}$ such that $X_k^\mathsf{T} X_k = kI_r$ for each $k \ge 1$, we can prove $q_2 \ge 1/2$. The proof is complete. □

Even though the function ρ_1 in Theorem 3.12 can only define a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$, global error bounds can still be established if we add a suitable power of $\|\sigma(X)-\mathbf{1}\|_2$ or $\|X^\mathsf{T} X - I_r\|_\mathrm{F}$ to ρ_1. This will be detailed in Remark 3.14 after we prove the following proposition.

Proposition 3.13. *Let ϕ_1 and ϕ_2 be two nonnegative functions on $\mathbb{R}^{n\times r}$. If there exist positive constants γ_1, γ_2, c_1 and c_2 such that*

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \le \gamma_1\phi_1(X) \quad \textit{when} \quad \phi_1(X) \le c_1, \tag{3.35}$$

$$\operatorname{dist}(X, \mathbb{S}^{n,r}) \le \gamma_2\phi_2(X) \quad \textit{when} \quad \operatorname{dist}(X, \mathbb{S}^{n,r}) \ge c_2. \tag{3.36}$$

Then $\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \le \max\{\gamma_1, \gamma_2, c_1^{-1}(2\sqrt{r}+c_2)\}[\phi_1(X)+\phi_2(X)]$ *for all* $X \in \mathbb{R}^{n\times r}$.

Proof. Fix an $X \in \mathbb{R}^{n\times r}$. We only consider the situation where $\phi_1(X) > c_1$, due to (3.35). Note that

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \le 2\sqrt{r} + \operatorname{dist}(X, \mathbb{S}^{n,r}). \tag{3.37}$$

If $\operatorname{dist}(X, \mathbb{S}^{n,r}) < c_2$, then (3.37) implies that

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \le c_1^{-1}(2\sqrt{r}+c_2)\phi_1(X).$$

If $\operatorname{dist}(X, \mathbb{S}^{n,r}) \ge c_2$, then (3.36) and (3.37) imply that

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \le \max\{2c_1^{-1}\sqrt{r}, \gamma_2\}[\phi_1(X)+\phi_2(X)].$$

The proof is complete. □

Remark 3.14. Suppose that $1 < r < n$, $0 < q_1 \le 1/2$, and $0 < q_2 \le 1/2$. According to Theorem 3.12, Proposition 3.13, and Lemma 2.4, $\rho_1(X) + \|\sigma(X) - \mathbf{1}\|_2^q$ with $q \ge 1$ defines a global error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$. So does $\rho_1(X) + \|X^\mathsf{T} X - I_r\|_\mathrm{F}^q$ with $q \ge 1/2$. However, the powers in ρ_1 cannot be greater than $1/2$ even with the additional terms for the global error bounds. The same can be said about ρ_2.

3.4 Linear regularity of $\mathbb{R}_+^{n\times r}$ and $\mathbb{S}^{n,r}$

Before ending this section, we briefly mention that our analysis enables us to characterize the linear regularity of $\mathbb{R}_+^{n\times r}$ and $\mathbb{S}^{n,r}$ for $r \in \{1,\ldots,n\}$.

A pair of sets $\mathcal{A}_1$ and $\mathcal{A}_2$ in $\mathbb{R}^{n\times r}$ with $\mathcal{A}_1\cap\mathcal{A}_2 \neq \emptyset$ are said to be boundedly linearly regular if for any bounded set $\mathcal{T} \subset \mathbb{R}^{n\times r}$ there exists a constant γ such that

$$\operatorname{dist}(X,\, \mathcal{A}_1 \cap \mathcal{A}_2) \;\le\; \gamma \max\{\operatorname{dist}(X,\, \mathcal{A}_1),\; \operatorname{dist}(X,\, \mathcal{A}_2)\} \tag{3.38}$$

for all $X \in \mathcal{T}$, and they are linearly regular if (3.38) holds for all $X \in \mathbb{R}^{n\times r}$. Linear regularity is a fundamental concept in optimization and is closely related to error bounds. See [21] and [5, Section 8.5] for more details. Note that we can replace the maximum in (3.38) with a summation without essentially changing the definition of (boundedly) linear regularity.

Proposition 3.15 clarifies whether $\mathbb{R}_+^{n\times r}$ and $\mathbb{S}^{n,r}$ are linearly regular.

Proposition 3.15. *The two sets $\mathbb{R}_+^{n\times r}$ and $\mathbb{S}^{n,r}$ are linearly regular if and only if $r = 1$ or $r = n$.*

Proof. Recall that $\operatorname{dist}(X,\, \mathbb{R}_+^{n\times r}) = \|X_-\|_{\mathrm{F}}$ and $\operatorname{dist}(X,\, \mathbb{S}^{n,r}) = \|\sigma(X) - \mathbf{1}\|_2$ for $X \in \mathbb{R}^{n\times r}$. The "if" part of this proposition holds because of the global error bounds in Theorems 3.1 and 3.3. The "only if" part holds because $\|X_-\|_{\mathrm{F}} + \|\sigma(X) - \mathbf{1}\|_2$ does not define a global error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ when $1 < r < n$, as we can see from (a) of Theorem 3.12. ☐

Proposition 3.15 remains true if we change "linearly regular" to "boundedly linearly regular". The "if" part is weakened after this change, and the other part holds because $\|X_-\|_{\mathrm{F}}+\|\sigma(X)-\mathbf{1}\|_2$ does not define a local error bound for $\mathbb{S}_+^{n,r}$ relative to $\mathbb{R}^{n\times r}$ when $1 < r < n$ according to (a) of Theorem 3.12.

4 Error bounds for the sign-constrained Stiefel manifold

This section will establish the error bounds for $\mathbb{S}_S^{n,r}$ based on those already proved for $\mathbb{S}_+^{n,r}$.

4.1 A special case

First, we consider the special case with

$$\mathcal{P} = \{1,\ldots,r_1\} \;\text{ and }\; \mathcal{N} = \emptyset,$$

where $r_1 \in \{1,\ldots,r\}$. Define $r_2 = r - r_1$ henceforth. In this case, $\mathbb{S}_S^{n,r}$ reduces to

$$\mathbb{S}_{r_1,+}^{n,r} \;\coloneqq\; \left\{X = (X_1, X_2) \mid X_1 \in \mathbb{R}_+^{n\times r_1},\; X_2 \in \mathbb{R}^{n\times r_2},\; X^{\mathsf{T}} X = I_r\right\}, \tag{4.1}$$

with $\mathbb{S}_{r_1,+}^{n,r}$ being $\mathbb{S}_+^{n,r}$ if $r_1 = r$.

Note that the results established in Sections 2 and 3 are still valid when r is replaced with r_1 or r_2. In the sequel, we will apply these results directly without restating this fact.

Lemma 4.1. *Suppose that $r_1 < r$. Consider matrices $Y_1 \in \mathbb{R}^{n\times r_1}$ and $Y_2 \in \mathbb{R}^{n\times r_2}$. If $Y_1^\mathsf{T} Y_2 = 0$, then there exists a matrix Z that is a projection of Y_2 onto $\mathbb{S}^{n,r_2}$ and satisfies $Y_1^\mathsf{T} Z = 0$.*

Proof. Define $k = n - \operatorname{rank}(Y_1)$. Take a matrix $V \in \mathbb{S}^{n,k}$ such that range(V) is the orthogonal complement of range(Y_1) in $\mathbb{R}^n$. Since $k \ge r - r_1 = r_2$, the matrix $V^\mathsf{T} Y_2 \in \mathbb{R}^{k\times r_2}$ has a polar decomposition UP with $U \in \mathbb{S}^{k,r_2}$ and $P \in \mathbb{R}^{r_2\times r_2}$, the latter being positive semidefinite. Define $Z = VU \in \mathbb{R}^{n\times r_2}$. Then

$$ZP = VUP = VV^\mathsf{T} Y_2 = Y_2,$$

where the last equality holds because range(Y_2) $\subset$ range(V) according to $Y_1^\mathsf{T} Y_2 = 0$, and VV^T is the orthogonal projection onto range(V). Besides, $Z^\mathsf{T} Z = U^\mathsf{T} V^\mathsf{T} V U = I_{r_2}$. Thus ZP is a polar decomposition of Y_2. Hence Z is a projection of Y_2 onto $\mathbb{S}^{n,r_2}$ by Lemma 2.3. Moreover, $Y_1^\mathsf{T} Z = Y_1^\mathsf{T} V U = 0$. □

Note that $\mathbb{S}^{n,r}_{r_1,+}$ can also be formulated as

$$\mathbb{S}^{n,r}_{r_1,+} \;=\; \Big\{(X_1, X_2) \mid X_1 \in \mathbb{S}^{n,r_1}_+,\; X_2 \in \mathbb{S}^{n,r_2},\; X_1^\mathsf{T} X_2 = 0\Big\}.$$

This formulation motivates us to develop the following lemma, which provides a global error bound for $\mathbb{S}^{n,r}_{r_1,+}$ relative to $\mathbb{R}^{n\times r}$.

Lemma 4.2. *Suppose that $r_1 < r$. For any matrix $X = (X_1, X_2)$ with $X_1 \in \mathbb{R}^{n\times r_1}$ and $X_2 \in \mathbb{R}^{n\times r_2}$, we have*

$$\operatorname{dist}(X, \mathbb{S}^{n,r}_{r_1,+}) \;\le\; (2\|X_2\|_2 + 1) \operatorname{dist}(X_1, \mathbb{S}^{n,r_1}_+) + \operatorname{dist}(X_2, \mathbb{S}^{n,r_2}) + 2\|X_1^\mathsf{T} X_2\|_\mathrm{F}. \tag{4.2}$$

Proof. Let Y_1 be a projection of X_1 onto $\mathbb{S}^{n,r_1}_+$ and $Y_2 = (I_n - Y_1 Y_1^\mathsf{T}) X_2 \in \mathbb{R}^{n\times r_2}$. Then $Y_1^\mathsf{T} Y_2 = 0$. By Lemma 4.1, there exists a matrix Z that is a projection of Y_2 onto $\mathbb{S}^{n,r_2}$ with $Y_1^\mathsf{T} Z = 0$. Define $\bar{X} = (Y_1, Z)$, which lies in $\mathbb{S}^{n,r}_{r_1,+}$. Let us estimate $\|X - \bar{X}\|_\mathrm{F}$. It is clear that

$$\begin{aligned}\|X - \bar{X}\|_\mathrm{F} &\le \|(X_1, X_2) - (Y_1, Y_2)\|_\mathrm{F} + \|(Y_1, Y_2) - (Y_1, Z)\|_\mathrm{F} \\ &\le \|X_1 - Y_1\|_\mathrm{F} + \|X_2 - Y_2\|_\mathrm{F} + \|Y_2 - Z\|_\mathrm{F}.\end{aligned}$$

Since $\|Y_2 - Z\|_\mathrm{F} = \|\sigma(Y_2) - \mathbf{1}\|_2$ (Lemma 2.4) and $\|\sigma(X_2) - \sigma(Y_2)\|_2 \le \|X_2 - Y_2\|_\mathrm{F}$ (Lemma 2.2), it holds that $\|Y_2 - Z\|_\mathrm{F} \le \|\sigma(X_2) - \mathbf{1}\|_2 + \|X_2 - Y_2\|_\mathrm{F}$. Therefore,

$$\|X - \bar{X}\|_\mathrm{F} \;\le\; \|X_1 - Y_1\|_\mathrm{F} + \|\sigma(X_2) - \mathbf{1}\|_2 + 2\|X_2 - Y_2\|_\mathrm{F}. \tag{4.3}$$

Meanwhile, recalling that $Y_2 = (I_n - Y_1 Y_1^\mathsf{T}) X_2$ and $Y_1 \in \mathbb{S}^{n,r_1}$, we have

$$\|X_2 - Y_2\|_\mathrm{F} = \|Y_1 Y_1^\mathsf{T} X_2\|_\mathrm{F} \;=\; \|Y_1^\mathsf{T} X_2\|_\mathrm{F} \;\le\; \|(Y_1 - X_1)^\mathsf{T} X_2\|_\mathrm{F} + \|X_1^\mathsf{T} X_2\|_\mathrm{F}. \tag{4.4}$$

Plugging (4.4) into (4.3) while noting $\|(Y_1 - X_1)^\mathsf{T} X_2\|_\mathrm{F} \le \|X_1 - Y_1\|_\mathrm{F} \|X_2\|_2$, we obtain

$$\|X - \bar{X}\|_\mathrm{F} \;\le\; (2\|X_2\|_2 + 1)\|X_1 - Y_1\|_\mathrm{F} + \|\sigma(X_2) - \mathbf{1}\|_2 + 2\|X_1^\mathsf{T} X_2\|_\mathrm{F}.$$

This implies inequality (4.2), because $\|X_1 - Y_1\|_\mathrm{F} = \operatorname{dist}(X_1, \mathbb{S}^{n,r_1}_+)$ by the definition of Y_1, and $\|\sigma(X_2) - \mathbf{1}\|_2 = \operatorname{dist}(X_2, \mathbb{S}^{n,r_2})$ by Lemma 2.4. □

In light of Lemma 4.2, we can establish error bounds for $\mathbb{S}^{n,r}_{r_1,+}$ using those for $\mathbb{S}^{n,r}_{+}$, as will be done in Propositions 4.3 and 4.4. To this end, it is useful to note for any matrix $X = (X_1, X_2)$ that

$$\|X^{\mathsf T}X - I_r\|_{\mathrm F} \;\ge\; \max\left\{\|X_1^{\mathsf T}X_1 - I_{r_1}\|_{\mathrm F},\; \|X_2^{\mathsf T}X_2 - I_{r_2}\|_{\mathrm F},\; \sqrt{2}\|X_1^{\mathsf T}X_2\|_{\mathrm F}\right\}. \tag{4.5}$$

Proposition 4.3. *For any matrix $X \in \mathbb{R}^{n\times r}$ with x_1 being its first column, we have*

$$\mathrm{dist}(X,\, \mathbb{S}^{n,r}_{1,+}) \;\le\; 7\sqrt{r}\left(\|(x_1)_-\|_2 + \|X^{\mathsf T}X - I_r\|_{\mathrm F}\right). \tag{4.6}$$

Moreover, if $\|X^{\mathsf T}X - I_r\|_{\mathrm F} < 1/3$, then

$$\mathrm{dist}(X,\, \mathbb{S}^{n,r}_{1,+}) \;\le\; 7\left(\|(x_1)_-\|_2 + \|X^{\mathsf T}X - I_r\|_{\mathrm F}\right). \tag{4.7}$$

Proof. If $r = 1$, then (4.6) and (4.7) hold because of Theorem 3.1. Hence we suppose that $r > 1$ in the sequel. We first assume $\|X^{\mathsf T}X - I_r\|_{\mathrm F} < 1/3$ and establish (4.7). Let X_2 be the matrix containing the last $r-1$ columns of X. According to Theorem 3.1 and Lemma 2.4,

$$\mathrm{dist}(x_1,\, \mathbb{S}^{n,1}_{+}) \;\le\; 2\|(x_1)_-\|_2 + \left|x_1^{\mathsf T}x_1 - 1\right|, \tag{4.8}$$

$$\mathrm{dist}(X_2,\, \mathbb{S}^{n,r-1}) \;\le\; \|X_2^{\mathsf T}X_2 - I_{r-1}\|_{\mathrm F}. \tag{4.9}$$

Plugging (4.8) and (4.9) into Lemma 4.2 while noting (4.5), we have

$$\begin{aligned}\mathrm{dist}(X,\, \mathbb{S}^{n,r}_{1,+}) \;&\le\; (2\|X_2\|_2 + 1)\cdot 2\|(x_1)_-\|_2 + \left[(2\|X_2\|_2+1) + 1 + \sqrt{2}\right]\|X^{\mathsf T}X - I_r\|_{\mathrm F}\\ &\le\; 7\left(\|(x_1)_-\|_2 + \|X^{\mathsf T}X - I_r\|_{\mathrm F}\right),\end{aligned}$$

where the second inequality uses the fact that $\|X_2\|_2^2 \le \|X^{\mathsf T}X - I_r\|_2 + 1 \le 4/3$.

To prove (4.6), we now only need to focus on the case with $\|X^{\mathsf T}X - I_r\|_{\mathrm F} \ge 1/3$. In this case,

$$\mathrm{dist}(X, \mathbb{S}^{n,r}_{1,+}) \;\le\; \mathrm{dist}(X, \mathbb{S}^{n,r}) + 2\sqrt{r} \;\le\; \|X^{\mathsf T}X - I_r\|_{\mathrm F} + 6\sqrt{r}\|X^{\mathsf T}X - I_r\|_{\mathrm F},$$

which implies (4.6). The proof is complete. □

Proposition 4.4. *For any matrix $X \in \mathbb{R}^{n\times r}$ with X_1 being its submatrix containing the first r_1 columns, we have*

$$\mathrm{dist}(X,\, \mathbb{S}^{n,r}_{r_1,+}) \;\le\; 15 r^{\frac{3}{4}}\left(\|(X_1)_-\|_{\mathrm F}^{\frac12} + \|X^{\mathsf T}X - I_r\|_{\mathrm F}^{\frac12}\right). \tag{4.10}$$

Moreover, if $\|(X_1)_-\|_{\mathrm F} + \|X^{\mathsf T}X - I_r\|_{\mathrm F} < 1/(3\sqrt{r})$, then

$$\mathrm{dist}(X,\, \mathbb{S}^{n,r}_{r_1,+}) \;\le\; 15\sqrt{r}\left(\|(X_1)_-\|_{\mathrm F}^{\frac12} + \|X^{\mathsf T}X - I_r\|_{\mathrm F}^{\frac12}\right). \tag{4.11}$$

Proof. If $r_1 = r$, then (4.10) and (4.11) hold because of Theorem 3.10. Hence we suppose that $r_1 < r$ in the sequel. We first assume $\|(X_1)_-\|_{\mathrm{F}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}} < 1/(3\sqrt{r})$ and establish (4.11). Let X_2 be the matrix containing the last $r_2 = r - r_1$ columns of X. According to (4.5), our assumption implies

$$\|(X_1)_-\|_{\mathrm{F}} + \|X_1^\mathsf{T} X_1 - I_{r_1}\|_{\mathrm{F}} < \frac{1}{3\sqrt{r_1}}, \quad \|X_2^\mathsf{T} X_2 - I_{r_2}\|_{\mathrm{F}} \le \frac{1}{3}.$$

Hence Theorem 3.10 and Lemma 2.4 yield

$$\mathrm{dist}(X_1, \mathbb{S}_+^{n,r_1}) \le 4\sqrt{r_1}\left(\|(X_1)_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X_1^\mathsf{T} X_1 - I_{r_1}\|_{\mathrm{F}}^{\frac{1}{2}}\right), \tag{4.12}$$

$$\mathrm{dist}(X_2, \mathbb{S}^{n,r_2}) \le \|X_2^\mathsf{T} X_2 - I_{r_2}\|_{\mathrm{F}} \le \frac{1}{\sqrt{3}}\|X_2^\mathsf{T} X_2 - I_{r_2}\|_{\mathrm{F}}^{\frac{1}{2}}. \tag{4.13}$$

In addition, inequality (4.5) and our assumption also provide

$$\|X_1^\mathsf{T} X_2\|_{\mathrm{F}} \le \frac{1}{\sqrt{2}}\|X^\mathsf{T} X - I_r\|_{\mathrm{F}} \le \frac{1}{\sqrt{6}}\|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}}. \tag{4.14}$$

Plugging (4.12)–(4.14) into Lemma 4.2 while noting (4.5), we obtain

$$\begin{aligned}\mathrm{dist}(X, \mathbb{S}_{r_1,+}^{n,r}) &\le \left[4\sqrt{r_1}(2\|X_2\|_2 + 1) + \frac{1}{\sqrt{3}} + \frac{2}{\sqrt{6}}\right]\left(\|(X_1)_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}}\right)\\ &\le 15\sqrt{r}\left(\|(X_1)_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}}\right),\end{aligned}$$

where the second inequality uses the fact that $\|X_2\|_2^2 \le \|X^\mathsf{T} X - I_r\|_2 + 1 \le 4/3$.

Now we prove (4.10). By the same technique as the proof of (3.28), we have

$$\mathrm{dist}(X, \mathbb{S}_{r_1,+}^{n,r}) \le 5r^{\frac{3}{4}}\left(\|(X_1)_-\|_{\mathrm{F}}^{\frac{1}{2}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}}\right)$$

when $\|(X_1)_-\|_{\mathrm{F}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}} \ge 1/(3\sqrt{r})$. Combining this with (4.11), we conclude that (4.10) is valid. The proof is complete. □

4.2 The general case

We now present the error bounds for $\mathbb{S}_S^{n,r}$, detailed in Theorems 4.5–4.7. Theorems 4.5 and 4.6 can be proved using Proposition 4.3 and Theorem 3.3, respectively. We omit the proofs because they are essentially the same as that of Theorem 4.7 below.

Theorem 4.5. *Suppose that $|\mathcal{P}| + |\mathcal{N}| = 1$. For any matrix $X \in \mathbb{R}^{n\times r}$, we have*

$$\mathrm{dist}(X, \mathbb{S}_S^{n,r}) \le 7\sqrt{r}\left(\|(S\circ X)_-\|_{\mathrm{F}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}\right).$$

Moreover, if $\|X^\mathsf{T} X - I_r\|_{\mathrm{F}} < 1/3$, then

$$\mathrm{dist}(X, \mathbb{S}_S^{n,r}) \le 7\left(\|(S\circ X)_-\|_{\mathrm{F}} + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}\right).$$

Theorem 4.6. *Suppose that $|\mathcal{P}|+|\mathcal{N}|=n$. For any matrix $X\in\mathbb{R}^{n\times n}$, we have*

$$\operatorname{dist}(X,\,\mathbb{S}_S^{n,n}) \;\le\; 9n\,(\|(S\circ X)_-\|_{\mathrm{F}}+\|\sigma(X)-\mathbf{1}\|_2)\,.$$

Moreover, if $\|(S\circ X)_-\|_{\mathrm{F}}+\|\sigma(X)-\mathbf{1}\|_2<1/(4\sqrt{n})$, then

$$\operatorname{dist}(X,\,\mathbb{S}_S^{n,n}) \;\le\; 8\sqrt{n}\,(\|(S\circ X)_-\|_{\mathrm{F}}+\|\sigma(X)-\mathbf{1}\|_2)\,.$$

Theorem 4.7. *For any matrix $X\in\mathbb{R}^{n\times r}$, we have*

$$\operatorname{dist}(X,\,\mathbb{S}_S^{n,r}) \;\le\; 15r^{\frac{3}{4}}\left(\|(S\circ X)_-\|_{\mathrm{F}}^{\frac{1}{2}}+\|X^\mathsf{T}X-I_r\|_{\mathrm{F}}^{\frac{1}{2}}\right). \tag{4.15}$$

Moreover, if $\|(S\circ X)_-\|_{\mathrm{F}}+\|X^\mathsf{T}X-I_r\|_{\mathrm{F}}<1/(3\sqrt{r})$, then

$$\operatorname{dist}(X,\,\mathbb{S}_S^{n,r}) \;\le\; 15\sqrt{r}\left(\|(S\circ X)_-\|_{\mathrm{F}}^{\frac{1}{2}}+\|X^\mathsf{T}X-I_r\|_{\mathrm{F}}^{\frac{1}{2}}\right). \tag{4.16}$$

Proof. Let $\mathcal{Q}=\{1,\ldots,r\}\setminus(\mathcal{P}\cup\mathcal{N})$. With $M_{\mathcal{P}}$, $M_{\mathcal{N}}$, and $M_{\mathcal{Q}}$ being the submatrices of I_r containing the columns indexed by $\mathcal{P}$, $\mathcal{N}$, and $\mathcal{Q}$, respectively, we take the permutation matrix

$$\Pi \;=\; (M_{\mathcal{P}},\; M_{\mathcal{N}},\; M_{\mathcal{Q}}) \;\in\; \mathbb{R}^{r\times r}.$$

In addition, we take the diagonal matrix $D\in\mathbb{R}^{r\times r}$ with $D_{j,j}=-1$ if $j\in\mathcal{N}$ and $D_{j,j}=1$ otherwise. Define $r_1=|\mathcal{P}|+|\mathcal{N}|$. If $r_1=0$, then (4.15) and (4.16) hold because of Lemma 2.4. Hence we suppose that $r_1\ge 1$ in the sequel.

Consider any matrix $X\in\mathbb{R}^{n\times r}$. Let $Y=XD\Pi$, and $\bar{Y}$ be the projection of Y onto $\mathbb{S}_{r_1,+}^{n,r}$ defined in (4.1). Set $\bar{X}=\bar{Y}\Pi^\mathsf{T}D$, which lies in $\mathbb{S}_S^{n,r}$. Then

$$\operatorname{dist}(X,\,\mathbb{S}_S^{n,r}) \;\le\; \|X-\bar{X}\|_{\mathrm{F}} \;=\; \|Y\Pi^\mathsf{T}D-\bar{Y}\Pi^\mathsf{T}D\|_{\mathrm{F}} \;=\; \|Y-\bar{Y}\|_{\mathrm{F}}.$$

Invoking Proposition 4.4, we have

$$\|Y-\bar{Y}\|_{\mathrm{F}} \;\le\; 15r^{\frac{3}{4}}\left(\|(Y_1)_-\|_{\mathrm{F}}^{\frac{1}{2}}+\|Y^\mathsf{T}Y-I_r\|_{\mathrm{F}}^{\frac{1}{2}}\right),$$

where Y_1 is the submatrix of Y containing the first r_1 columns. It is straightforward to verify that $\|(Y_1)_-\|_{\mathrm{F}}=\|(S\circ X)_-\|_{\mathrm{F}}$ and $\|Y^\mathsf{T}Y-I_r\|_{\mathrm{F}}=\|X^\mathsf{T}X-I_r\|_{\mathrm{F}}$. Hence we obtain (4.15). The bound (4.16) can be established in a similar way. □

5 Exact penalties for optimization on the nonnegative Stiefel manifold

In this section, as an application of the error bounds established in this paper, we consider exact penalties for optimization problem (1.5). For simplicity, we will focus on the special case with

$$\mathbb{S}_S^{n,r}=\mathbb{S}_+^{n,r},$$

applying the bounds in Section 3. Essentially the same results can be established in the general case by exploiting the bounds in Section 4. The exact penalty results only require (local) Lipschitz continuity of F, and hence can be applied to nonsmooth optimization, for example, F involving a group sparse regularization term [27].

The exactness of penalty methods for problem (1.5) with $\mathbb{S}^{n,r}_S = \mathbb{S}^{n,r}_+$ has been studied in [12, 24]. In [12], an error bound is established for $\mathbb{S}^{n,r}_+$ relative to the set

$$\{X \in \mathbb{R}^{n\times r}_+ : (X^\mathsf{T} X)_{j,j} = 1,\ j = 1, \dots, r\},$$

and then the bound is used to analyze a penalty method. However, the error bound in [12] cannot be used to derive the values of ν and q in (1.2)–(1.4). In [24], the authors consider the penalty problem (1.6) with $q = 1$, and show this problem has the same global minimizers as problem (1.5) if each global optimal solution of (1.5) has no zero rows. Our exact penalty results only need the Lipschitz continuity of the objective function F in (1.5).

The error bounds (1.2)–(1.4) established in this paper enable us to have the exactness of the penalized problem

$$\min\left\{F(X) + \mu\left(\|X_-\|^{q_1}_{\ell_p} + \|X^\mathsf{T} X - I_r\|^{q_2}_{\ell_p}\right) : X \in \mathcal{S}\right\} \tag{5.1}$$

for solving (1.5) with $\mathbb{S}^{n,r}_S = \mathbb{S}^{n,r}_+$ only under the (local) Lipschitz continuity of function F. Here the set $\mathcal{S} \subset \mathbb{R}^{n\times r}$ is a set that contains $\mathbb{S}^{n,r}_+$, while the parameters μ, p, q_1, and q_2 are all positive. If $p = 2$ and $q_1 = q_2 = q$, then the penalized problem (5.1) reduces to problems (1.6) and (1.7) when $\mathcal{S}$ equals $\mathbb{S}^{n,r}$ and $\mathbb{R}^{n\times r}_+$, respectively.

During the revision of this paper, a very recent work [17] studied another exact penalty problem for (1.5) with $\mathbb{S}^{n,r}_S = \mathbb{S}^{n,r}_+$ based on an error bound for $\mathbb{S}^{n,r}_+$ relative to the set

$$\{X \in \mathbb{R}^{n\times r}_+ : (X^\mathsf{T} X)_{j,j} \le 1,\ j = 1, \dots, r\}. \tag{5.2}$$

Since our error bounds for $\mathbb{S}^{n,r}_+$ are established relative to $\mathbb{R}^{n\times r}$, we allow the feasible set of our penalty problem to be any set $\mathcal{S}$ containing $\mathbb{S}^{n,r}_+$, whereas the feasible set in [17] can only be the set (5.2). In addition, with the error bounds established in Section 4, our results can be readily extended to the case where $\mathbb{S}^{n,r}_S$ is a sign-constrained Stiefel manifold other than $\mathbb{S}^{n,r}_+$, which is not considered in [17].

Due to the equivalence between norms, it is indeed possible to establish the exactness of (5.1) when the entry-wise ℓ_p-norm is changed to other ones. We choose to use the entry-wise ℓ_p-norm in (5.1) because it is easy to evaluate.

5.1 Exactness for Lipschitz continuous objective functions

Theorem 5.1 presents the exactness of problem (5.1) regarding global optimizers when the objective function $F : \mathcal{S} \to \mathbb{R}$ is an L-Lipschitz continuous function, namely

$$|F(X) - F(Y)| \;\le\; L\|X - Y\|_{\mathrm{F}} \tag{5.3}$$

for all X and Y in $\mathcal{S}$, where $L \in (0, \infty)$ is a Lipschitz constant of F with respect to the Frobenius norm. Note that the global Lipschitz continuity of the objective function F is assumed on a set $\mathcal{S}$ containing $\mathbb{S}_+^{n,r}$. For example, if $F(X) = \operatorname{trace}(X^\mathsf{T} A^\mathsf{T} AX)$ and $\mathcal{S} = \{X \in \mathbb{R}^{n\times r} : \|X\|_{\mathrm{F}} \le \gamma\}$ with $\gamma > \sqrt{r}$, then the global Lipschitz continuity of F holds on $\mathcal{S}$ with the Lipschitz constant $L = 2\gamma\|A\|_2^2$. Indeed, our theory holds even if F is undefined out of $\mathcal{S}$. The proof of Theorem 5.1 is standard and we include it in Appendix A for completeness.

Theorem 5.1 (Exact penalty (5.1) with F being Lipschitz continuous)**.** *Suppose that $\mathcal{S} \subset \mathbb{R}^{n\times r}$ is a set containing $\mathbb{S}_+^{n,r}$, $F : \mathcal{S} \to \mathbb{R}$ is an L-Lipschitz function, and $p \ge 1$ is a constant. If $0 < q \le 1/2$ and $\mu > 5Lr^{\frac{3}{4}} \max\left\{1,\, (nr)^{\frac{p-2}{4p}}\right\}$, then*

$$\operatorname{Argmin}\{F(X) : X \in \mathbb{S}_+^{n,r}\} = \operatorname{Argmin}\left\{F(X) + \mu\big(\|X_-\|_{\ell_p}^q + \|X^\mathsf{T} X - I_r\|_{\ell_p}^{\frac{1}{2}}\big) : X \in \mathcal{S}\right\}.$$

Theorem 5.2 presents the exactness of problem (5.1) regarding local minimizers when F is locally Lipschitz continuous on $\mathcal{S}$, meaning that for any $\bar{X} \in \mathcal{S}$ there exists a constant $L \in (0, \infty)$ such that (5.3) holds for all X and Y in a certain neighborhood of $\bar{X}$ in $\mathcal{S}$. We will refer to this L as a Lipschitz constant of F around $\bar{X}$. The proof of Theorem 5.2 is also given in Appendix A.

Theorem 5.2 (Exact penalty (5.1) with F being locally Lipschitz continuous)**.** *Let $\mathcal{S} \subset \mathbb{R}^{n\times r}$ be a set containing $\mathbb{S}_+^{n,r}$, $F : \mathcal{S} \to \mathbb{R}$ be a locally Lipschitz continuous function, and $p \ge 1$ be a constant. Suppose that $0 < q_1 \le 1/2$ and $0 < q_2 \le 1/2$. For any local minimizer X^* of F on $\mathbb{S}_+^{n,r}$, X^* is also a local minimizer of*

$$\min\left\{F(X) + \mu(\|X_-\|_{\ell_p}^{q_1} + \|X^\mathsf{T} X - I_r\|_{\ell_p}^{q_2}) : X \in \mathcal{S}\right\} \tag{5.4}$$

for all $\mu > 4L^*\sqrt{r}\max\left\{1,\, (nr)^{\frac{q_1(p-2)}{2p}},\, r^{\frac{q_2(p-2)}{p}}\right\}$, where L^* is a Lipschitz constant of F around X^*. Conversely, if X^* lies in $\mathbb{S}_+^{n,r}$ and there exists a constant μ such that X^* is a local minimizer of (5.4), then X^* is also a local minimizer of F on $\mathbb{S}_+^{n,r}$.

Suppose that $p \le 2$. It is noteworthy that the thresholds for μ in Theorems 5.1 and 5.2 are independent of n (even the dependence on r is mild). This is favorable in practice, as r can be much smaller than n in applications. We also note that the second part of Theorem 5.2 requires $X^* \in \mathbb{S}_+^{n,r}$. This is indispensable without additional assumptions on the problem structure (see [5, Remark 9.1.1]).

5.2 The exponents in the penalty term

When $1 < r < n$, the requirements on the exponents of $\|X_-\|_{\mathrm{F}}$ and $\|X^{\mathsf{T}}X - I_r\|_{\mathrm{F}}$ in Theorems 5.1 and 5.2 cannot be relaxed. This is elaborated in Proposition 5.3, with $\mathcal{S} = \mathbb{R}^{n\times r}$ being an example. Similar results can be proved for $\mathcal{S} = \mathbb{S}^{n,r}$ and $\mathcal{S} = \mathbb{R}^{n\times r}_+$.

Proposition 5.3. *Suppose that $1 < r < n$, $p \ge 1$, $q_1 > 0$, and $q_2 > 0$. Define the function $\rho(X) = \|X_-\|_{\ell_p}^{q_1} + \|X^{\mathsf{T}}X - I_r\|_{\ell_p}^{q_2}$ for $X \in \mathbb{R}^{n\times r}$. There exists a Lipschitz continuous function $F : \mathbb{R}^{n\times r} \to \mathbb{R}$ such that the following statements hold.*

(a) $\operatorname{Argmin}\{F(X) : X \in \mathbb{S}^{n,r}_+\} = \mathbb{S}^{n,r}_+$.

(b) *If $q_1 > 1/2$ or $q_2 \ne 1/2$, then any $X^* \in \mathbb{S}^{n,r}_+$ is not a global minimizer of $F + \mu\rho$ on $\mathbb{R}^{n\times r}$ for any $\mu > 0$.*

(c) *If $q_1 > 1/2$ or $q_2 > 1/2$, then there exists an $X^* \in \mathbb{S}^{n,r}_+$ that is not a local minimizer of $F + \mu\rho$ on $\mathbb{R}^{n\times r}$ for any $\mu > 0$.*

Proof. Define

$$F(X) \;=\; -\operatorname{dist}(X, \mathbb{S}^{n,r}_+) \quad \text{for} \quad X \in \mathbb{R}^{n\times r}.$$

Then F is Lipschitz continuous on $\mathbb{R}^{n\times r}$. We will justify (a)–(c) one by one.

(a) This holds because F takes a constant value 0 on $\mathbb{S}^{n,r}_+$.

(b) Assume for contradiction that there exists an $X^* \in \mathbb{S}^{n,r}_+$ such that X^* is a global minimizer of $F + \mu^*\rho$ on $\mathbb{R}^{n\times r}$ for a certain $\mu^* > 0$. Then

$$F(X) + \mu^*\rho(X) \;\ge\; F(X^*) + \mu^*\rho(X^*) \;=\; 0 \quad \text{for all} \quad X \in \mathbb{R}^{n\times r}.$$

By the definition of F, we then have $\operatorname{dist}(X, \mathbb{S}^{n,r}_+) \le \mu^*\rho(X)$ for all $X \in \mathbb{R}^{n\times r}$. Hence ρ defines a global error bound for $\mathbb{S}^{n,r}_+$ relative to $\mathbb{R}^{n\times r}$, contradicting (b) of Theorem 3.12 (note that $\|\cdot\|_{\ell_p}$ and $\|\cdot\|_{\mathrm{F}}$ are equivalent norms).

(c) According to (b) of Theorem 3.12, the function ρ does not define a local error bound for $\mathbb{S}^{n,r}_+$ relative to $\mathbb{R}^{n\times r}$. Thus there is a sequence $\{X_k\} \subset \mathbb{R}^{n\times r}$ such that

$$\|(X_k)_-\|_{\mathrm{F}} + \|X_k^{\mathsf{T}}X_k - I_r\|_{\mathrm{F}} \;\le\; k^{-1}, \tag{5.5}$$

$$\operatorname{dist}(X_k, \mathbb{S}^{n,r}_+) \;>\; k\rho(X_k) \tag{5.6}$$

for each $k \ge 1$. According to (5.5), $\|X_k^{\mathsf{T}}X_k\|_{\mathrm{F}} \le \sqrt{r} + k^{-1}$. Thus $\{X_k\}$ has a subsequence $\{X_{k_\ell}\}$ that converges to a certain point X^*. Using (5.5) again, we have $\|X^*_-\|_{\mathrm{F}} + \|(X^*)^{\mathsf{T}}X^* - I_r\|_{\mathrm{F}} = 0$, and hence $X^* \in \mathbb{S}^{n,r}_+$. It remains to show that X^* is not a local minimizer of $F + \mu\rho$ for any $\mu > 0$. Assume for contradiction that X^* is such a local minimizer for a certain $\mu^* > 0$. Then for all sufficiently large ℓ,

$$F(X_{k_\ell}) + \mu^*\rho(X_{k_\ell}) \;\ge\; F(X^*) + \mu^*\rho(X^*) \;=\; 0.$$

By the definition of F, we then have $\operatorname{dist}(X_{k_\ell}, \mathbb{S}^{n,r}_+) \le \mu^*\rho(X_{k_\ell})$, contradicting (5.6). The proof is complete. □

When $r = 1$ or $r = n$, since the exponents of $\|X_-\|_{\mathrm{F}}$ and $\|X^\top X - I_r\|_{\mathrm{F}}$ in the error bounds can be increased from 1/2 to 1, their exponents in the penalty term of (5.1) can be taken from a larger range while keeping the exactness of (5.1). This is briefly summarized in Remark 5.4.

Remark 5.4. Suppose that $r = 1$ or $r = n$. If F is Lipschitz continuous on $\mathcal{S}$, then we can establish a result similar to Theorem 5.1 for $0 < q_1 \leq 1$ and $1/2 \leq q_2 \leq 1$ based on the error bound (3.11). When F is only locally Lipschitz continuous, similar to Theorem 5.2, the exactness of problem (5.1) regarding local minimizers can be established if $0 < q_1 \leq 1$ and $0 < q_2 \leq 1$. Proposition 5.3 can also be adapted to the case of $r = 1$ or $r = n$. It is also worth noting that $\mathbb{S}_+^{n,n}$ is precisely the set of $n \times n$ permutation matrices, and hence $\min\{F(X) : X \in \mathbb{S}_+^{n,n}\}$ represents optimization problems over permutation matrices.

6 Penalty methods for (1.5)

When $\mathbb{S}_S^{n,r} = \mathbb{S}_+^{n,r}$, problem (1.5) reduces to the nonnegative orthogonal constrained optimization problem

$$\min_{X \in \mathbb{S}_+^{n,r}} F(X). \tag{6.1}$$

Many papers use penalty methods for problem (6.1) with penalty functions $\|\cdot\|_{\mathrm{F}}^2$, $\|\cdot\|_{\mathrm{F}}$ or $\|.\|_{\ell_1}$ of X_- or $X^\top X - I_r$, e.g., [1, 18, 28, 30]. However, there is not a satisfactory answer in existing literature whether the penalty problem using $\|\cdot\|_{\mathrm{F}}^2$, $\|.\|_{\mathrm{F}}$ or $\|\cdot\|_{\ell_1}$ is an exact penalty regarding local and global minimizers of problem (6.1) for a Lipschitz continuous objective function.

In 2024, the authors of [24] proved that the penalty problem

$$\min_{X \in \mathbb{S}^{n,r}} F(X) + \mu\|X_-\|_{\ell_1} \tag{6.2}$$

is a global exact penalty for problem (6.1) under the assumption that any global minimizer has no zero rows and F satisfies a second-order calmness condition in a neighborhood of any global minimizer of (6.1). Moreover, they aimed to show that such strong assumption cannot be removed by Example 3.9 in [24], which is as follows

$$\min_{X \in \mathbb{S}_+^{3,2}} f(X) := -2X_{1,1} - 2X_{2,2} - X_{3,1} - X_{3,2}. \tag{6.3}$$

The authors of [24] claimed $X^* = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}^\top$ is a global minimizer of (6.3), but is not a solution of the penalty problem

$$\min_{X \in \mathbb{S}^{3,2}} f(X) + \mu\|X_-\|_{\ell_1}$$

for any $\mu > 0$. However, X^* is not a global minimizer of (6.3), as $f(X^*) = -4 > -\sqrt{5}-2 = f(\hat{X})$, where $\hat{X} = \begin{bmatrix} 2/\sqrt{5} & 0 & 1/\sqrt{5} \\ 0 & 1 & 0 \end{bmatrix}^\top$. Thus the claim with this example in [24] is wrong.

In this paper, we give a warning for the penalty problem (6.2) in the case where the objective function is only Lipschitz continuous. From Proposition 5.3, we know that there is a Lipschitz continuous function F such that any global (local) minimizer of (6.1) is not a global (local) minimizer of (6.2) for any $\mu > 0$. On the other hand, from Theorem 5.1 and Theorem 5.2, we know that

$$\min_{X \in \mathbb{S}^{n,r}} F(X) + \mu \|X_-\|_{\ell_1}^q$$

is an exact penalty problem for (6.1) regarding global and local minimizers for $\mu > 5Lr^{\frac{3}{4}}$ and $q \in (0, 1/2]$, where L is a Lipschitz constant of F. Our results provide theoretical warning and guarantee for penalty methods of nonnegative orthogonal constrained optimization problem (6.1).

Note that Remark 5.4 can be extended to the case $|\mathcal{P}| + |\mathcal{N}| = 1$ or $|\mathcal{P}| + |\mathcal{N}| = n$. In particular, the penalty problem

$$\min_{X \in \mathbb{S}^{n,r}} F(X) + \mu \|(S \circ X)_-\|_{\ell_1}$$

is an exact penalty problem of (1.5) with $S_{i,1} = 1$ and $S_{i,j} = 0$, for $j \neq 1, i = 1, \ldots, n$.

Consider the following sparse trace maximization problem [4]

$$\min_{X \in \mathbb{S}^{n,r}} -\text{tr}(X^\top A^\top AX) + \lambda \|X\|_{\ell_1}, \tag{6.4}$$

where $A \in \mathbb{R}^{m \times n}$ is a given matrix. If $A^\top A$ is a positive or an irreducible nonnegative matrix, then by the Perron-Frobenius theorem, the largest eigenvalue of $A^\top A$ is positive and the corresponding eigenvector is positive. Hence, for a dense nonnegative data matrix A, it is interesting to consider

$$\min_{X \in \mathbb{S}_S^{n,r}} -\text{tr}(X^\top A^\top AX) + \lambda \|T \circ X\|_{\ell_1}, \tag{6.5}$$

with $S_{i,1} = 1$, $S_{i,j} = 0$, $T_{i,1} = 0, T_{i,j} = 1$, for $j \neq 1, i = 1, \ldots, n$. Since the objective function of (6.5) is Lipschitz continuous with Lipschitz constant $L = 2\|A\|_2^2 + r\lambda\sqrt{n}$ over $\mathbb{S}^{n,r}$, our results show that

$$\min_{X \in \mathbb{S}^{n,r}} -\text{tr}(X^\top A^\top AX) + \lambda \|T \circ X\|_{\ell_1} + \mu \|(S \circ X)_-\|_{\ell_1} \tag{6.6}$$

is an exact penalty problem of (6.5) with $\mu > 5Lr^{\frac{3}{4}}$.

In [4], Chen et. al proposed a ManPG (Manifold Proximal Gradient) algorithm to solve the following nonsmooth optimization problem

$$\min_{X \in \mathbb{S}^{n,r}} F(X) := f(X) + \rho(X),$$

where f is smooth, ∇f is Lipschitz continuous and ρ is nonsmooth, convex and Lipschitz continuous. The objective functions in problem (6.4) and problem (6.6) satisfy these conditions. Numerical results in [4] show that ManPG outperforms some existing algorithms for solving problem (6.4). We compare the two models (6.4) and (6.6) for sparse trace maximization problem by using the code of [4] downloaded from `https://github.com/chenshixiang/ManPG`, with the same initial points that are randomly generated by the code. Other algorithms for solving nonsmooth matrix optimization over $\mathbb{S}^{n,r}$ can be found in [32] and its references. Moreover, we can also replace the orthogonal constraint by adding a penalty term $\|X^\top X - I_r\|_{\ell_1}$ to (6.6).

6.1 Synthetic simulations

For given m, n, we randomly generated 20 nonnegative matrices and then normalized the columns by Matlab functions as follows

$$A = \text{rand}(m, n), \quad A = \text{normc}(A).$$

For each randomly generated matrix A, we use ManPG to find an approximate solution $\hat{X}$ of (6.4) and (6.6), respectively. The reconstructed matrix and its relative reconstruction error (RRE) and percentage of explained variance (PEV) [31] by using $\hat{X}$ are defined by

$$\hat{A} = A\hat{X}(\hat{X}^\top \hat{X})^{-1}\hat{X}^\top, \quad \text{RRE} = \frac{\|A - \hat{A}\|_\text{F}}{\|A\|_\text{F}}, \quad \text{PEV} = \frac{\text{tr}(\hat{A}^\top \hat{A})}{\text{tr}(A^\top A)}(\times 100\%). \tag{6.7}$$

In Table 2 and Table 3, we report the average values of RRE and PEV of $\hat{A}$ by using the randomly generated 20 nonnegative matrices A for each m and n to compare models (6.4) and (6.6) with $r = 10$. All computed solutions $\hat{X}$ for calculating RRE and PEV in Table 2 and Table 3, satisfy

$$\|\hat{X}^\top \hat{X} - I_r\|_\text{F} \le 10^{-14} \quad \text{and} \quad \|\hat{X}^\top \hat{X} - I_r\|_\text{F} + \|(S \circ \hat{X})_-\|_{\ell_1} \le 10^{-14},$$

for model (6.4) and model (6.6), respectively.

$m = 40,\ n = 30$							
λ, μ	$0.6, 150$	$0.6, 170$	$0.6, 190$	$0.6, 200$	$1, 100$	$1,\ 110$	$1,\ 130$
model (6.4)	0.4029	0.4029	0.4029	0.4029	0.4046	0.4046	0.4046
model (6.6)	0.3999	0.3992	0.3988	0.3953	0.4029	0.4008	0.3981
$\lambda = 0.6,\ \mu = 100$							
m, n	$50, 25$	$50, 50$	$80, 25$	$80, 40$	$80, 80$	$200,\ 25$	$200,\ 50$
model (6.4)	0.3811	0.4427	0.3846	0.4315	0.4652	0.3860	0.4464
model (6.6)	0.3806	0.4409	0.3843	0.4284	0.4636	0.3847	0.4451

Table 2: Comparison on RRE with different (m, n, λ, μ) by randomly generated A

$m = 40,\ n = 30$							
λ, μ	$0.6, 150$	$0.6, 170$	$0.6, 190$	$0.6, 200$	$1, 100$	$1,\ 110$	$1,\ 130$
model (6.4)	0.8376	0.8376	0.8376	0.8376	0.8363	0.8363	0.8363
model (6.6)	0.8400	0.8406	0.8410	0.8410	0.8376	0.8391	0.8404
$\lambda = 0.6,\ \mu = 100$							
m, n	$50, 25$	$50, 50$	$80, 25$	$80, 40$	$80, 80$	$200, 25$	$200, 50$
model (6.4)	0.8547	0.8040	0.8520	0.8138	0.7836	0.8510	0.8007
model (6.6)	0.8551	0.8055	0.8523	0.8164	0.7850	0.8520	0.8019

Table 3: Comparison on PEV with different (m, n, λ, μ) by randomly generated A

6.2 Numerical results using Yale face dataset

The Yale Face dataset contains 165 GIF format gray scale images of 15 individuals with 11 images for each subject, and one for each different facial expression or configuration. From `http://www.cad.zju.edu.cn/home/dengcai/Data/FaceData.html`, we download the 165×1024 facial image matrix F_{ace}. The $(15 \times (i-1) + t)$th row of F_{ace} is the tth image of the ith person, with $i = 1, \ldots, 15$ and $t = 1, \ldots, 11$. Each row of F_{ace} defines a 32×32 nonnegative matrix. We use the first 55 rows of F_{ace}, which include 11 images of each of the first five persons, to get 55 32×32 nonnegative matrices and then use Matlab function `normc` to normalize each of these matrices.

For each 32×32 matrix A, we use ManPG to find an approximate solution $\hat{X}$ of (6.4) and (6.6), respectively. We compute the reconstructed matrix $\hat{A}$ and its RRE and PEV by using computed $\hat{X}$ as (6.7).

From Table 2, Table 3 and Figure 1, we can see that in almost every case, the reconstructed matrix $\hat{A}$ by model (6.6) has lower values RRE and higher values PEV than that computed by model (6.4). In our numerical experiments, we only restricted the power of the penalty term to be one, but did not restrict the penalty parameter $\mu > 5Lr^{\frac{3}{4}}$.

7 Conclusions

We present the error bounds (1.2)–(1.4) with explicit values of ν and q in Theorems 3.1, 3.3 and 3.10 for $\mathbb{S}_S^{n,r} = \mathbb{S}_+^{n,r}$. Furthermore, we show that these error bounds cannot hold with $q > 1/2$ when $1 < r < n$ in Proposition 3.11, and point out that they cannot hold with $q > 1$ for any $r \in \{1, \ldots, n\}$ in Remark 3.4. In Section 4 we present the error bounds (1.2)–(1.4) with explicit values of ν and q in Theorems 4.5–4.7 for the sign-constrained Stiefel manifold. The exponent q in the error bounds is $1/2$ for any $r \in \{1, \ldots, n\}$ and can take the value 1 for $|\mathcal{P}| + |\mathcal{N}| \in \{1, n\}$. The new error bounds help us to establish the exactness of penalty problems (1.6)–(1.8) for problem (1.5). Compared with existing results on error bounds for the set $\mathbb{S}_+^{n,r}$ and penalty methods for minimization with nonnegative orthogonality constraints, our

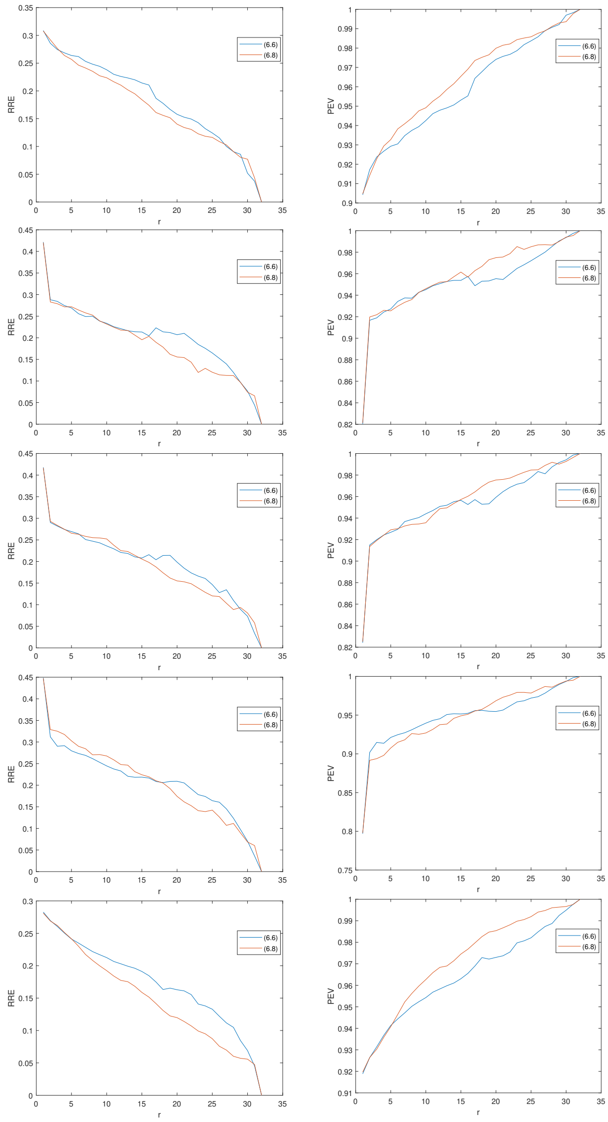

Figure 1: Row i ($i = 1, \ldots, 5$) shows average values of RRE and PEV of the reconstructed matrix $\hat{A}$ using 11 images for the ith person by models (6.4) with $\lambda = 1$ and (6.6) with $\lambda = 1, \mu = 6$, respectively, for $r = 1, \ldots, 32$.

results have explicit values of the error bound parameters and penalty parameters, and do not need any condition other than the (local) Lipschitz continuity of the objective function for the exact penalty. Moreover, exponents in our error bounds are independent of the dimension of the underlying space.

A Appendix. Proofs of Theorems 5.1 and 5.2

We first present the following lemma on a simple inequality between the entry-wise ℓ_p-norm and the Frobenius norm. Its proof is elementary and hence omitted.

Lemma A.1. *For any $X \in \mathbb{R}^{n\times r}$ and any $p \geq 1$,*

$$\|X\|_{\mathrm{F}} \;\leq\; \max\left\{1,\; (nr)^{\frac{p-2}{2p}}\right\} \|X\|_{\ell_p}.$$

The proofs of Theorems 5.1 and 5.2 are as follows.

Proof of Theorem 5.1. Define the function $\rho(X) = \|X_-\|_{\ell_p}^q + \|X^\mathsf{T} X - I_r\|_{\ell_p}^{\frac{1}{2}}$ for $X \in \mathcal{S}$, and set $\nu = 5r^{\frac{3}{4}} \max\left\{1,\, (nr)^{\frac{p-2}{4p}}\right\}$. By (3.34) and Lemma A.1, we have

$$\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;\leq\; 5r^{\frac{3}{4}} \left(\|X_-\|_{\mathrm{F}}^q + \|X^\mathsf{T} X - I_r\|_{\mathrm{F}}^{\frac{1}{2}}\right) \;\leq\; \nu\rho(X) \quad \text{for} \quad X \in \mathcal{S}.$$

For any $X \in \mathcal{S}$, setting $\bar{X}$ to a projection of X onto $\mathbb{S}_+^{n,r}$, and combining the L-Lipschitz continuity of F with the above error bound, we have

$$F(\bar{X}) \;\leq\; F(X) + L\operatorname{dist}(X, \mathbb{S}_+^{n,r}) \;\leq\; F(X) + \mu\rho(X).$$

This implies that

$$\inf\{F(X) : X \in \mathbb{S}_+^{n,r}\} \;\leq\; \inf\{F(X) + \mu\rho(X) : X \in \mathcal{S}\}.$$

Meanwhile, $\inf\{F(X) : X \in \mathbb{S}_+^{n,r}\} \;\geq\; \inf\{F(X) + \mu\rho(X) : X \in \mathcal{S}\}$ as ρ is zero on $\mathbb{S}_+^{n,r} \subset \mathcal{S}$. Thus

$$\inf\{F(X) : X \in \mathbb{S}_+^{n,r}\} \;=\; \inf\{F(X) + \mu\rho(X) : X \in \mathcal{S}\}. \tag{A.1}$$

For any $X^* \in \operatorname{Argmin}\{F(X) : X \in \mathbb{S}_+^{n,r}\}$, we have $\rho(X^*) = 0$ and

$$F(X^*) + \mu\rho(X^*) \;=\; F(X^*) \;=\; \inf\{F(X) : X \in \mathbb{S}_+^{n,r}\},$$

which together with (A.1) ensures $X^* \in \operatorname{Argmin}\{F(X) + \mu\rho(X) : X \in \mathcal{S}\}$.

Now take any $X^* \in \operatorname{Argmin}\{F(X) + \mu\rho(X) : X \in \mathcal{S}\}$, and let $\bar{X}^*$ be a projection of X^* onto $\mathbb{S}_+^{n,r}$. Then we have

$$F(X^*) + \mu\rho(X^*) \;\leq\; F(\bar{X}^*) + \mu\rho(\bar{X}^*) \;=\; F(\bar{X}^*) \;\leq\; F(X^*) + \nu L\rho(X^*).$$

This leads to $\rho(X^*) = 0$, as $\mu > \nu L$ and $\rho(X^*) \geq 0$. Hence X^* lies in $\mathbb{S}_+^{n,r}$, and

$$F(X^*) \;=\; F(X^*) + \mu\rho(X^*) \;=\; \inf\{F(X) + \mu\rho(X) : x \in \mathcal{S}\},$$

which implies that $X^* \in \operatorname{Argmin}\{F(X) : X \in \mathbb{S}_+^{n,r}\}$ with the help of (A.1). We complete the proof. $\square$

Proof of Theorem 5.2. Define the function $\rho(X) = \|X_-\|_{\ell_p}^{q_1} + \|X^\mathsf{T} X - I_r\|_{\ell_p}^{q_2}$ for $X \in \mathcal{S}$, and set $\nu = 4\sqrt{r}\max\left\{1,\, (nr)^{\frac{q_1(p-2)}{2p}},\, r^{\frac{q_2(p-2)}{p}}\right\}$. For any $X \in \mathbb{S}_+^{n,r}$ and $Y \in \mathcal{S}$ with $\|Y - X\|_\mathrm{F} < 1/(6\sqrt{r})$, we have

$$\|Y_-\|_\mathrm{F} + \|\sigma(Y) - \mathbf{1}\|_2 \;\leq\; \|Y - X\|_\mathrm{F} + \|\sigma(Y) - \sigma(X)\|_2 \;\leq\; 2\|Y - X\|_\mathrm{F} \;<\; \frac{1}{3\sqrt{r}},$$

where the first inequality is because $X_- = 0$ and $\sigma(X) - \mathbf{1} = 0$, while the second invokes Lemma 2.2. Hence (3.26) and Lemma A.1 yield

$$\begin{aligned}
&\operatorname{dist}(Y, \mathbb{S}_+^{n,r}) \\
&\leq 4\sqrt{r}\left(\|Y_-\|_\mathrm{F}^{q_1} + \|Y^\mathsf{T} Y - I_r\|_\mathrm{F}^{q_2}\right) \\
&\leq 4\sqrt{r}\left(\max\left\{1,\, (nr)^{\frac{q_1(p-2)}{2p}}\right\}\|Y_-\|_{\ell_p}^{q_1} + \max\left\{1,\, (r^2)^{\frac{q_2(p-2)}{2p}}\right\}\|Y^\mathsf{T} Y - I_r\|_{\ell_p}^{q_2}\right) \\
&\leq \nu\rho(Y).
\end{aligned}$$

Given a local minimizer X^* of F on $\mathbb{S}_+^{n,r}$, there exists a $\delta \in (0, 1/(3\sqrt{r}))$ such that X^* is a global minimizer of F on $\mathbb{S}_+^{n,r} \cap \mathcal{B}(X^*, \delta)$ and F is L^*-Lipschitz continuous in the same set.

It suffices to demonstrate that X^* is a global minimizer of $F + \mu\rho$ on $\mathcal{S} \cap \mathcal{B}(X^*, \delta/2)$ for all $\mu > \nu L^*$. Take any point $Y \in \mathcal{S} \cap \mathcal{B}(X^*, \delta/2)$, let $\bar{Y}$ be a projection of Y onto $\mathbb{S}_+^{n,r}$, and note that $\bar{Y}$ lies in $\mathcal{B}(X^*, \delta)$, which is because

$$\|\bar{Y} - X^*\|_\mathrm{F} \;\leq\; \|\bar{Y} - Y\|_\mathrm{F} + \|Y - X^*\|_\mathrm{F} \;\leq\; \|X^* - Y\|_\mathrm{F} + \|Y - X^*\|_\mathrm{F} \;<\; \delta.$$

Then, using the fact that $\rho(X^*) = 0$, we have

$$F(X^*) + \mu\rho(X^*) = F(X^*) \leq F(\bar{Y}) \leq F(Y) + L^* \operatorname{dist}(Y, \mathbb{S}_+^{n,r}) \leq F(Y) + \mu\rho(Y),$$

which is what we desire.

If X^* is a local minimizer of $F + \mu\rho$ on $\mathcal{S}$, and X^* happens to lie in $\mathbb{S}_+^{n,r}$, then

$$F(X^*) \;=\; F(X^*) + \mu\rho(X^*) \;\leq\; F(Y) + \mu\rho(Y) \;=\; F(Y)$$

for any Y that is close to X^* and located in $\mathbb{S}_+^{n,r} \subset \mathcal{S}$. Hence X^* is also a local minimizer of F on $\mathbb{S}_+^{n,r}$. We complete the proof. $\square$

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