
A Framework of Constraint Preserving Update Schemes for Optimization on Stiefel Manifold

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Abstract This paper considers optimization problems on the Stiefel manifold $X^T X = I_p$, where $X \in \mathbb{R}^{n \times p}$ is the variable and I_p is the p -by- p identity matrix. A framework of constraint preserving update schemes is proposed by decomposing each feasible point into the range space of X and the null space of X^T . While this general framework can unify many existing schemes, a new update scheme with low complexity cost is also discovered. Then we study a feasible Barzilai-Borwein-like method under the new update scheme. The global convergence of the method is established with an adaptive nonmonotone line search. The numerical tests on the nearest low-rank correlation matrix problem, the Kohn-Sham total energy minimization and a specific problem from statistics demonstrate the efficiency of the new method. In particular, the new method performs remarkably well for the nearest low-rank correlation matrix problem in terms of speed and solution quality and is considerably competitive with the widely used SCF iteration for the Kohn-Sham total energy minimization.

Keywords Stiefel manifold · orthogonality constraint · sphere constraint · range space · null space · Barzilai-Borwein-like method · feasible · global convergence · adaptive nonmonotone line search · low-rank correlation matrix · Kohn-Sham total energy minimization · heterogeneous quadratic functions

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1 Introduction

In this paper, we consider general feasible methods for optimization on the Stiefel manifold,

$$\min_{X \in \mathbb{R}^{n \times p}} \mathcal{F}(X), \quad \text{s.t. } X^T X = I_p, \quad (1.1)$$

where I_p is the p -by- p identity matrix and $\mathcal{F}(X): \mathbb{R}^{n \times p} \rightarrow \mathbb{R}$ is a differentiable function. The feasible set $\mathcal{S}_{n,p} := \{X \in \mathbb{R}^{n \times p} : X^T X = I_p\}$ is referred to as the Stiefel manifold, which was due to Stiefel in 1935 [48].

Problem (1.1) captures many applications, for instance, nearest low-rank correlation matrix problem [25, 38, 44], linear eigenvalue problem [23, 45], Kohn-Sham total energy minimization [53], orthogonal Procrustes problem [19, 47], maximization of sums of heterogeneous quadratic functions from statistics [9, 40], sparse principal component analysis [16, 30, 58], leakage interference minimization [33, 37], joint diagonalization (blind source separation) [29, 50] and determining a minimal set of localized orbitals from

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atomic chemistry [10]. For other applications, we refer interested readers to [18, 52] and the references therein. In general, problem (1.1) is difficult to solve due to the nonconvexity of the orthogonality constraint. In fact, some of the above examples, including the maxcut problem and the leakage interference minimization [33], are NP-hard.

With the wide applicability and fundamental difficulty, problem (1.1) has attracted many researchers. Based on the geometric structure, Rapcsák [40, 41] reformulated it as a smooth nonlinear program by introducing a new coordinate representation. From the point of view of manifold, some authors proposed a variety of feasible algorithms to solve problem (1.1). These algorithms include steepest descent methods [1, 3, 34, 35], Barzilai-Borwein (BB) method [52], conjugate gradient methods [2, 3, 18], trust region methods [3, 55], Newton methods [3, 18], quasi-Newton methods [46] and subspace methods [54]. Unlike the unconstrained case, it is not trivial to keep the whole iterations in the Stiefel manifold and the concept of retraction has played an important role (see [4, Theorem 15] and [3, Definition 4.1.1] for a detailed description on retractions). Simply speaking, the retraction defines an update scheme which preserves the orthogonality constraint. The existing update schemes employed by the aforementioned methods are some specific choices of retractions. They can be classified into two types: geodesic-like and projection-like update schemes. Briefly speaking, geodesic-like update schemes preserve the constraint by moving a point along the geodesic or quasi-geodesic while projection-like update schemes do so by (approximately) projecting a point into the constraint. We will delve into the details of these update schemes in §2.1.

In this paper, we firstly develop a framework of constraint preserving update schemes based on a novel idea; *i.e.*, decomposing each feasible point into the range space of X and the null space of X^\top . This framework can not only unify most existing schemes including a kind of geodesic, gradient projection, Manton's projection, polar decomposition, QR factorization and Wen-Yin update schemes (they will be mentioned in §2.1), but also leads to the discovery of a new scheme with low complexity cost.

Secondly, under the new update scheme, we look for a suitable descent feasible curve along which the objective function can achieve a certain decrease by taking a suitable stepsize. Then the original problem can be treated as an unconstrained optimization problem. We consider to combine the efficient BB method [7] with our new update scheme. To ensure the global convergence, we adopt the adaptive nonmonotone line search [11], leading to an adaptive feasible Barzilai-Borwein-like (AFBB) method for problem (1.1). Note that certain feasible BB-like method with a different nonmonotone line search was first studied in [52], but the convergence issue was not discussed there. We prove the global convergence of the AFBB method in the numerical sense under some mild assumptions. Although our update scheme is also a retraction, the convergence of retraction-based line search methods in [3] cannot be applied to our methods. To the best of our knowledge, this is the first global convergence result for feasible methods with nonmonotone line search for optimization on the Stiefel manifold. Furthermore, our convergence analysis can also be extended to feasible BB-like methods based on monotone or some other nonmonotone Armijo-type line search techniques.

Thirdly, we extend the proposed update scheme and algorithm to deal with optimization with multiple generalized orthogonality constraints:

$$\min_{X_1 \in \mathbb{C}^{n_1 \times p_1}, \dots, X_q \in \mathbb{C}^{n_q \times p_q}} \mathcal{F}(X_1, \dots, X_q), \quad \text{s.t.} \quad X_1^* H_1 X_1 = K_1, \dots, X_q^* H_q X_q = K_q, \quad (1.2)$$

where $H_1 \in \mathbb{R}^{n_1 \times n_1}, \dots, H_q \in \mathbb{R}^{n_q \times n_q}$ are symmetric positive semidefinite matrices, and $K_1 \in \mathbb{R}^{p_1 \times p_1}, \dots, K_q \in \mathbb{R}^{p_q \times p_q}$ are symmetric positive definite matrices. Note that problem (1.1) is a special case of problem (1.2).

Finally, to demonstrate the efficiency of the proposed method, we apply the new method to a variety of problems. For the nearest low-rank correlation matrix problem, our new method performs remarkably well in terms of speed and solution quality. We also modify the new method to deal with the extra fixed constraints for the nearest low-rank correlation matrix problem through the augmented Lagrangian function. The preliminary numerical results show the potential of the new method to handle some more general constraints beyond the sphere constraints. For the Kohn-Sham total energy minimization problem arising in electronic structure calculations, the new method is considerably competitive with the widely used SCF iteration.

The rest of this paper is organized as follows. In §2, we review the existing update schemes and give the first-order optimality condition of problem (1.1). In §3, we introduce our framework of constraint preserving update schemes and propose a new update scheme. Some properties of the new update scheme and

comparisons with existing update schemes are also stated in this section. We present the AFBB method in §4.1, establish its global convergence in §4.2 and then discuss how to deal with the cumulative feasibility error during the iterations in §4.3. The AFBB method is also extended to more general problems in §5. Some numerical tests on an extensive collection of problems are presented to demonstrate the efficiency of our AFBB method in §6. Finally, conclusions are drawn in the last section.

Notation: For matrix $M \in \mathbb{R}^{n \times n}$, we define $\text{sym}(M) = (M + M^\top)/2$. The maximal and minimal eigenvalues of M are denoted by $\lambda_{\max}(M)$ and $\lambda_{\min}(M)$, respectively. We use $\text{diag}(M)$ to stand for the vector formed by the diagonal entries of M . Meanwhile, we use $\text{Diag}(\theta_1, \dots, \theta_n)$ to represent the diagonal matrix whose diagonal entries are $\theta_1, \dots, \theta_n$. The set of n -by- n symmetric matrices is denoted by \mathcal{S}^n . For $S \in \mathcal{S}^n$, if S is positive semidefinite (positive definite), we mark $S \succeq 0$ ($S \succ 0$). The Euclidean inner product of two matrices $A, B \in \mathbb{R}^{m \times n}$ is defined as $\langle A, B \rangle = \text{tr}(A^\top B)$, where $\text{tr}(\cdot)$ is the trace operator. We denote by $A_{(i)}$ the i -th column of A . The decomposition $A = \text{qr}(A)\text{upp}(A)$ is the unique QR factorization with $\text{qr}(A) \in \mathbb{R}^{n \times p}$ being a matrix with orthonormal columns and $\text{upp}(A) \in \mathbb{R}^{p \times p}$ an upper triangular matrix with positive diagonal entries. The condition number of A is defined as $\text{cond}(A) = \left(\frac{\lambda_{\max}(A^\top A)}{\lambda_{\min}(A^\top A)}\right)^{1/2}$. Denote by e_i the i -th unit vector of an appropriate size. For $X \in \mathcal{S}_{n,p}$, we define $P_X = I_n - \frac{1}{2}XX^\top$. The gradient of \mathcal{F} with respect to X is $G := \mathcal{D}\mathcal{F}(X) = \left(\frac{\partial \mathcal{F}(X)}{\partial X_{ij}}\right)$, whereas the gradient in the tangent space is denoted by $\nabla \mathcal{F}$.

2 Preliminaries

2.1 Overview of existing update schemes

Given any tangent direction $D \in \mathbb{R}^{n \times p}$ satisfying $X^\top D + D^\top X = 0$ with $X \in \mathcal{S}_{n,p}$, we briefly review the geodesic-like and projection-like update schemes. Note that the parameter $\tau \geq 0$ in the following update schemes is some stepsize.

Geodesic-like update schemes. In 1998, Edelman *et al.* [18] proposed a computable geodesic update scheme, in which the iterations lie in the curve defined by

$$Y_{\text{geol}}(\tau; X) = [X, Q] \exp\left(\tau \begin{bmatrix} -X^\top D & -R^\top \\ R & 0 \end{bmatrix}\right) \begin{bmatrix} I_p \\ 0 \end{bmatrix}, \quad (2.1)$$

where $QR = -(I_n - XX^\top)D$ is the unique QR factorization of $-(I_n - XX^\top)D$. This strategy requires computing the exponential of a $2p$ -by- $2p$ matrix and the QR factorization of an n -by- p matrix at each iteration. Consequently, the flops will be high when $p \geq n/2$. Another geodesic approach is proposed by Abrudan *et al.* [1]. Given an n -by- n skew-symmetric matrix A_1 , they considered the curve $Y_{\text{geo2}}(\tau) = \exp(-\tau A_1)X$. Comparing with (2.1), this formula can efficiently deal with the case when $p \geq n/2$. Nevertheless, it still requires great efforts to compute the exponential of an n -by- n matrix. To avoid computing exponentials of matrices, Nishimori and Akaho [35] proposed a kind of quasi-geodesic approach. Given an n -by- n skew-symmetric matrix A_2 , a special case of their update schemes is the Cayley transformation scheme

$$Y_{\text{qgc}}(\tau; X) = \left(I_n - \frac{\tau}{2}A_2\right)^{-1} \left(I_n + \frac{\tau}{2}A_2\right)X. \quad (2.2)$$

The computation cost for (2.2) is $O(n^3)$. This is considerably high even for small p . In 2010, by some clever derivations, Wen and Yin [52] developed a simple and efficient constraint preserving update scheme, known as the Crank-Nicholson-like update scheme. This scheme is equivalent to the Cayley transformation update scheme. Their update scheme is described as follows:

$$Y_{\text{wy}}(\tau; X) = X - \tau U \left(I_{2p} + \frac{\tau}{2}V^\top U\right)^{-1} V^\top X, \quad (2.3)$$

where $U = [P_X D, X]$, $V = [X, -P_X D] \in \mathbb{R}^{n \times 2p}$. For convenience, we call it Wen-Yin update scheme throughout this paper. Formula (2.3) has the lowest computation complexity per iteration among the existing geodesic-like approaches when $p < n/2$. However, when $p \geq n/2$, the cost is still expensive. To deal with this case, a low-rank update scheme is explored in [52]. They were also the first to combine the feasible update scheme with the nonmonotone curvilinear search for optimization with orthogonality constraints.

Projection-like update schemes. In spite of the nonconvexity of the Stiefel manifold, it is possible to preserve the constraint by the projection. The projection of a rank p matrix $C \in \mathbb{R}^{n \times p}$ onto $\mathcal{S}_{n,p}$ is defined as the unique solution of

$$\min_{X \in \mathbb{R}^{n \times p}} \|X - C\|_F, \quad \text{s.t. } X^\top X = I_p, \quad (2.4)$$

where $\|\cdot\|_F$ is the Frobenius norm. For any symmetric positive definite matrix $B \in \mathbb{R}^{p \times p}$, denote by $B^{1/2}$ the unique *square root* of B . It is easy to see that the solution of (2.4) is $\mathcal{P}_{\mathcal{S}_{n,p}}(C) = C(C^\top C)^{-1/2}$. Then we can extend the gradient projection method for optimization with convex constraints for solving (1.1), yielding the update scheme

$$Y_{\text{gp}}(\tau; X) = \mathcal{P}_{\mathcal{S}_{n,p}}(X - \tau G). \quad (2.5)$$

In fact, the famous power method [23] for the extreme eigenvalue problem of symmetric matrix is a special case of this gradient projection update scheme. Manton [34] considered another different projection scheme

$$Y_{\text{mp}}(\tau; X) = \mathcal{P}_{\mathcal{S}_{n,p}}(X - \tau D).$$

Absil *et al.* [3] proposed the polar decomposition

$$Y_{\text{pd}}(\tau; X) = (X - \tau D)(I_p + \tau^2 D^\top D)^{-1/2}. \quad (2.6)$$

The polar decomposition is equivalent to Manton's projection update scheme, but has lower complexity cost¹. It is then mainly considered in this paper. It is worth noting that the QR factorization update scheme

$$Y_{\text{qr}}(\tau; X) = \text{qr}(X - \tau D) \quad (2.7)$$

proposed in [3] can be regarded as an approximation to the polar decomposition update scheme.

2.2 First-order optimality condition

To begin with, we introduce some basic concepts related to the Stiefel manifold as in [18]. For any $X \in \mathcal{S}_{n,p}$, define the tangent space at X as $\mathcal{T}_X := \{\Delta : X^\top \Delta + \Delta^\top X = 0\}$. There are two different metrics on \mathcal{T}_X . The first one is the *Euclidean metric* $d_e(\Delta, \Delta) = \langle \Delta, \Delta \rangle$, which is independent of the point X . The second one is the *canonical metric* $d_c(\Delta, \Delta) = \langle \Delta, P_X \Delta \rangle$, which is related to X . Then the projection of any $Z \in \mathbb{R}^{n \times p}$ onto the tangent space \mathcal{T}_X under the Euclidean or canonical metric is $\mathcal{P}_{\mathcal{T}}(Z) = Z - X \text{sym}(X^\top Z)$.

The gradient $\nabla \mathcal{F} \in \mathcal{T}_X$ of a differential function $\mathcal{F}(X) : \mathbb{R}^{n \times p} \rightarrow \mathbb{R}$ on the Stiefel manifold is defined such that

$$\langle G, \Delta \rangle = d_c(\nabla \mathcal{F}, \Delta) \equiv \langle \nabla \mathcal{F}, P_X \Delta \rangle \quad (2.8)$$

for all tangent vectors Δ at X . Solving (2.8) for $\nabla \mathcal{F}$ such that $X^\top \nabla \mathcal{F}$ is skew-symmetric yields

$$\nabla \mathcal{F} = G - X G^\top X.$$

Notice that $\nabla \mathcal{F}$ is not the projection of G onto the tangent space at X . The latter should be $G - X \text{sym}(X^\top G)$.

We now give the first-order optimality condition without proof. It is analogous to Lemma 2.1 in [52].

Lemma 2.1 (First-order optimality condition) *Suppose X is a local minimizer of problem (1.1). Then X satisfies the first-order optimality condition*

$$\mathcal{D}_X \mathcal{L}(X, \Lambda) = G - X G^\top X = 0;$$

i.e., $\nabla \mathcal{F} = 0$, with the associated Lagrange multiplier $\Lambda = G^\top X$. Besides, $\nabla \mathcal{F} = 0$ if and only if

$$G - X(2\rho G^\top X + (1 - 2\rho)X^\top G) = 0, \quad \text{for any } \rho > 0.$$

¹ In [34], Manton used the SVD decomposition of $X - \tau D$ to obtain the projection, and the cost is higher than that of the polar decomposition.

3 Constraint Preserving update schemes

For a feasible point $X \in \mathcal{S}_{n,p}$, denote $\mathcal{R}_X = \{XR : R \in \mathbb{R}^{p \times p}\}$ and $\mathcal{N}_X = \{W \in \mathbb{R}^{n \times p} : X^\top W = 0\}$ to be the range space of X and the null space of X^\top , respectively. It is well known that the two spaces are orthogonal to each other and their sum forms the whole space $\mathbb{R}^{n \times p}$. As a result, any point in $\mathbb{R}^{n \times p}$ can uniquely be decomposed into the sum of two points, which belong to the two spaces, respectively. With this observation, we introduce our idea for a framework of constraint preserving update schemes for problem (1.1).

Given a matrix W in the null space \mathcal{N}_X , consider the following curve

$$Y(\tau; X) = XR(\tau) + WN(\tau), \quad (3.1)$$

where $R(\tau), N(\tau) \in \mathbb{R}^{p \times p}$ and $\tau \geq 0$ is some parameter. In other words, this curve can be divided into two parts; *i.e.*, $XR(\tau)$ in the range space of X and $WN(\tau)$ in the null space of X^\top . Our goal is to determine appropriate $R(\tau)$ and $N(\tau)$ such that the curve $Y(\tau; X)$ is still feasible; *i.e.*, $Y^\top Y = I_p$ (notice that if there is no confusion, we will write $Y(\tau; X)$ as $Y(\tau)$ or even simply Y , *etc.*). If we assume that $R(\tau) = \tilde{R}(\tau)Z(\tau)$ and $N(\tau) = \tilde{N}(\tau)Z(\tau)$, where $Z(\tau)$ is always invertible, the curve (3.1) can be expressed by

$$Y(\tau; X) = \left(X\tilde{R}(\tau) + W\tilde{N}(\tau) \right) Z(\tau). \quad (3.2)$$

The condition that $Y^\top Y = I_p$ requires

$$Z(\tau)^\top \left(\tilde{R}(\tau)^\top \tilde{R}(\tau) + \tilde{N}(\tau)^\top W^\top W \tilde{N}(\tau) \right) Z(\tau) = I_p,$$

or, equivalently,

$$Z(\tau)^{-\top} Z(\tau)^{-1} = \tilde{R}(\tau)^\top \tilde{R}(\tau) + \tilde{N}(\tau)^\top W^\top W \tilde{N}(\tau). \quad (3.3)$$

Once W , $\tilde{R}(\tau)$ and $\tilde{N}(\tau)$ have been determined in some way, $Z(\tau)$ can be calculated by (3.3). Then $R(\tau)$, $N(\tau)$ and hence the whole curve $Y(\tau; X)$ will be given.

Now we focus on the choices of W , $\tilde{R}(\tau)$ and $\tilde{N}(\tau)$. As $Y(\tau; X)$ with $\tau \geq 0$ is a curve starting from the current iteration X , it is natural to impose that $Y(0; X) = X$. To meet this condition, by (3.2), we may ask

$$\tilde{R}(0) = I_p, \quad \tilde{N}(0) = 0, \quad Z(0) = I_p. \quad (3.4)$$

With these choices, we further have by (3.2) that

$$Y'(0; X) = X \left(\tilde{R}'(0) + Z'(0) \right) + W\tilde{N}'(0). \quad (3.5)$$

Assume that some matrix E is chosen, which is intended for $-Y'(0; X)$; *i.e.*, $E = -Y'(0; X)$. Then (3.5) holds if

$$W = -(I_n - XX^\top)E, \quad \tilde{R}'(0) + Z'(0) = -X^\top E, \quad \tilde{N}'(0) = I_p. \quad (3.6)$$

In the following, we consider three approaches of choosing $\tilde{R}(\tau)$, $\tilde{N}(\tau)$ and $Z(\tau)$ such that (3.3) holds.

Approach I. Consider the simple case that $Z(\tau) \equiv I_p$. This, with the second equation in (3.6), indicates that $\tilde{R}'(0) = -X^\top E$. Denoting $\mathcal{A}(\tau) = \begin{bmatrix} \tilde{R}(\tau) \\ W\tilde{N}(\tau) \end{bmatrix}$, we know from (3.4) and (3.6) that

$$\mathcal{A}'(0) = \begin{bmatrix} -X^\top E & B \\ W & F \end{bmatrix} \begin{bmatrix} I_p \\ 0 \end{bmatrix} \quad \text{and} \quad \mathcal{A}(0) = \begin{bmatrix} I_p \\ 0 \end{bmatrix},$$

where $B \in \mathbb{R}^{n \times p}$, $F \in \mathbb{R}^{p \times p}$. Solving the above ordinary differential equations, we get that

$$\mathcal{A}(\tau) = \exp \left(\tau \begin{bmatrix} -X^\top E & B \\ W & F \end{bmatrix} \right) \begin{bmatrix} I_p \\ 0 \end{bmatrix}. \quad (3.7)$$

Since $Z(\tau) \equiv I_p$, we know from (3.3) and the definition of $\mathcal{A}(\tau)$ that

$$Y(\tau) = [X, I_p] \mathcal{A}(\tau),$$

and $\mathcal{A}(\tau)^\top \mathcal{A}(\tau) = I_p$. It follows that the matrix inside the brackets of (3.7) will be skew-symmetric. This means that $B = -W^\top$, $F + F^\top = 0$ and $X^\top E + E^\top X = 0$ (*i.e.*, $E \in \mathcal{T}_X$). Let $W = QR$ be the unique QR

factorization of W and assume that F takes the form $F = Q\tilde{F}Q^\top$, where $\tilde{F} \in \mathbb{R}^{p \times p}$ is any skew-symmetric matrix. Then we can write

$$\begin{aligned} Y(\tau) &= [X, I_p] \exp \left(\tau \begin{bmatrix} I_p & 0 \\ 0 & Q \end{bmatrix} \begin{bmatrix} -X^\top E & -R^\top \\ R & \tilde{F} \end{bmatrix} \begin{bmatrix} I_p & 0 \\ 0 & Q^\top \end{bmatrix} \right) \begin{bmatrix} I_p \\ 0 \end{bmatrix} \\ &= [X, Q] \exp \left(\tau \begin{bmatrix} -X^\top E & -R^\top \\ R & \tilde{F} \end{bmatrix} \right) \begin{bmatrix} I_p \\ 0 \end{bmatrix}, \end{aligned} \quad (3.8)$$

where the second equality is due that Q has orthonormal columns. The update scheme (3.8) can be regarded as a generalized geodesic update scheme, since letting $\tilde{F} = 0$, (3.8) reduces to the geodesic update scheme (2.1).

In the next two approaches, to satisfy the conditions $\tilde{N}(0) = 0$ and $\tilde{N}'(0) = I_p$, we choose

$$\tilde{N}(\tau) = \tau I_p. \quad (3.9)$$

Noticing that $\frac{\partial Z(\tau)^{-1}}{\partial \tau} = -Z(\tau)^{-1}Z'(\tau)Z(\tau)^{-1}$ and using (3.3) and (3.9), we can get that

$$Z'(0)^\top + Z'(0) = -\left(\tilde{R}'(0)^\top + \tilde{R}'(0)\right).$$

This, with the second condition in (3.6), means that $X^\top E$ must be a skew-symmetric matrix; *i.e.*, $E \in \mathcal{T}_X$.

Approach II. To meet (3.3) and $\tilde{R}(0) = I_p$, we consider to choose

$$\tilde{R}(\tau) = I_p + \tau \tilde{R}'(0). \quad (3.10)$$

Since $\tilde{N}(\tau) = \tau I_p$, we can get $Z(\tau)$ from (3.3) by the polar decomposition or the Cholesky factorization.

If by the polar decomposition, $Z(\tau)$ and $Z'(\tau)$ are always symmetric. In this case, it is easy to show that $Y(\tau; X) = \mathcal{P}_{\mathcal{S}_{n,p}}(X\tilde{R}(\tau) + W\tilde{N}(\tau))$, which with (3.6), (3.9) and (3.10) further implies that

$$Y(\tau; X) = \mathcal{P}_{\mathcal{S}_{n,p}}(X - \tau E - \tau XZ'(0)), \quad (3.11)$$

where $Z'(0)$ is any p -by- p symmetric matrix. If $Z'(0) = 0$, (3.11) reduces to the ordinary polar decomposition or Manton's projection update scheme. If $Z'(0) = \text{sym}(X^\top G)$ and $E = G - X\text{sym}(X^\top G)$, it becomes the ordinary gradient projection update scheme.

If by the Cholesky factorization, $Z(\tau)$ and $Z'(\tau)$ are always upper triangular. Similarly, we can derive

$$Y(\tau; X) = \text{qr}(X - \tau E - \tau XZ'(0)), \quad (3.12)$$

where $Z'(0)$ is any p -by- p upper triangular matrix. When $Z'(0) = 0$, (3.12) reduces to the ordinary QR factorization update scheme.

Approach III. In this approach, we regard $\tilde{R}(\tau)$ as some function of $Z(\tau)$. To solve (3.3) easily, we may assume

$$\tilde{R}(\tau) = 2I_p - Z(\tau)^{-1}. \quad (3.13)$$

Substituting (3.9) and (3.13) into (3.3) leads to

$$Z(\tau)^{-\top} + Z(\tau)^{-1} = 2I_p + \frac{\tau^2}{2}W^\top W.$$

Consequently, $Z(\tau)$ must be of the form

$$Z(\tau) = \left(I_p + \frac{\tau^2}{4}W^\top W + L(\tau) \right)^{-1}, \quad (3.14)$$

where $L(\tau)$ is any p -by- p skew-symmetric matrix with $L(0) = 0$. Notice that the above inverse always exists since $L(\tau)$ is skew-symmetric. The relations (3.13) and (3.14) indicate that $\tilde{R}'(0) = Z'(0) = -L'(0)$. Further, by the second relation in (3.6), we must have that $L'(0) = \frac{1}{2}X^\top E$. Thus we can choose

$$L(\tau) = g(\tau)X^\top E,$$

where $g(\tau)$ is any function satisfying $g(0) = 0$ and $g'(0) = 1/2$. For simplicity, we choose $g(\tau) = \tau/2$. See §4.2 and §6.4 for more choices of $g(\tau)$.

To sum up, given any matrix $E \in \mathcal{T}_X$, we can define the following update scheme

$$\begin{cases} W = -(I_n - XX^\top)E, \\ J(\tau) = I_p + \frac{\tau^2}{4}W^\top W + \frac{\tau}{2}X^\top E, \\ Y(\tau; X) = (2X + \tau W)J(\tau)^{-1} - X. \end{cases} \quad (3.15)$$

Some geometrical meanings of the above scheme will be discussed in the paragraph before Lemma 3.3.

A few remarks on the framework and the direction E are made here. Firstly, it follows from (3.8), (3.11) and (3.12) that the framework can unify the famous geodesic, gradient projection, polar decomposition and QR factorization update schemes. Meanwhile, it can yield generalized geodesic, polar decomposition or QR factorization update scheme by choosing different \tilde{F} or $Z'(0)$. We will mainly consider the new update scheme (3.15) in the remainder of this paper. Secondly, like unconstrained optimization, many possible choices for E , for instance, the gradient descent, conjugate gradient, or quasi-Newton direction, can be used under the update scheme (3.15). However, we focus on the gradient descent direction in §3.1 due to its simplicity.

3.1 Choice of E

In this subsection, we consider to seek an appropriate E such that the update scheme $Y(\tau; X)$ given by (3.15) defines a descent curve.

Lemma 3.1 *For any feasible point $X \in \mathcal{S}_{n,p}$, consider the curve given by (3.15), where $E = D_\rho$ and*

$$D_\rho = (I_n - (1 - 2\rho)XX^\top)\nabla\mathcal{F} = G - X(2\rho G^\top X + (1 - 2\rho)X^\top G), \quad \rho > 0. \quad (3.16)$$

Then the following properties hold:

- (i) $Y(\tau)^\top Y(\tau) = I_p$;
- (ii) $Y'(0) = -D_\rho$ is a descent direction and

$$\mathcal{F}'_\tau(Y(0)) := \left. \frac{\partial \mathcal{F}(Y(\tau))}{\partial \tau} \right|_{\tau=0} \leq -\min\{\rho, 1\} \|\nabla\mathcal{F}\|_{\mathbb{F}}^2;$$

- (iii) for any $\tau > 0$ and any p -by- p orthogonal matrix Q_p , we have $YQ_p \neq X$;
- (iv) $\text{cond}(J) \leq (5 + v^2)/4$, where $v = \tau \|D_\rho\|_{\mathbb{F}}$.

In particular, if $p = n$, $Y(\tau) = X(2J^{-1} - I_n)$ and $J = I_n + \frac{\tau}{2}X^\top E$; if $p = 1$, the matrices X, Y, G reduce to the vectors x, y, g , respectively, and the update scheme becomes

$$y(\tau) = \left(\frac{2 + \tau x^\top g}{1 + \frac{\tau^2}{4}(g^\top g - (x^\top g)^2)} - 1 \right) x - \frac{\tau}{1 + \frac{\tau^2}{4}(g^\top g - (x^\top g)^2)} g.$$

Proof The fact that $X^\top D_\rho$ is skew-symmetric implies that J is invertible, thus $Y(\tau)$ is well-defined. (i) follows from the construction of the update scheme (3.15).

Meanwhile, we know that $Y'(0) = -D_\rho$, which with the chain rule shows that

$$\mathcal{F}'_\tau(Y(0)) = -\langle G, D_\rho \rangle = -\langle \nabla\mathcal{F}, P_X D_\rho \rangle,$$

where the second equality is due to $D_\rho \in \mathcal{T}_X$ and the definition (2.8) of $\nabla\mathcal{F}$. Recall that $P_X = I_n - \frac{1}{2}XX^\top$. Substituting (3.16) into the above equation yields

$$\mathcal{F}'_\tau(Y(0)) = -\langle \nabla\mathcal{F}, (I_n + (\rho - 1)XX^\top)\nabla\mathcal{F} \rangle \leq -\min\{\rho, 1\} \|\nabla\mathcal{F}\|_{\mathbb{F}}^2.$$

So (ii) is true.

We prove (iii) by contradiction. Multiplying X^\top from both sides the expression of $Y(\tau)$ in (3.15) and using $X^\top W = 0$, we get that $2J^{-1} - I_p = X^\top Y$. Assume that there exists a p -by- p orthogonal matrix Q_p such that $Y = XQ_p$. Then we have $2J^{-1} - I_p = Q_p$; i.e., $2I_p - J = Q_p J$. It follows from $(2I_p - J)^\top (2I_p - J) = (Q_p J)^\top Q_p J$ and $Q_p^\top Q_p = I_p$ that

$$J^\top + J = 4I_p,$$

which is a contradiction to the definition of J . The contradiction shows the truth of (iii).

For (iv), it is obvious that $\|J\|_2 \leq 1 + \frac{\tau^2}{4}\|W\|_{\mathbb{F}}^2 + \frac{\tau}{2}\|X^T D_\rho\|_{\mathbb{F}}$, where $\|\cdot\|_2$ is the spectral norm. It follows from $-D_\rho = W - XX^T D_\rho$ and $X^T W = 0$ that $\|D_\rho\|_{\mathbb{F}}^2 = \|W\|_{\mathbb{F}}^2 + \|X^T D_\rho\|_{\mathbb{F}}^2$. Notice that $v = \tau\|D_\rho\|_{\mathbb{F}}$. Then we have

$$\|J\|_2 \leq 1 + \frac{v^2}{4} \cdot \frac{\|W\|_{\mathbb{F}}^2}{\|D_\rho\|_{\mathbb{F}}^2} + \frac{v}{2} \cdot \frac{\|X^T D_\rho\|_{\mathbb{F}}}{\|D_\rho\|_{\mathbb{F}}} \leq 1 + \max_{0 \leq t \leq 1} \left(\frac{v^2}{4}(1-t^2) + \frac{v}{2}t \right) \leq (5+v^2)/4.$$

On the other hand, the relation $2J^{-1} = X^T Y + I_p$ indicates that $\|J^{-1}\|_2 \leq 1$. Thus (iv) is true.

In the case that $p = 1$ or n , it is not difficult to simplify the corresponding update schemes and we omit the details here. Thus, we complete the proof. \square

Before we proceed, several remarks on Lemma 3.1 are in order. Firstly, without otherwise specification, we will always choose $E = D_\rho$ in the remainder of this paper. In this case, by (3.15) and the definition of D_ρ , we must have that

$$W = -(I_n - XX^T)D_\rho \equiv -(I_n - XX^T)G. \quad (3.17)$$

There are two special choices of ρ . One is $\rho = 1/2$, yielding $Y'(0) = -\nabla\mathcal{F}$; the other one is $\rho = 1/4$ yielding $Y'(0) = -G + X\text{sym}(X^T G)$. Generally, the two directions are not the same except the case when $X^T G = G^T X$. We will compare the two directions in §6.4; the results therein shows that $\rho = 1/4$ is a better choice. Secondly, recalling that the Grassmann manifold $\mathcal{G}_{n,p}$ is defined as the set of all p -dimensional subspaces of an n -dimensional space, any two orthogonal matrices whose columns span the same p -dimensional subspace can be regarded as the same point in $\mathcal{G}_{n,p}$. By (iii) of Lemma 3.1, we know that any $Y(\tau)$ with $\tau > 0$ and X must be different points in $\mathcal{G}_{n,p}$. Thus our update scheme can be also used for optimization on the Grassmann manifold, that is, problem (1.1) with the additional homogeneity assumption that $\mathcal{F}(XQ_p) = \mathcal{F}(X)$, where Q_p is any p -by- p orthogonal matrix. Finally, statement (iv) of Lemma 3.1 indicates that the condition number of J can be controlled by the term $\tau\|D_\rho\|_{\mathbb{F}}$, this fact will guide us to set a safeguard for the stepsize, as addressed in (4.4).

As mentioned before, one typical choice of E is $E = D_\rho$. Consider the case when $p \approx n$, it is quite expensive to calculate J^{-1} directly. However, in this case we may construct a low-rank matrix E so that J^{-1} can be cheaply obtained. The following lemma shows the possibility of choosing a rank-2 matrix E , with which J^{-1} can be analytically given and fast computed. Similarly, we may also form a rank- $2r$ matrix E with $1 \leq r < n/2$ in the same vein. Nevertheless, it is worth noting that seeking an appropriate low-rank matrix E faces a trade-off between the computational cost and the quality of the search curve.

Lemma 3.2 *For any feasible $X \in \mathcal{S}_{n,p}$, define $D^{(i)} = G_{(i)}e_i^T - X_{(i)}G_{(i)}^T X$. Consider the curve $Y(\tau)$ given by (3.15) with $E = D^{(q)}$, where q is the column index given by*

$$q := \arg \max_{i=1,\dots,p} \langle G, D^{(i)} \rangle = \arg \max_{i=1,\dots,p} e_i^T (G^T \nabla \mathcal{F}) e_i. \quad (3.18)$$

Then we have that

$$J^{-1} = I_p - \frac{1}{1+\alpha} [e_q, b] \begin{bmatrix} \alpha & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} e_q^T \\ b^T \end{bmatrix}, \quad (3.19)$$

where $\alpha = \frac{\tau^2}{4} G_{(q)}^T (I_n - X_{(q)} X_{(q)}^T) G_{(q)}$, $b = \frac{\tau}{2} X_{-q}^T G_{(q)}$ and $X_{-q} = X - X_{(q)} e_q^T$. Moreover, $Y(\tau)$ is a descent curve satisfying

$$\mathcal{F}'_\tau(Y(0)) \leq -\frac{1}{2p} \|\nabla \mathcal{F}\|_{\mathbb{F}}^2.$$

Proof The relation $\langle G, D^{(i)} \rangle = e_i^T (G^T \nabla \mathcal{F}) e_i$ can be easily verified from the definition of $D^{(i)}$. With the definition of $D^{(q)}$ and $X^T X = I_p$, we have that

$$X^T D^{(q)} = X^T G_{(q)} e_q^T - e_q G_{(q)}^T X = \frac{2}{\tau} (b e_q^T - e_q b^T) \in \mathcal{T}_X.$$

Thus $Y(\tau)$ is well-defined. Moreover, we have that

$$W = -(I_n - XX^T)D^{(q)} = -(I_n - XX^T)G_{(q)} e_q^T$$

Hence, the matrix $J = I_p + \frac{\tau^2}{4}W^\top W + \frac{\tau}{2}X^\top D^{(q)}$ can be expressed as

$$J = I_p + \xi e_q e_q^\top + b e_q^\top - e_q b^\top = I_p + [e_q, b] \begin{pmatrix} \left[\begin{array}{cc} \xi & -1 \\ 1 & 0 \end{array} \right] \left[\begin{array}{c} e_q^\top \\ b^\top \end{array} \right] \end{pmatrix}, \quad (3.20)$$

where $\xi = \frac{\tau^2}{4}G_{(q)}^\top(I_n - XX^\top)G_{(q)}$. By the formulations of b and ξ , we easily see that

$$e_q^\top b = 0, \quad \xi = \alpha - b^\top b.$$

Applying the SMW formula to (3.20) and using the above relations, we can obtain (3.19).

Moreover, notice that $\nabla \mathcal{F} = \sum_{i=1}^p D^{(i)}$. Thus we have

$$p \mathcal{F}'_\tau(Y(0)) = -p \langle G, D^{(q)} \rangle \leq -\langle G, \nabla \mathcal{F} \rangle \leq -\frac{1}{2} \|\nabla \mathcal{F}\|_{\mathbb{F}}^2,$$

where the first inequality follows from the choice of q in (3.18) and the second one is due to (ii) of Lemma 3.1. The proof is completed. \square

Geometrically, the proposed framework is not geodesic exact for the case when $p = 1$. Instead, it can be regarded as a generalized gradient projection scheme. In the special case when there always holds $X^\top G \equiv G^\top X$, we can explicitly get the projection operator of new update scheme (3.15). Notice that the condition $X^\top G \equiv G^\top X$ holds for a wide range of problems, such as the linear eigenvalue problem and the vector case ($p = 1$) of problem (1.1).

Lemma 3.3 *Assume that $X^\top G \equiv G^\top X$ for any feasible point $X \in \mathcal{S}_{n,p}$. Then the update scheme (3.15) with $E = D_\rho$ can be expressed by*

$$Y(\tau) = \mathcal{P}_{\mathcal{S}_{n,p}} \left(X \left(I_p + \tau X^\top G - \frac{\tau^2}{4} G^\top (I_n - XX^\top) G \right) - \tau G \right).$$

Proof The condition $X^\top G \equiv G^\top X$ implies that $X^\top D_\rho = 0$, which with (3.15) means that $J = I_p + \frac{\tau^2}{4}W^\top W$. Rewrite $Y(\tau)$ in (3.15) as

$$Y(\tau) = (X(2I_p - J) + \tau W)J^{-1}.$$

Thus it follows from $Y(\tau)^\top Y(\tau) = I_p$ and the above expressions of $Y(\tau)$ and J that

$$(X(2I_p - J) + \tau W)^\top (X(2I_p - J) + \tau W) = J^2.$$

Recalling the definition of $\mathcal{P}_{\mathcal{S}_{n,p}}(\cdot)$ for (2.4), we have that

$$\begin{aligned} Y(\tau) &= \mathcal{P}_{\mathcal{S}_{n,p}}(X(2I_p - J) + \tau W) \\ &= \mathcal{P}_{\mathcal{S}_{n,p}} \left(X \left(I_p + \tau X^\top G - \frac{\tau^2}{4} G^\top (I_n - XX^\top) G \right) - \tau G \right), \end{aligned}$$

where the second equality uses (3.17). This completes the proof. \square

3.2 Comparison with the existing update schemes

To begin with, we address a relationship between the update scheme (3.15) and the Wen-Yin update scheme. We show that the Wen-Yin update scheme can be regarded as a special member of the update scheme (3.15) with $g(\tau) = \tau/2$ under the condition that $I_p + \frac{\tau}{4}X^\top D$ is invertible. Notice that this invertible condition is indispensable for the well definition of the Wen-Yin update scheme, but is not necessary for the validity of the update scheme (3.15).

Lemma 3.4 *Assume that $T = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix}$, where T_{22} and $T_{11} - T_{12}T_{22}^{-1}T_{21}$ are invertible. Then T is invertible and*

$$T^{-1} = \begin{bmatrix} (T_{11} - T_{12}T_{22}^{-1}T_{21})^{-1} & -(T_{11} - T_{12}T_{22}^{-1}T_{21})^{-1}T_{12}T_{22}^{-1} \\ -T_{22}^{-1}T_{21}(T_{11} - T_{12}T_{22}^{-1}T_{21})^{-1} & T_{22}^{-1}T_{21}(T_{11} - T_{12}T_{22}^{-1}T_{21})^{-1}T_{12}T_{22}^{-1} + T_{22}^{-1} \end{bmatrix}.$$

Proposition 3.1 *For any feasible point $X \in \mathcal{S}_{n,p}$, if the tangent direction $D \in \mathcal{T}_X$ is such that $I_p + \frac{\tau}{4}X^\top D$ is invertible, the update scheme (2.3) is well-defined and it is equivalent to the update scheme (3.15) with $g(\tau) = \tau/2$ and $E = D$.*

Proof First, we show that the update scheme (2.3) is well-defined, provided that $I_p + \frac{\tau}{4}X^\top D$ is invertible. Consider the update scheme (2.3) with $U = [P_X D, X]$ and $V = [X, -P_X D]$. It follows from $P_X = I_n - \frac{1}{2}XX^\top$ that $X^\top P_X D = \frac{1}{2}X^\top D$. Combining this with $X^\top X = I_p$ and $X^\top D$ being skew-symmetric, we can rewrite

$$I_{2p} + \frac{\tau}{2}V^\top U = \begin{bmatrix} I_p + \frac{\tau}{4}X^\top D & \frac{\tau}{2}I_p \\ -\frac{\tau}{2}D^\top P_X^\top P_X D & I_p + \frac{\tau}{4}X^\top D \end{bmatrix}. \quad (3.21)$$

Moreover, we derive that

$$W^\top W = D^\top (I_n - XX^\top) D = D^\top P_X^\top P_X D + \frac{1}{4}(X^\top D)^2,$$

which with (3.15) implies that

$$J = \left(I_p + \frac{\tau}{4}X^\top D \right)^2 + \frac{\tau^2}{4}D^\top P_X^\top P_X D.$$

Plugging this into (3.21) yields

$$I_{2p} + \frac{\tau}{2}V^\top U := \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} = \begin{bmatrix} I_p + \frac{\tau}{4}X^\top D & \frac{\tau}{2}I_p \\ \frac{2}{\tau} \left((I_p + \frac{\tau}{4}X^\top D)^2 - J \right) & I_p + \frac{\tau}{4}X^\top D \end{bmatrix}, \quad (3.22)$$

where $T_{ij} \in \mathbb{R}^{p \times p}$ ($i, j \in \{1, 2\}$). By simple calculations, we know that

$$T_{11} - T_{12}T_{22}^{-1}T_{21} = \left(I_p + \frac{\tau}{4}X^\top D \right)^{-1} J.$$

Thus it follows from Lemma 3.4 that $I_{2p} + \frac{\tau}{2}V^\top U$ is invertible and the update scheme (2.3) is well-defined.

We now prove the equivalence. With Lemma 3.4 and (3.22), some tedious manipulations yield that $(I_{2p} + \frac{\tau}{2}V^\top U)^{-1} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}$, where

$$\begin{aligned} M_{11} &= J^{-1}(I_p + \frac{\tau}{4}X^\top D), & M_{12} &= -\frac{\tau}{2}J^{-1}, \\ M_{21} &= \frac{2}{\tau}(I_p - M_{22}(I_p + \frac{\tau}{4}X^\top D)), & M_{22} &= (I_p + \frac{\tau}{4}X^\top D)J^{-1}. \end{aligned}$$

Direct calculations show that

$$M_{11} + \frac{1}{2}M_{12}X^\top D = J^{-1}, \quad \tau \left(M_{21} + \frac{1}{2}M_{22}X^\top D \right) = 2I_p - 2 \left(I_p + \frac{\tau}{4}X^\top D \right) J^{-1}. \quad (3.23)$$

Finally, we can obtain

$$\begin{aligned} Y_{\text{wy}}(\tau) &= X - \tau [P_X D, X] \left(\begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} \begin{bmatrix} I_p \\ \frac{1}{2}X^\top D \end{bmatrix} \right) \\ &= X - \tau \left(\frac{1}{2}XX^\top D - W \right) \left(M_{11} + \frac{1}{2}M_{12}X^\top D \right) - \tau X \left(M_{21} + \frac{1}{2}M_{22}X^\top D \right) \\ &= (2X + \tau W)J^{-1} - X, \end{aligned}$$

where the first equality uses (2.3) and $X^\top X = I_p$, the second and third equalities are due to $P_X D = \frac{1}{2}XX^\top D - W$ and (3.23), respectively. The proof is completed. \square

For a fixed feasible point $X \in \mathcal{S}_{n,p}$, assume that the gradient G has been computed. We now compare the computational costs of several aforementioned constraint preserving update schemes. To do so, we review the computational costs of some basic matrix operations. Given $A \in \mathbb{R}^{n_1 \times n_2}$ and $B \in \mathbb{R}^{n_2 \times n_2}$, computing AB needs $2n_1n_2^2$ flops while computing $A^\top A$ only needs $n_1n_2^2$ flops. Computing $\text{qr}(A)$ by the modified Gram-Schmidt algorithm needs $2n_1n_2^2$ flops (here $n_1 \geq n_2$). If B is symmetric, computing the eigenvalue decomposition $B = P\Sigma P^\top$ with orthogonal $P \in \mathbb{R}^{n_2 \times n_2}$ and diagonal $\Sigma \in \mathbb{R}^{n_2 \times n_2}$ by the symmetric QR algorithm needs $9n_2^3$ flops. If B is skew-symmetric, computing the exponential of B needs $10n_2^3$ flops. If B

Table 3.1 Computational cost for different update schemes

update schemes	$1 < p < n$		$p = 1$		$p = n$	
	first τ	new τ	first τ	new τ	first τ	new τ
$Y_{\text{gp}}(2.5), \text{any } D$	$3np^2 + 2np + \frac{32}{3}p^3$	$3np^2 + 2np + \frac{32}{3}p^3$	$5n$	$5n$	$\frac{41}{3}n^3$	$\frac{41}{3}n^3$
$Y_{\text{geol}}(2.1), D = D_\rho$	$10np^2 + np + 80p^3$	$4np^2 + 80p^3$	$7n$	$3n$	$14n^3$	$12n^3$
$Y_{\text{pd}}(2.6), D = D_\rho$	$7np^2 + 3np + \frac{32}{3}p^3$	$2np^2 + 2np + \frac{32}{3}p^3$	$7n$	$3n$	$\frac{53}{3}n^3$	$\frac{38}{3}n^3$
$Y_{\text{qr}}(2.7), D = D_\rho$	$6np^2 + 3np$	$2np^2 + 2np$	$7n$	$3n$	$6n^3$	$2n^3$
$Y_{\text{wy}}(2.3), D = D_\rho$	$9np^2 + 2np + \frac{40}{3}p^3$	$4np^2 + np + \frac{40}{3}p^3$	$7n$	$3n$	$\frac{67}{3}n^3$	$\frac{52}{3}n^3$
$Y_{\text{wy}}(2.3), D = D_{1/2}$	$7np^2 + np + \frac{40}{3}p^3$	$4np^2 + np + \frac{40}{3}p^3$	$7n$	$3n$	$\frac{61}{3}n^3$	$\frac{52}{3}n^3$
$Y(3.15), D = D_\rho$	$7np^2 + 2np + \frac{5}{3}p^3$	$2np^2 + 3np + \frac{2}{3}p^3$	$7n$	$3n$	$\frac{14}{3}n^3$	$\frac{8}{3}n^3$

is symmetric positive definite, computing $B^{1/2}$ needs $10n_2^3$ flops. In addition, if B is nonsingular, solving the matrix equation $BT = A^\top$ by the Gauss elimination with partial pivoting needs $2n_1n_2^2 + 2n_2^3/3$ flops. It follows that computing B^{-1} needs $8n_2^3/3$ flops. We refer interested readers to [23] for more details.

In the following computational cost analysis, we take the new update scheme (3.15) and the Wen-Yin update scheme (2.3) as examples. Notice that comparing with $O(np^2)$ or $O(n^3)$, the $O(p^2)$ term is omitted for $1 \leq p \leq n$. Consider the case that $1 < p < n$. To analyze the computational cost for (3.15), since $E = D_\rho$ and hence $W = -G + XX^\top G$, we can rewrite the feasible curve as

$$Y(\tau; X) = \left(X \left(\frac{2}{\tau} I_p + X^\top G \right) - G \right) \left(\frac{J(\tau)}{\tau} \right)^{-1} - X,$$

and

$$J(\tau) = I_p + \frac{\tau^2}{4} (G^\top G - G^\top X X^\top G) + \rho \tau (X^\top G - G^\top X).$$

Forming $J(\tau)$ needs $3np^2 + p^3$ flops involving computing $X^\top G$, $G^\top G$ and $(G^\top X)(X^\top G)$. The final assembly for $Y(\tau)$ consists of involving solving one matrix equation and performing one matrix multiplication and two matrix subtractions, and hence needs $4np^2 + 2np + 2p^3/3$ flops. Therefore, the total cost of forming $Y(\tau; X)$ in (3.15) for any τ is $7np^2 + 2np + 5p^3/3$. While doing backtracking line searches, we need to update $Y(\tau; X)$ for a different τ . Denote the first trial and the new trial stepsizes by τ_{first} and τ_{new} , respectively. It is easy to see that

$$Y(\tau_{\text{new}}; X) = \left(X \left(\frac{2}{\tau_{\text{first}}} I_p + X^\top G \right) - G + \left(\frac{2}{\tau_{\text{new}}} - \frac{2}{\tau_{\text{first}}} \right) X \right) \left(\frac{J(\tau_{\text{new}})}{\tau_{\text{new}}} \right)^{-1} - X.$$

As $X \left(\frac{2}{\tau_{\text{first}}} I_p + X^\top G \right) - G$ is already computed in $Y(\tau_{\text{first}}; X)$, we store this matrix and hence only need $2np^2 + 3np + 2p^3/3$ to compute $Y(\tau_{\text{new}}; X)$.

To analyze the computational cost for the Wen-Yin update scheme (2.3), we see that it takes $3np^2$ and $2np^2 + np$ flops to form $I_{2p} + \frac{\tau}{2} V^\top U$ and $P_X D_\rho$, respectively. The final assembly for $Y(\tau)$ needs $4np^2 + np + 40p^3/3$ flops. Hence, the total cost for the Wen-Yin update scheme is $9np^2 + 2np + 40p^3/3$. When $\rho = 1/2$, we see from [52] that $U = [G, X]$, $V = [X, -G]$ in (2.3) which implies that there is no need to compute $P_X D_{1/2}$ any more, and the total cost for forming the Wen-Yin update scheme can be reduced to $7np^2 + np + 40p^3/3$. The cost for updating $Y(\tau)$ with a new τ is $4np^2 + np + 40p^3/3$ since $V^\top U$ can be stored and the main work involves solving a matrix equation and the final assembly. In the case that $p = 1$ or n , the cost for the update schemes (3.15) and (2.3) can be easily obtained in a similar analysis. We omit the details here.

In Table 3.1, we list the cost of the aforementioned update schemes without giving more details. In the table, the column “first τ ” gives the cost of computing a feasible point with the first trial stepsize of τ_{first} , whereas the column “new τ ” provides the cost of getting a new feasible point with a new stepsize of τ_{new} . Table 3.1 tells us that the ordinary gradient projection actually has the lowest complexity cost while the scheme (2.7) based on the QR factorization and our update scheme (3.15) are strong candidates. Although by Proposition 3.1, our update scheme and the Wen-Yin update scheme are equivalent under some assumption, the former has a low complexity cost especially for large p , as shown in Table 3.1. As pointed in [4], however, the choice of the update scheme can affect the number of iterations required for solving the optimization problem. Hence, a lower complexity cost at each iteration does not necessarily imply a

higher efficiency on the whole. Actually, how to seek a constraint preserving update scheme which can find the global minimizer with a higher probability and at a faster speed is still an open problem. This remains under investigation.

4 Adaptive feasible BB-like (AFBB) method and global convergence

In this section, we focus on the adaptive feasible BB-like method and its global convergence. We also propose a strategy to control the feasibility error in practical computations.

4.1 Adaptive feasible BB-like method

To provide an efficient scheme, we must also pay much attention on choosing the stepsize τ in the constraint preserving update scheme (3.15) with $E = D_\rho$. Although there is only one parameter, its choice proves very important to the efficiency of the scheme. Since BB-like methods need less storage and are very efficient for unconstrained optimization problems [13, 20, 43, 57] and special constrained optimization problems [8, 11, 12, 52], we consider to use some BB-like stepsize in the scheme (3.15).

Denote $S_{k-1} = X_k - X_{k-1}$ and $Y_{k-1} = D_{\rho,k} - D_{\rho,k-1}$, where $X_k = Y(\tau_{k-1}; X_{k-1})$. Similar to the unconstrained case, we can get the large and short BB stepsizes as follows:

$$\tau_k^{\text{LBB}} = \frac{\langle S_{k-1}, S_{k-1} \rangle}{|\langle S_{k-1}, Y_{k-1} \rangle|} \quad \text{and} \quad \tau_k^{\text{SBB}} = \frac{|\langle S_{k-1}, Y_{k-1} \rangle|}{\langle Y_{k-1}, Y_{k-1} \rangle}.$$

In the numerical experiments in §6, we adopt the following alternative BB (ABB) stepsize [11]

$$\tau_k^{\text{ABB}} = \begin{cases} \tau_k^{\text{SBB}}, & \text{for odd } k; \\ \tau_k^{\text{LBB}}, & \text{for even } k. \end{cases} \quad (4.1)$$

If J_{k-1}^{-1} is stored in updating X_k , we can freely get $\langle S_{k-1}, S_{k-1} \rangle = 4p - 4\text{tr}(J_{k-1}^{-1})$ which is due to the feasibility of X_k and X_{k-1} and $X_{k-1}^\top X_k = 2J_{k-1}^{-1} - I_p$. Thus, computing the ABB stepsize needs at most $6np$ flops.

Although BB-like methods prove efficient for nonlinear optimization, its heavy nonmonotonicity in function values makes the global convergence analysis difficult. Up to now, the unmodified BB method is only showed to be globally convergent in the strongly convex quadratic case [42] and the convergence is R -linear [14]. It is shown in [27] that the unmodified BB method needs not converge for the extreme eigenvalue problem, which is a special case of problem (1.1). Thus we consider to incorporate the ABB stepsize with the Armijo-type line search which requires τ_k to satisfy

$$\mathcal{F}(Y_k(\tau_k)) \leq \mathcal{F}_r + \delta \tau_k \mathcal{F}'_r(Y(0; X_k)),$$

for some constant $\delta \in (0, 1)$, and \mathcal{F}_r is the so-called ‘‘reference function value’’, satisfying $\mathcal{F}_r \geq \mathcal{F}_k$. In this paper, we consider to update \mathcal{F}_r by the adaptive strategy proposed in [11]. This strategy can not only guarantee the convergence, but can keep the efficiency of the unmodified BB method since only few line search procedures will be invoked during the iterations. Denote by $\mathcal{F}_{\text{best}}$ the current best function value and by \mathcal{F}_c the maximum objective value since the value of $\mathcal{F}_{\text{best}}$ was found. Initially, we set $\mathcal{F}_r := +\infty$, $\mathcal{F}_{\text{best}} = \mathcal{F}_c = \mathcal{F}(X_0)$. Let L be a preselected positive integer. The following is a detailed description of the aforementioned adaptive strategy.

$$\begin{aligned} & \text{if } \mathcal{F}_{k+1} < \mathcal{F}_{\text{best}} \\ & \quad \mathcal{F}_{\text{best}} = \mathcal{F}_{k+1}, \mathcal{F}_c = \mathcal{F}_{k+1}, l = 0, \\ & \text{else} \\ & \quad \mathcal{F}_c = \max\{\mathcal{F}_c, \mathcal{F}_{k+1}\}, l = l + 1, \\ & \quad \text{if } l = L, \mathcal{F}_r = \mathcal{F}_c, \mathcal{F}_c = \mathcal{F}_{k+1}, l = 0, \quad \text{end} \\ & \text{end} \end{aligned} \quad (4.2)$$

For other nonmonotone line search methods, interested readers can refer to [15, 24, 43, 51, 56].

Now we give a detailed description of the AFBB method.

Algorithm 4.1 (Adaptive Feasible BB-like Method)

Step 0 Given $X_0 \in \mathcal{S}_{n,p}$, $\epsilon, \rho > 0$, $0 < \sigma, \delta < 1$, $\epsilon_{\min}, \epsilon_{\max} > 0$, $\Delta, L > 0$ and set $k := 0$.

Step 1 If $\|D_{\rho,k}\|_{\mathbb{F}} \leq \epsilon$, stop.

Step 2 Find the least nonnegative integer i_k satisfying

$$\mathcal{F}(Y(\delta^{i_k} \tau_k^{(1)}; X_k)) \leq \mathcal{F}_r + \delta \sigma^{i_k} \tau_k^{(1)} \mathcal{F}'_{\tau}(Y(0; X_k)), \quad (4.3)$$

and set $\tau_k := \sigma^{i_k} \tau_k^{(1)}$.

Step 3 Update $X_{k+1} = Y(\tau_k; X_k)$ by (3.15) and \mathcal{F}_r by (4.2).

Step 4 Calculate $\tau_k^{(0)}$ by a certain BB stepsize and set

$$\tau_k^{(1)} := \max \left\{ \epsilon_{\min} / \|D_{\rho,k}\|_{\mathbb{F}}, \min \left\{ \tau_k^{(0)}, \min \{ \epsilon_{\max} / \|D_{\rho,k}\|_{\mathbb{F}}, \Delta \} \right\} \right\}. \quad (4.4)$$

Step 5 $k := k + 1$. Go to Step 1.

4.2 Convergence of the AFBB method

In this subsection, we establish the global convergence result of Algorithm 4.1 in the numerical sense.

Theorem 4.1 *Let $\{X_k : k \geq 0\}$ be the sequence generated by Algorithm 4.1 with $\epsilon = 0$. Assume that $\mathcal{F}(X)$ is differentiable and that its gradient $\mathcal{D}\mathcal{F}(X)$ is Lipschitz continuous on $\mathcal{S}_{n,p}$ with Lipschitz constant L_0 , that is,*

$$\|\mathcal{D}\mathcal{F}(X) - \mathcal{D}\mathcal{F}(Y)\|_{\mathbb{F}} \leq L_0 \|X - Y\|_{\mathbb{F}}, \quad \text{for all } X, Y \in \mathcal{S}_{n,p}.$$

Then we have either $D_{\rho,k} = 0$ for some finite k or

$$\liminf_{k \rightarrow \infty} \|D_{\rho,k}\|_{\mathbb{F}} = 0. \quad (4.5)$$

Proof The sketch of proof is as follows (see [26] for more details). Firstly, for the update scheme (3.15), we can show (see Lemma 4.4 of [26]) that

$$\|Y_k(t_k) - Y_k(0)\|_{\mathbb{F}} \leq \frac{2 + \epsilon_{\max}}{2} t_k \|D_{\rho,k}\|_{\mathbb{F}}, \quad \|Y'_k(t_k) - Y'_k(0)\|_{\mathbb{F}} \leq \frac{4 + \epsilon_{\max}}{2} t_k \|D_{\rho,k}\|_{\mathbb{F}}^2, \quad (4.6)$$

where $Y_k(t_k)$ and $Y'_k(t_k)$ stand for $Y(t_k; X_k)$ and $Y'(t_k; X_k)$, respectively.

Secondly, since $\mathcal{D}\mathcal{F}(X)$ is Lipschitz continuous on the compact set $\mathcal{S}_{n,p}$, there exists a constant $c_0 > 0$ such that

$$\|\mathcal{D}\mathcal{F}(X)\|_{\mathbb{F}} \leq c_0, \quad \text{for all } X \in \mathcal{S}_{n,p}.$$

By employing (4.6), we can verify [26] that the stepsizes $\{\tau_k\}$ are bounded below, as addressed by

$$\tau_k \geq \min\{c, \tau_k^{(1)}\},$$

where $c = \frac{2\sigma(1-\delta)\min\{\rho,1\}}{c_1 \max\{2\rho,1\}^2}$ and $c_1 = \frac{4+\epsilon_{\max}}{2} c_0 + \frac{2+\epsilon_{\max}}{2} L_0$.

Thirdly, denote $\mathcal{F}_r, \mathcal{F}_c, \mathcal{F}_{\text{best}}, l$ at the k -th iteration by $\mathcal{F}_r^k, \mathcal{F}_c^k, \mathcal{F}_{\text{best}}^k, l^k$, respectively. It follows from (4.3), the second statement of Lemma 3.1, $\tau_k \geq \min\{c, \tau_k^{(1)}\}$ and $\|D_{\rho,k}\|_{\mathbb{F}} \leq \max\{2\rho, 1\} \|\nabla \mathcal{F}_k\|_{\mathbb{F}}$ that

$$\mathcal{F}_{k+1} \leq \mathcal{F}_r^k - \delta c_2 \|D_{\rho,k}\|_{\mathbb{F}}^2, \quad (4.7)$$

where $c_2 = \frac{\min\{c, \tau_k^{(1)}\} \min\{\rho, 1\}}{\max\{2\rho, 1\}^2}$. Assume that $D_{\rho,k} = 0$ will not happen after finite iterations. Numerically, if $\mathcal{F}_{k+1} < \mathcal{F}_{\text{best}}$, we must have that $\mathcal{F}_{k+1} \leq \mathcal{F}_{\text{best}} - \epsilon_{\text{mach}}$, where ϵ_{mach} is the machine precision again. By this, we can show [26] that $l^k = L$ holds for infinite number of times. Define the infinite set $\mathcal{K} := \{k_i : l^{k_i} = L\}$. If the relation (4.5) is false, then there must exist a positive constant $c_3 > 0$ such that $\|D_{\rho,k}\|_{\mathbb{F}} \geq c_3$ for all sufficiently large k . Then we obtain by (4.7) that

$$\mathcal{F}_j \leq \mathcal{F}_r^{k_i} - \varepsilon_1 \quad \text{for all } k_i < j \leq k_{i+1}, \quad (4.8)$$

where $\varepsilon_1 = \frac{\delta c_3 \min\{\rho, 1\} \min\{c, c_3, \epsilon_{\min}\}}{\max\{2\rho, 1\}^2}$ is a positive constant. Moreover, by the definition of \mathcal{F}_r , we know that $\mathcal{F}_r^{k_{i+1}} \leq \max_{k_i < j \leq k_{i+1}} \mathcal{F}_j$, which with (4.8) implies that for all $k_i \in \mathcal{K}$,

$$\mathcal{F}_r^{k_{i+1}} \leq \mathcal{F}_r^{k_i} - \varepsilon_1.$$

Since \mathcal{K} is an infinite set, the summation of the above relation over \mathcal{K} leads to a contradiction to the boundedness of $\mathcal{F}(X)$ in the feasible set. Therefore (4.5) must be true. This completes the proof. \square

Several remarks on the convergence are made here. Firstly, we note that Theorem 4.1 still holds for a certain nonlinear $g(\tau)$, provided that $|g(\tau)/\tau|$ is bounded above. Secondly, we point out that inequality (4.6), the basis for proving (4.7), is a crucial ingredient in establishing the convergence. Actually, this inequality also holds for the gradient projection, the polar decomposition or the Wen-Yin update scheme, but with different constant before the term t_k . Thus similar convergence results can be established for the three schemes in the framework of Algorithm 4.1. Thirdly, with the key inequalities in (4.6), we can similarly prove the global convergence of the feasible BB-like methods based on the monotone line search, or the nonmonotone line searches proposed in [24, 56]. Finally, we know from (4.4) that the sequence $\{\tau_k : k \geq 0\}$ is bounded above. This, with $v_k = \tau_k \|D_{\rho,k}\|_{\mathbb{F}}$ and Theorem 4.1, indicates that either $v_k = 0$ for some finite k or $\liminf_{k \rightarrow \infty} v_k = 0$. Combining this with statement (iv) of Lemma 3.1, we have either $\text{cond}(J_k) = 1$ for some finite k or $\liminf_{k \rightarrow \infty} \text{cond}(J_k) = 1$.

4.3 Controlling feasibility errors

The update scheme (3.15) is so constructed that $Y(\tau)^\top Y(\tau) = I_p$ always holds. In practical computations, however, the orthogonality constraint may be violated after several iterations. As will be seen, it is mainly due to the numerical errors occurred on the multiplication $X^\top W$, which should be exactly equal to zero in theory. In the following, we give a detailed analysis for this phenomenon and then propose a strategy for controlling the feasibility errors.

Now we assume that all the arithmetics are exact, but the orthogonality constraint may be violated at X . Denote $\Xi_X = X^\top X - I_p$, $\Xi_Y = Y^\top Y - I_p$. It is easy to verify from the definition (3.15) of J that

$$(2I_p - J)^\top (2I_p - J) + \tau^2 W^\top W = J^\top J.$$

Performing respectively the left and right multiplications by $J^{-\top}$ and J^{-1} on both sides of the above equation, we obtain

$$(2J^{-1} - I_p)^\top (2J^{-1} - I_p) + \tau^2 J^{-\top} W^\top W J^{-1} = I_p, \quad (4.9)$$

which implies that

$$\|2J^{-1} - I_p\|_2 \leq 1. \quad (4.10)$$

Rewrite $Y(\tau)$ in update scheme (3.15) as $Y(\tau) = X(2J^{-1} - I_p) + \tau W J^{-1}$. This, with (4.9) and $X^\top X = \Xi_X + I_p$, implies that

$$\Xi_Y = (2J^{-1} - I_p)^\top \Xi_X (2J^{-1} - I_p) + \tau (2J^{-1} - I_p)^\top X^\top W J^{-1} + \tau J^{-\top} W^\top X (2J^{-1} - I_p). \quad (4.11)$$

It follows from $W = -(I_n - X X^\top) D_\rho$ in (3.15) and the definition of Ξ_X that $X^\top W = \Xi_X X^\top D_\rho$. Then by the Cauchy inequality, (4.11), (4.10), $\|J^{-1}\|_2 \leq 1$ and $\tau \|D_\rho\|_{\mathbb{F}} \leq \epsilon_{\max}$, we know that

$$\|\Xi_Y\|_{\mathbb{F}} \leq (1 + 2\tau \|X^\top D_\rho\|_{\mathbb{F}}) \|\Xi_X\|_{\mathbb{F}} \leq \left(1 + 2\epsilon_{\max} \sqrt{1 + \|\Xi_X\|_2}\right) \|\Xi_X\|_{\mathbb{F}}, \quad (4.12)$$

showing that the feasibility of Y may be out of control after some iterations.

To control the feasibility errors, we propose an approach, in which the matrix W in the scheme is replaced by

$$\widehat{W} = -(I_n - X(X^\top X)^{-1} X^\top) G = -(I_n - X(X^\top X)^{-1} X^\top) D_\rho. \quad (4.13)$$

Notice that when $X^\top X$ is exactly I_p , \widehat{W} reduces to $-(I_n - X X^\top) D_\rho$ which is identical to the original W in (3.15) corresponding to $E = D_\rho$. Denote by \widehat{Y} the new Y computed by using \widehat{W} and define $\widehat{\Xi}_Y = \widehat{Y}^\top \widehat{Y} - I$. Noting that $X^\top \widehat{W} \equiv 0$, similarly to the deriving of (4.11), we obtain that

$$\widehat{\Xi}_Y = (2J^{-1} - I_p)^\top \Xi_X (2J^{-1} - I_p),$$

which with (4.10) implies that $\|\widehat{\Xi}_Y\|_{\mathbb{F}} \leq \|\Xi_X\|_{\mathbb{F}}$. Thus, with $np^2 + 8p^3/3$ extra flops for computing the \widehat{W} in (4.13), we can efficiently control the cumulative feasibility errors. Considering that $X^\top \widehat{W}$ is not exactly zero in practical computations, we may reasonably assume that $\|X^\top - X^\top X(X^\top X)^{-1} X^\top\|_{\mathbb{F}}$ is in the same order as the machine precision ϵ_{mach} . Then we have $\|X^\top \widehat{W}\|_{\mathbb{F}} \leq O(\epsilon_{\text{mach}}) \|D_\rho\|_{\mathbb{F}}$. Following the analysis of deriving (4.12), we have that

$$\|\widehat{\Xi}_Y\|_{\mathbb{F}} \leq \|\Xi_X\|_{\mathbb{F}} + 2\epsilon_{\max} O(\epsilon_{\text{mach}}),$$

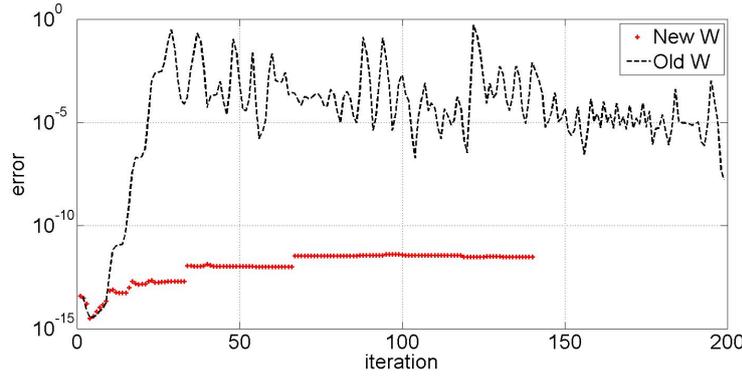


Fig. 4.1 The error of feasibility during iterations

which significantly improves the bound in (4.12).

To illustrate the usefulness of the above strategy, we take a typical example, which is to calculate the sum of the four largest eigenvalue of matrix “S3DKT3M2” from UF Sparse Matrix Collection [17]. We tried two versions of Algorithm 4.1, in which the original W and the modified \widehat{W} in (4.13) are used respectively. The corresponding parameters are chosen according to §6.1. Figure 4.3 depicts the error of the feasibility versus the iteration number. From this figure, we see that the feasibility errors during the iterations are efficiently controlled by using \widehat{W} .

5 Several extensions

In this section, we mention some extensions of the constraint preserving update scheme (3.15) and the AFBB method. At first, we consider a special case of (1.2); *i.e.*, optimization with the generalized orthogonality constraint,

$$\min_{X \in \mathbb{C}^{n \times p}} \mathcal{F}(X), \quad \text{s.t. } X^*HX = K, \quad (5.1)$$

where $H \in \mathbb{R}^{n \times n}$ is a symmetric positive semidefinite (not necessarily symmetric positive definite) matrix and $K \in \mathbb{R}^{p \times p}$ is a symmetric positive definite matrix. The first-order optimality condition of problem (5.1) is as follows.

Lemma 5.1 *Suppose X is a local minimizer of problem (5.1). Then X satisfies the first-order optimality condition $\nabla \mathcal{F} := G - HXG^*XK^{-1} = 0$, with the associated Lagrange multiplier $\Lambda = G^*XK^{-1}$. Moreover, $\nabla \mathcal{F} = 0$ if and only if $D := GX^*H^2X - HXG^*HX = 0$.*

Proof The first statement can be easily verified. For the second one, we first assume that $\nabla \mathcal{F} = 0$. Then, we know that $G = HXK^{-1}X^*G$. Substituting $HXK^{-1}X^*G$ for the second G in the definition of D yields

$$D = (G - HXG^*XK^{-1})X^*H^2X = \nabla \mathcal{F}X^*H^2X = 0.$$

Now we assume that $D = 0$. Noting that $D = (GX^*H - HXG^*)HX$, we can obtain

$$\langle G, D \rangle = \langle GX^*H, GX^*H - HXG^* \rangle = \frac{1}{2} \|GX^*H - HXG^*\|_F^2, \quad (5.2)$$

which with $D = 0$ means that $GX^*H - HXG^* = 0$. Noting that $\nabla \mathcal{F} = (GX^*H - HXG^*)XK^{-1}$, we can see that $\nabla \mathcal{F} = 0$. The proof is completed. \square

Similar to the analysis in §3, we can give the following feasible update scheme for (5.1).

Lemma 5.2 *For any feasible point X with $X^*HX = K$, let $W = -(I_n - XK^{-1}X^*H)D$ and $J(\tau) = K + \frac{\tau^2}{4}W^*HW + \frac{1}{2}\tau X^*HD$. Consider the curve given by*

$$Y(\tau) = (2X + \tau W)J^{-1}K - X. \quad (5.3)$$

Then we have that

- (i) $Y(\tau)^*HY(\tau) = K$;
- (ii) $Y'(0) = -D$ is a descent direction and $\mathcal{F}'_\tau(Y(0)) \leq -\frac{1}{2}\|XK^{-1}\|_2^{-2}\|\nabla\mathcal{F}\|_F^2$;
- (iii) $\text{cond}(J) \leq \frac{5+v^2}{4}\text{cond}(K)$, where $v = \frac{\tau\|H^{\frac{1}{2}}D\|_F}{\sqrt{\|K\|_2}}$.

Proof Since X^*HD is skew-Hermitian, J is invertible and hence $Y(\tau)$ is well-defined. Rewriting $Y(\tau) = X(2J^{-1}K - I_p) + \tau WJ^{-1}K$ and noting $X^*HW = 0$, we can easily verify (i). Moreover, it is not difficult to verify that $Y'(0) = -D$. It follows from $\nabla\mathcal{F} = (GX^*H - HXG^*)XK^{-1}$ that

$$\|\nabla\mathcal{F}\|_F \leq \|XK^{-1}\|_2\|GX^*H - HXG^*\|_F.$$

Combing the above inequality with (5.2), $\mathcal{F}'_\tau(Y(0)) = \langle G, Y'(0) \rangle$ and $Y'(0) = -D$, we have that

$$\mathcal{F}'_\tau(Y(0)) = -\frac{1}{2}\|GX^*H - HXG^*\|_F^2 \leq -\frac{1}{2}\|XK^{-1}\|_2^{-2}\|\nabla\mathcal{F}\|_F^2.$$

So (ii) is true.

For (iii), it follows from $D = -W + XK^{-1}X^*HD$ and $X^*HW = 0$ that $D^*HD = W^*HW + D^*HXX^{-1}X^*HD$. Thus there holds

$$\|H^{\frac{1}{2}}D\|_F^2 = \|H^{\frac{1}{2}}W\|_F^2 + \|K^{-\frac{1}{2}}X^*HD\|_F^2.$$

Meanwhile, it is easy to see that

$$\|J\|_2 \leq \|K\|_2 + \frac{\tau^2}{4}\|H^{\frac{1}{2}}W\|_F^2 + \frac{\tau}{2}\|K^{\frac{1}{2}}\|_2\|K^{-\frac{1}{2}}X^*HD\|_F.$$

Plugging $\tau = \frac{\sqrt{\|K\|_2}}{\|H^{\frac{1}{2}}D\|_F}v$ into the above equality yields

$$\begin{aligned} \|J\|_2 &\leq \|K\|_2 + \frac{\|K\|_2 v^2}{4} \cdot \frac{\|H^{\frac{1}{2}}W\|_F^2}{\|H^{\frac{1}{2}}D\|_F^2} + \frac{\|K\|_2 v}{2} \cdot \frac{\|K^{-\frac{1}{2}}X^*HD\|_F}{\|H^{\frac{1}{2}}D\|_F} \\ &\leq \|K\|_2 + \|K\|_2 \cdot \max_{0 \leq t \leq 1} \left(\frac{v^2}{4}(1-t^2) + \frac{v}{2}t \right) \\ &\leq \frac{5+v^2}{4}\|K\|_2. \end{aligned} \tag{5.4}$$

On the other hand, we see from (5.3), $X^*HW = 0$ and $X^*HX = K$ that $2J^{-1} = K^{-1}(X^*HY)K^{-1} + K^{-1}$, which indicates that $\|J^{-1}\|_2 \leq \|K^{-1}\|_2$. Combing this with (5.4) gives (iii). The proof is completed. \square

With the help of the above lemma, we can design the AFBB method for problem (5.1) similar to Algorithm 4.1. Global convergence results can also be established.

Finally, we point out that our scheme and algorithm can naturally be extended to (1.2), since the variables X_1, \dots, X_p are separated in the constraints.

6 Numerical Results

In this section, we present numerical results on a variety of problems to illustrate the efficiency of our AFBB method. We implemented AFBB in Matlab R2012a. All experiments were performed in Matlab under a Linux operating system on a Thinkpad T420 Laptop with an Intel[®] dual core CPU at 2.60GHz \times 2 and 4GB of RAM.

6.1 Stopping criteria

Define $\text{tol}_k^x := \frac{\|X_k - X_{k-1}\|_F}{\sqrt{n}}$ and $\text{tol}_k^f := \frac{|\mathcal{F}_k - \mathcal{F}_{k+1}|}{|\mathcal{F}_k|+1}$. We terminate the algorithm if one of the following holds: (i) $k \geq \text{MaxIter}$; (ii) $\|D_{\rho,k}\|_F \leq \epsilon \|D_{\rho,0}\|_F$; (iii) $\text{tol}_k^x \leq \epsilon_x$ and $\text{tol}_k^f \leq \epsilon_f$; (iv) $\text{mean}([\text{tol}_{k-\min\{k,T\}+1}^x, \dots, \text{tol}_k^x]) \leq 10\epsilon_x$ and $\text{mean}([\text{tol}_{k-\min\{k,T\}+1}^f, \dots, \text{tol}_k^f]) \leq 10\epsilon_f$, where MaxIter is the maximal iteration number. These criteria are the same as those used in [52] except that we replace $\|\nabla \mathcal{F}_k\|_F \leq \epsilon$ therein by criterion (ii) here. Unless otherwise specified, we set $\epsilon = 10^{-5}$, $\epsilon_x = 10^{-5}$, $\epsilon_f = 10^{-8}$, $T = 5$ and $\text{MaxIter} = 3000$.

The other parameters for AFBB are given as follows:

$$\rho = 0.25, \sigma = 0.5, \delta = 0.001, \epsilon_{\min} = 10^{-8}, \epsilon_{\max} = 10^8, \Delta = 10^{10}, L = 3.$$

The initial trial stepsize $\tau_0^{(1)}$ at the first iteration is chosen to be $0.5 \|D_{\rho,0}\|_F^{-1}$. The ABB stepsize (4.1) is used for computing the trial stepsize $\tau_k^{(0)}$. The ‘‘tic-toc’’ command in Matlab is used to obtain the CPU time in seconds elapsed by each code. After the iterations, if $\|X^T X - I_p\|_F \geq 10^{-14}$, a re-orthogonality procedure will be performed to enhance the feasibility.

6.2 Nearest low-rank correlation matrix problem

Given $C \in \mathcal{S}^n$ and a nonnegative weight matrix $H \in \mathcal{S}^n$, the nearest low-rank correlation matrix problem is given by

$$\min_{X \in \mathcal{S}^n} \frac{1}{2} \|H \odot (X - C)\|_F^2, \quad \text{s.t.} \quad \text{diag}(X) = e, \quad \text{rank}(X) \leq r, \quad X \succeq 0, \quad (6.1)$$

where \odot is the Hadama product operator of two matrices, $e \in \mathbb{R}^n$ is the vector with all ones, $r < n$ is a given positive integer number. A usual weight is $H = \mathbf{1}$, where $\mathbf{1} \in \mathbb{R}^{n \times n}$ represents the matrix with all ones.

To deal with the nonconvex rank constraints $\text{rank}(X) \leq r$, as used in the geometric optimization method [25], majorization method [38], and trigonometric parametrization method [44], we rewrite $X = V^T V$ with $V = [V_1, \dots, V_n] \in \mathbb{R}^{r \times n}$. Consequently, we get the equivalent formulation of (6.1) as follows:

$$\min_{V \in \mathbb{R}^{r \times n}} \theta(V; H, C) := \frac{1}{2} \|H \odot (V^T V - C)\|_F^2, \quad \text{s.t.} \quad \|V_i\|_2 = 1, \quad i = 1, \dots, n, \quad (6.2)$$

which is the minimization of a quartic polynomial over spheres. Among many approaches to solve problem (6.1), we compared our algorithm with several state-of-the-art methods; *i.e.*, the majorized penalty approach (PenCorr²) [22], the sequential semismooth Newton method (SemiNewton) [32], and the Wen-Yin nonmonotone BB method (OptM³) proposed in [52]. For more comprehensive literature reviews, see [22, 32].

We chose the initial point of problem (6.2) in the same way as in the majorization method. Specifically, we selected the modified PCA [21] of C ; *i.e.*, C_{pca} , to be the initial point in AFBB or OptM. Let C have the eigenvalue decomposition $C = P \text{Diag}(\lambda_1, \dots, \lambda_n) P^T$, where $P^T P = I_n$ and $\lambda_1 \geq \dots \geq \lambda_n$. Define $A_r = \text{Diag}(\lambda_1, \dots, \lambda_r)$ and denote by P_1 the first r columns of P . Then the i -th column of C_{pca} is $[C_{\text{pca}}]_{(i)} = z_i / \|z_i\|$, where $z_i = P_1 [A_r^{1/2}]_{(i)}$, $i = 1, \dots, r$. In case of $\lambda_i \leq 0$ for some $1 \leq i \leq r$, we first solved the following problem:

$$\tilde{C} = \arg \min_{X \in \mathcal{S}^n} \frac{1}{2} \|X - C\|_F^2, \quad \text{s.t.} \quad \text{diag}(X) = e, \quad X \succ 0$$

by the semismooth Newton method [39] and then set the initial point as \tilde{C}_{pca} . Note that SemiNewton and PenCorr also have their own efficient ways to generate good initial points.

We list the test problems from [22, 28, 31, 32, 38] as follows. For the case when $H \neq \mathbf{1}$, we may need to use the incomplete C . More specifically, the entries of C , corresponding to the nonzero weights, will be set to be zeros.

Ex. 1^[32]: The matrix C is the 387×387 one-day correlation matrix (as of Oct. 10, 2008) from the lagged datasets of RiskMetrics.⁴

² It can be downloaded from <http://www.math.nus.edu.sg/~matsundf/#Codes>.

³ It can be downloaded from <http://optman.blogs.rice.edu/>.

⁴ Dr. Qingna Li provided us this matrix kindly.

Ex. 2^[38]: $H = \mathbf{1}$, $n = 500$, the entries

$$C_{ij} = \exp\left(-\gamma_1|i-j| - \frac{\gamma_2|t_i - t_j|}{\max\{i, j\}^{\gamma_3} - \gamma_4|\sqrt{i} - \sqrt{j}|}\right)$$

for $i, j = 1, \dots, n$ with $\gamma_1 = 0, \gamma_2 = 0.480, \gamma_3 = 1.511, \gamma_4 = 0.186$.

Ex. 3^[22]: $n = 500$, the entries $C_{ij} = 0.5 + 0.5e^{-0.05|i-j|}$ for $i, j = 1, \dots, n$. The weight matrix H is either $\mathbf{1}$ or a random matrix whose entries are uniformly distributed in $[0.1, 10]$ except for 200 entries in $[0.01, 100]$.

Ex. 4^[22]: $n = 943$, C is based on 100,000 ratings for 1682 movies by 943 users from MovieLens data sets. It can be download from <http://www.grouplens.org/node/73>. The weight matrix H is either $\mathbf{1}$ or the one provided by T. Fushiki at Institute of Statistical Mathematics in Japan.

Ex. 5-9^[28, 31]: We consider the five gene correlation matrices \widehat{C} : Lymph, ER, Arabidopsis, Leukemia and Hereditary bc. For the sake of comparison, as done in [28], we perturb \widehat{C} to

$$C = (1 - \gamma)\widehat{C} + \gamma F,$$

where $\gamma = 0.05$ and F is a random symmetric matrix with entries uniformly distributed in $[-1, 1]$. The corresponding weight matrix H is either $\mathbf{1}$ or the one created by Example 2 in [28].

In our implementation, all the parameters of each solver were set to be their default values except the termination criteria of OptM were changed to the ones in §6.1. The numerical results are reported in Tables 6.1 – 6.3. In these tables, “nlmres⁰” and “nlmres” represent the initial and returned residual $\|H \odot (X - C)\|_F$, respectively. The terms “time” and “feasi” denote the CPU time and the violation of $\text{diag}(X) = e$, respectively, and “nfgc” stands for the total number of function and gradient evaluations. Note that CPU time of OptM or AFBB includes the CPU time for generating the initial point by the modified PCA. To further show the efficiency of our approach, we considered to implement AFBB starting from a random X_0 , denoted by “AFBB-rand X_0 ”. For space consideration, we only list the results of AFBB-rand X_0 for $H = \mathbf{1}$. They are reported in the last five columns of Table 6.2.

From the results, we know that AFBB performs better than OptM in terms of the residual, the CPU time and the number of function and gradient evaluations. Again, in the case when $H = \mathbf{1}$, AFBB not only runs considerably faster than SemiNewton and PenCorr, but also always find a better solution in terms of the residual except for the problem with large r ; in the case when $H \neq \mathbf{1}$, our AFBB shows great advantage over PenCorr in terms of the solution quality and CPU time. Besides, although AFBB-rand X_0 performs worse than AFBB, it still can solve the problem in a reasonable time and is comparable with SemiNewton and PenCorr. Apart from the ABB stepsize, another reason for the efficiency of AFBB is its low complexity cost per iteration. The dominated cost of AFBB at each iteration is computing the function value and the gradient in (6.1). For special $H = \mathbf{1}$ and general H , the costs are $2n^2r + 3nr^2$ and $3n^2r$, respectively. In contrast, SemiNewton and PenCorr need to solve iteratively a series of least squares correlation matrix problems without the rank constraint, whose cost is very expensive.

Here we should notice that PenCorr is a general and powerful package since it can deal with more general constraints such as lower and upper bound constraints. While it is not known yet how to extend AFBB efficiently in this situation, we shall consider a possible extension of the problem (6.1) with some given entries of the matrix X . More exactly, it is required that $X_{ij} = q_{ij}$ for $(i, j) \in \mathcal{B}_e$, where \mathcal{B}_e is the subset of $\{(i, j) | 1 \leq j < i \leq n\}$ satisfying $-1 \leq q_{ij} \leq 1$ for any $(i, j) \in \mathcal{B}_e$. Using the decomposition $X = V^T V$, the problem is now equivalent to

$$\begin{aligned} \min_{V \in \mathbb{R}^{r \times n}} \quad & \theta(V; H, C) \\ \text{s.t.} \quad & \|V_i\|_2 = 1, \quad i = 1, \dots, n, \\ & V_i^T V_j - q_{ij} = 0, \quad (i, j) \in \mathcal{B}_e. \end{aligned} \tag{6.3}$$

To deal with the extra nonlinear constraints, we introduce the augmented Lagrangian function (see [5, 36, 49]) of (6.3) as follows:

$$L_\mu(V, \Lambda) = \theta(V; H, C) + \frac{\mu}{2}\theta(V; H_e, \widehat{C} + \Lambda/\mu)$$

where $\mu > 0$ is the penalty parameter, Λ , H_e and \widehat{C} are matrices in $\mathbb{R}^{n \times n}$ with zero entries for all $(i, j) \notin \mathcal{B}_e$. Starting from the initial point C_{pca} or $\widetilde{C}_{\text{pca}}$, $\Lambda_0 = 0$, $\mu_0 > 0$, the procedure of the augmented Lagrangian

Table 6.1 Numerical results of the nearest low-rank correlation matrix problem with $H = 1$: SemiNewton, PenCorr

r	SemiNewton				PenCorr			
	nltmres ⁰	nltmres	time	feasi	nltmres ⁰	nltmres	time	feasi
Ex. 1, $n = 387$								
2	1.653e02	1.630e02	3.6	4e-15	1.653e02	1.623e02	12.3	1e-08
5	7.026e01	6.157e01	2.2	4e-15	7.026e01	6.111e01	8.1	5e-08
20	8.641e00	6.087e00	1.5	5e-15	8.641e00	6.066e00	2.3	6e-07
40	1.335e00	7.765e-01	1.3	7e-15	1.335e00	7.768e-01	1.1	2e-08
80	5.889e-02	3.228e-02	1.2	9e-15	5.889e-02	3.262e-02	0.7	1e-08
Ex. 2, $n = 500$								
2	1.509e02	1.447e02	2.2	4e-15	1.509e02	1.446e02	7.4	2e-07
5	5.030e01	4.117e01	1.9	4e-15	5.030e01	4.113e01	6.2	3e-08
20	1.050e01	5.282e00	2.1	6e-15	1.050e01	5.282e00	2.5	6e-08
50	3.989e00	1.342e00	2.4	8e-15	3.989e00	1.344e00	1.2	6e-07
100	1.888e00	4.640e-01	1.8	1e-14	1.888e00	4.645e-01	1.2	1e-07
125	1.467e00	3.275e-01	2.0	1e-14	1.467e00	3.278e-01	1.4	4e-08
Ex. 3, $n = 500$								
2	2.038e02	1.580e02	2.4	4e-15	2.038e02	1.564e02	17.8	4e-09
5	1.350e02	7.889e01	2.5	4e-15	1.350e02	7.883e01	5.4	3e-08
20	3.889e01	1.571e01	2.1	5e-15	3.889e01	1.571e01	3.0	8e-08
50	1.461e01	4.139e00	2.5	6e-15	1.461e01	4.139e00	1.2	5e-07
100	6.920e00	1.466e00	1.8	9e-15	6.920e00	1.466e00	1.4	2e-07
125	5.395e00	1.048e00	1.9	9e-15	5.395e00	1.048e00	1.4	3e-08
Ex. 4, $n = 943$								
5	4.410e02	4.136e02	18.8	6e-15	4.410e02	4.128e02	73.6	6e-08
20	2.943e02	2.888e02	22.7	7e-15	2.943e02	2.887e02	36.4	3e-08
50	2.765e02	2.773e02	26.6	1e-14	2.765e02	2.763e02	18.7	8e-08
100	2.758e02	2.761e02	26.6	1e-14	2.758e02	2.758e02	4.6	2e-08
200	2.758e02	2.758e02	20.1	1e-14	2.758e02	2.758e02	4.5	2e-08
250	2.758e02	2.758e02	27.3	1e-14	2.758e02	2.758e02	4.5	2e-08
Ex. 5, Lymph, $n = 587$								
2	3.681e02	3.429e02	7.9	5e-15	3.681e02	3.414e02	37.0	3e-09
5	2.068e02	1.803e02	6.5	5e-15	2.068e02	1.798e02	30.8	8e-10
20	8.225e01	6.042e01	4.5	5e-15	8.225e01	6.039e01	12.1	5e-08
50	3.916e01	2.620e01	5.0	8e-15	3.916e01	2.620e01	7.0	5e-07
100	1.980e01	1.474e01	3.6	1e-14	1.980e01	1.474e01	4.2	7e-08
200	1.169e01	1.157e01	5.2	2e-14	1.169e01	1.156e01	1.8	2e-08
Ex. 6, ER, $n = 692$								
2	4.169e02	4.132e02	8.8	5e-15	4.169e02	4.122e02	45.3	6e-10
5	2.258e02	2.111e02	8.9	5e-15	2.258e02	2.099e02	89.7	7e-09
20	8.115e01	6.414e01	5.8	6e-15	8.115e01	6.406e01	22.6	5e-08
50	4.088e01	2.845e01	6.8	8e-15	4.088e01	2.844e01	12.1	3e-08
100	2.343e01	1.763e01	7.5	1e-14	2.343e01	1.763e01	8.1	1e-08
200	1.475e01	1.447e01	6.1	2e-14	1.475e01	1.446e01	3.0	7e-08
Ex. 7, Arabidopsis, $n = 834$								
5	2.253e02	2.143e02	14.6	6e-15	2.253e02	2.132e02	58.6	4e-09
20	7.764e01	5.878e01	12.6	7e-15	7.764e01	5.858e01	47.1	3e-09
50	4.102e01	2.874e01	11.3	1e-14	4.102e01	2.874e01	14.4	9e-09
100	2.648e01	2.100e01	11.6	1e-14	2.648e01	2.100e01	12.6	2e-08
200	1.918e01	1.899e01	10.8	2e-14	1.918e01	1.894e01	4.3	2e-07
250	1.886e01	1.886e01	9.9	2e-14	1.886e01	1.886e01	5.4	6e-08
Ex. 8, Leukemia, $n = 1255$								
5	3.918e02	3.317e02	45.4	7e-15	3.918e02	3.309e02	140.6	2e-08
20	1.554e02	1.055e02	32.6	8e-15	1.554e02	1.055e02	87.0	2e-07
50	6.529e01	4.473e01	29.2	1e-14	6.529e01	4.473e01	33.4	4e-07
100	3.937e01	3.274e01	21.3	2e-14	3.937e01	3.274e01	28.9	4e-08
200	3.163e01	3.099e01	35.7	2e-14	3.163e01	3.095e01	12.3	7e-08
400	3.078e01	3.078e01	29.3	3e-14	3.078e01	3.078e01	7.6	2e-07
Ex. 9, Hereditary bc, $n = 1869$								
5	4.657e02	4.361e02	118.7	8e-15	4.657e02	4.357e02	342.8	6e-08
20	7.194e01	6.426e01	104.2	1e-14	7.194e01	6.425e01	163.0	9e-08
50	5.823e01	5.200e01	79.1	2e-14	5.823e01	5.199e01	112.1	8e-08
100	5.311e01	5.026e01	92.5	2e-14	5.311e01	5.026e01	109.2	3e-08
200	4.990e01	4.989e01	110.9	3e-14	4.990e01	4.970e01	36.5	6e-07
400	4.966e01	4.966e01	27.6	1e-09	4.966e01	4.966e01	23.7	4e-09

method is as follows:

$$\begin{cases} V_{k+1} := \arg \min_{V \in \mathbb{R}^{r \times n}} L_{\mu_k}(V, \Lambda_k), \quad \text{s.t.} \quad \|V_i\|_2 = 1, \quad i = 1, \dots, n, \\ \Lambda_{k+1} := \Lambda_k - \mu_k H_e \odot (V_k^T V_k - \hat{C}_k), \\ \mu_{k+1} := 10\mu_k. \end{cases} \quad (6.4)$$

Table 6.2 Numerical results of the nearest low-rank correlation matrix problem with $H = 1$: OptM, AFBB, AFBB-rand X_0

r	OptM					AFBB					AFBB-rand X_0				
	n lcmres ⁰	n lcmresi	time	feasi	n fge	n lcmres ⁰	n lcmres	time	feasi	n fge	n lcmres ⁰	n lcmres	time	feasi	n fge
Ex. 1, $n = 387$															
2	1.653e02	1.624e02	0.1	3e-15	31	1.653e02	1.624e02	0.1	3e-15	32	3.265e02	1.636e02	0.3	3e-15	88
5	7.026e01	6.109e01	0.1	3e-15	90	7.026e01	6.109e01	0.1	3e-15	80	2.995e02	6.109e01	0.2	3e-15	114
20	8.641e00	6.063e00	0.2	3e-15	145	8.641e00	6.063e00	0.2	3e-15	125	2.902e02	6.063e00	0.4	4e-15	273
40	1.335e00	7.756e-01	0.4	4e-15	166	1.335e00	7.759e-01	0.3	3e-15	151	2.896e02	7.755e-01	0.9	5e-15	478
80	5.887e-02	3.302e-02	0.3	3e-15	79	5.887e-02	3.266e-02	0.3	3e-15	85	2.895e02	4.705e-02	2.6	6e-15	876
Ex. 2, $n = 500$															
2	1.509e02	1.446e02	0.1	4e-15	14	1.509e02	1.446e02	0.1	3e-15	15	2.643e02	1.485e02	0.1	4e-15	40
5	5.030e01	4.113e01	0.1	4e-15	36	5.030e01	4.113e01	0.2	3e-15	39	2.293e02	4.113e01	0.2	4e-15	69
20	1.050e01	5.280e00	0.4	3e-15	127	1.050e01	5.280e00	0.4	3e-15	132	2.139e02	5.280e00	1.8	5e-15	808
50	3.989e00	1.340e00	1.1	3e-15	311	3.989e00	1.340e00	0.9	4e-15	259	2.118e02	1.342e00	2.6	6e-15	839
100	1.888e00	4.641e-01	1.7	4e-15	257	1.888e00	4.640e-01	1.1	4e-15	179	2.109e02	4.658e-01	6.1	8e-15	1015
125	1.467e00	3.276e-01	2.1	4e-15	234	1.467e00	3.276e-01	1.8	4e-15	239	2.111e02	3.291e-01	7.9	8e-15	1065
Ex. 3, $n = 500$															
2	2.038e02	1.564e02	0.2	4e-15	32	2.038e02	1.564e02	0.2	3e-15	33	1.836e02	1.689e02	0.2	4e-15	30
5	1.350e02	7.883e01	0.2	4e-15	56	1.350e02	7.883e01	0.2	3e-15	49	1.425e02	7.883e01	0.3	4e-15	91
20	3.889e01	1.571e01	0.3	3e-15	67	3.889e01	1.571e01	0.2	4e-15	56	1.212e02	1.571e01	0.7	5e-15	317
50	1.461e01	4.139e00	0.5	4e-15	94	1.461e01	4.139e00	0.5	4e-15	114	1.178e02	4.139e00	3.0	6e-15	717
100	6.920e00	1.466e00	0.8	4e-15	96	6.920e00	1.466e00	0.9	4e-15	111	1.162e02	1.467e00	5.5	8e-15	819
125	5.395e00	1.048e00	1.2	4e-15	135	5.395e00	1.048e00	1.0	4e-15	107	1.162e02	1.049e00	8.3	8e-15	957
Ex. 4, $n = 943$															
5	4.359e02	4.128e02	1.0	5e-15	120	4.359e02	4.128e02	0.8	5e-15	100	7.282e02	4.128e02	1.0	5e-15	147
20	2.930e02	2.887e02	2.3	6e-15	340	2.930e02	2.887e02	2.2	6e-15	321	7.083e02	2.887e02	1.8	7e-15	244
50	2.843e02	2.763e02	3.0	7e-15	252	2.843e02	2.763e02	2.4	7e-15	209	7.031e02	2.763e02	2.7	9e-15	243
100	2.948e02	2.758e02	3.3	7e-15	125	2.948e02	2.758e02	2.3	7e-15	105	7.023e02	2.758e02	2.8	1e-14	131
200	3.088e02	2.758e02	4.4	7e-15	109	3.088e02	2.758e02	3.7	7e-15	93	7.013e02	2.758e02	4.7	2e-14	109
250	3.129e02	2.758e02	5.8	7e-15	109	3.129e02	2.758e02	4.4	7e-15	83	7.012e02	2.758e02	5.6	2e-14	113
Ex. 5, Lymph, $n = 587$															
2	3.681e02	3.412e02	0.3	4e-15	116	3.681e02	3.412e02	0.3	4e-15	95	5.099e02	3.435e02	0.4	4e-15	266
5	2.064e02	1.797e02	0.4	4e-15	142	2.064e02	1.797e02	0.4	4e-15	136	4.639e02	1.798e02	0.3	4e-15	109
20	8.068e01	6.038e01	0.4	5e-15	85	8.068e01	6.038e01	0.3	4e-15	71	4.486e02	6.038e01	0.6	5e-15	171
50	3.619e01	2.620e01	0.6	5e-15	96	3.619e01	2.620e01	0.6	5e-15	105	4.470e02	2.620e01	1.2	7e-15	221
100	1.618e01	1.474e01	0.8	5e-15	87	1.618e01	1.474e01	0.7	6e-15	79	4.464e02	1.474e01	2.4	8e-15	323
200	1.540e01	1.156e01	2.3	5e-15	109	1.540e01	1.156e01	2.6	6e-15	117	4.458e02	1.156e01	6.6	1e-14	333
Ex. 6, ER, $n = 692$															
2	4.168e02	4.120e02	0.4	4e-15	105	4.168e02	4.120e02	0.4	4e-15	80	5.997e02	4.133e02	0.4	4e-15	118
5	2.257e02	2.097e02	0.6	5e-15	172	2.257e02	2.097e02	0.6	5e-15	166	5.464e02	2.099e02	0.8	4e-15	236
20	7.985e01	6.404e01	0.5	5e-15	89	7.985e01	6.404e01	0.5	5e-15	105	5.283e02	6.404e01	0.9	6e-15	205
50	3.769e01	2.844e01	1.3	5e-15	166	3.769e01	2.844e01	1.2	6e-15	155	5.264e02	2.844e01	2.0	8e-15	321
100	1.899e01	1.763e01	1.7	6e-15	106	1.899e01	1.763e01	1.4	6e-15	93	5.252e02	1.763e01	4.7	9e-15	398
200	1.933e01	1.446e01	4.1	6e-15	140	1.933e01	1.446e01	3.2	6e-15	117	5.245e02	1.446e01	9.5	1e-14	403
Ex. 7, Arabidopsis, $n = 834$															
5	2.252e02	2.132e02	0.6	5e-15	89	2.252e02	2.132e02	0.6	5e-15	92	6.557e02	2.128e02	0.8	5e-15	131
20	7.593e01	5.856e01	1.0	5e-15	158	7.593e01	5.856e01	1.0	5e-15	162	6.358e02	5.856e01	1.3	6e-15	215
50	3.646e01	2.874e01	1.2	6e-15	110	3.646e01	2.874e01	1.2	6e-15	97	6.326e02	2.874e01	2.5	8e-15	273
100	2.139e01	2.100e01	2.3	6e-15	127	2.139e01	2.100e01	2.2	6e-15	101	6.324e02	2.100e01	7.1	9e-15	459
200	2.991e01	1.894e01	6.2	6e-15	159	2.991e01	1.894e01	5.5	6e-15	166	6.312e02	1.894e01	11.1	1e-14	377
250	3.631e01	1.886e01	5.6	6e-15	129	3.631e01	1.886e01	5.7	6e-15	144	6.310e02	1.886e01	13.1	1e-14	321
Ex. 8, Leukemia, $n = 1255$															
5	3.906e02	3.309e02	1.6	6e-15	101	3.906e02	3.309e02	1.6	6e-15	97	9.105e02	3.309e02	1.7	6e-15	116
20	1.506e02	1.055e02	2.4	7e-15	164	1.506e02	1.055e02	2.1	7e-15	137	8.789e02	1.055e02	4.1	7e-15	360
50	5.703e01	4.473e01	2.1	7e-15	91	5.703e01	4.473e01	1.8	7e-15	69	8.740e02	4.473e01	5.9	1e-14	368
100	3.291e01	3.273e01	3.9	7e-15	118	3.291e01	3.273e01	4.1	7e-15	119	8.712e02	3.274e01	14.5	1e-14	557
200	4.583e01	3.095e01	8.0	7e-15	143	4.583e01	3.095e01	5.7	7e-15	99	8.706e02	3.095e01	23.8	2e-14	455
400	7.580e01	3.078e01	21.7	8e-15	188	7.580e01	3.078e01	22.9	7e-15	207	8.704e02	3.078e01	30.2	2e-14	266
Ex. 9, Hereditary bc, $n = 1869$															
5	4.651e02	4.357e02	3.5	7e-15	56	4.651e02	4.357e02	3.7	7e-15	63	1.362e03	4.358e02	4.5	7e-15	101
20	6.936e01	6.425e01	3.9	8e-15	64	6.936e01	6.425e01	3.9	8e-15	65	1.317e03	6.425e01	5.6	9e-15	141
50	5.256e01	5.199e01	7.0	8e-15	138	5.256e01	5.199e01	7.5	8e-15	148	1.309e03	5.200e01	16.5	1e-14	440
100	5.506e01	5.026e01	8.3	8e-15	113	5.506e01	5.026e01	7.7	8e-15	103	1.305e03	5.027e01	26.0	1e-14	473
200	8.384e01	4.970e01	13.7	8e-15	114	8.384e01	4.970e01	11.8	8e-15	99	1.304e03	4.970e01	31.9	2e-14	321
400	1.345e02	4.966e01	50.4	8e-15	250	1.345e02	4.966e01	42.4	7e-15	211	1.304e03	4.966e01	57.2	2e-14	288

The subproblem in (6.4) is a low-rank nearest correlation matrix problem and is solved inexactly by the AFBB method. Specifically, for the k -th subproblem, the main parameters of AFBB are set to be

$$\epsilon_k = \max\{0.1\epsilon_{k-1}, 10^{-5}\}, \epsilon_{x,k} = \max\{0.1\epsilon_{x,k-1}, 10^{-5}\}, \epsilon_{f,k} = \max\{0.1\epsilon_{f,k-1}, 10^{-8}\}, \text{MaxIter}_k = 2000,$$

where $\epsilon_0 = 10^{-1}, \epsilon_{x,0} = 10^{-3}, \epsilon_{f,0} = 10^{-5}$. Denoting $\nu_k = \sum_{(i,j) \in \mathcal{B}_e} |V_{k,i}^\top V_{k,j} - q_{i,j}|$, we terminate the procedure (6.4) when $\nu_{k+1} \leq 3 \times 10^{-8}$ or $|\nu_{k+1} - \nu_k| \leq 10^{-8}$.

Table 6.3 Numerical results of the nearest low-rank correlation matrix problem with $H \neq 1$: PenCorr, OptM, AFBB

r	PenCorr				OptM					AFBB				
	n lcmres ⁰	n lcmres	time	feasi	n lcmres ⁰	n lcmres	time	feasi	n fge	n lcmres ⁰	n lcmres	time	feasi	n fge
Ex. 3, $n = 500$, random H														
2	1.198e03	9.122e02	89.6	3e-09	1.198e03	9.120e02	0.4	3e-15	50	1.198e03	9.120e02	0.5	4e-15	48
5	7.944e02	4.541e02	53.3	8e-09	7.944e02	4.539e02	1.5	3e-15	201	7.944e02	4.539e02	0.7	3e-15	85
20	2.293e02	8.812e01	38.8	3e-07	2.293e02	8.809e01	1.6	4e-15	185	2.293e02	8.809e01	1.3	4e-15	156
50	8.607e01	2.195e01	48.4	9e-07	8.607e01	2.189e01	7.7	4e-15	787	8.607e01	2.189e01	7.1	4e-15	731
100	4.084e01	6.445e00	55.5	3e-07	4.084e01	6.295e00	38.5	4e-15	3116	4.084e01	6.289e00	38.1	4e-15	3011
125	3.184e01	4.057e00	73.9	9e-07	3.184e01	3.958e00	43.8	4e-15	2948	3.184e01	3.939e00	42.7	4e-15	3008
Ex. 4, $n = 943$, H is given by T. Fushiki														
5	1.590e04	1.148e04	1188.4	6e-07	1.541e04	1.139e04	31.2	5e-15	1525	1.541e04	1.139e04	39.7	5e-15	1951
20	7.722e03	5.219e03	1072.5	3e-07	8.005e03	5.194e03	17.4	6e-15	748	8.005e03	5.195e03	18.8	6e-15	821
50	5.211e03	3.719e03	706.5	2e-09	6.126e03	3.712e03	14.6	7e-15	533	6.126e03	3.712e03	16.3	7e-15	539
100	4.844e03	3.507e03	412.0	3e-07	6.443e03	3.503e03	14.4	7e-15	338	6.443e03	3.503e03	11.6	7e-15	269
200	4.844e03	3.505e03	378.5	3e-07	7.621e03	3.501e03	16.9	8e-15	318	7.621e03	3.501e03	13.8	8e-15	275
250	4.844e03	3.505e03	372.2	3e-07	8.023e03	3.501e03	16.7	8e-15	273	8.023e03	3.501e03	18.5	8e-15	324
Ex. 5, Lymph, $n = 587$, H is generated by Example 2 in [28]														
2	7.808e04	7.268e04	3290.7	4e-07	7.808e04	7.271e04	9.9	4e-15	1119	7.808e04	7.261e04	3.5	4e-15	384
5	4.495e04	3.827e04	2455.2	9e-07	4.490e04	3.822e04	11.9	4e-15	1244	4.490e04	3.822e04	3.5	4e-15	355
20	1.762e04	1.226e04	2014.1	1e-07	1.740e04	1.222e04	7.0	5e-15	652	1.740e04	1.222e04	2.6	5e-15	227
50	8.089e03	4.712e03	1480.5	7e-08	7.765e03	4.706e03	7.5	6e-15	562	7.765e03	4.704e03	6.6	5e-15	496
100	3.577e03	2.281e03	666.7	7e-08	3.497e03	2.280e03	11.0	6e-15	642	3.497e03	2.280e03	9.5	5e-15	574
200	1.993e03	1.906e03	76.3	9e-07	3.356e03	1.907e03	19.6	6e-15	742	3.356e03	1.906e03	11.8	6e-15	447
Ex. 6, ER, $n = 692$, H is generated by Example 2 in [28]														
2	8.994e04	8.830e04	6727.7	6e-07	8.995e04	8.822e04	18.3	4e-15	1512	8.995e04	8.821e04	4.9	4e-15	388
5	4.676e04	4.392e04	2502.8	3e-07	4.675e04	4.386e04	13.4	4e-15	1002	4.675e04	4.386e04	9.1	5e-15	677
20	1.721e04	1.284e04	4127.0	9e-07	1.700e04	1.282e04	7.8	5e-15	521	1.700e04	1.282e04	4.6	5e-15	300
50	8.626e03	5.233e03	1432.4	8e-08	8.284e03	5.227e03	9.0	6e-15	544	8.284e03	5.232e03	5.8	5e-15	349
100	4.370e03	2.922e03	1020.6	6e-08	4.180e03	2.920e03	16.7	6e-15	744	4.180e03	2.919e03	16.1	6e-15	717
200	2.642e03	2.538e03	98.4	7e-09	4.335e03	2.539e03	21.5	6e-15	644	4.335e03	2.539e03	10.7	6e-15	334
Ex. 7, Arabidopsis, $n = 834$, H is generated by Example 2 in [28]														
5	4.908e04	4.588e04	6912.6	3e-07	4.906e04	4.558e04	24.8	5e-15	1263	4.906e04	4.587e04	7.6	5e-15	379
20	1.693e04	1.225e04	3008.0	1e-07	1.665e04	1.225e04	11.9	6e-15	577	1.665e04	1.225e04	3.9	5e-15	181
50	8.503e03	5.421e03	3350.3	1e-07	7.971e03	5.413e03	15.5	7e-15	639	7.971e03	5.412e03	9.4	6e-15	391
100	4.865e03	3.722e03	1679.9	7e-08	4.677e03	3.720e03	17.7	6e-15	554	4.677e03	3.720e03	16.1	6e-15	513
200	3.587e03	3.488e03	140.2	2e-08	6.456e03	3.490e03	32.7	7e-15	713	6.456e03	3.488e03	21.9	6e-15	491
250	3.587e03	3.488e03	42.3	1e-07	7.823e03	3.490e03	31.2	7e-15	582	7.823e03	3.488e03	17.9	6e-15	344
Ex. 8, Leukemia, $n = 1255$, H is generated by Example 2 in [28]														
5	8.545e04	7.148e04	44049.6	5e-07	8.517e04	7.133e04	71.3	6e-15	1572	8.517e04	7.133e04	16.5	6e-15	352
20	3.320e04	2.203e04	22685.8	1e-07	3.218e04	2.200e04	52.4	7e-15	1026	3.218e04	2.200e04	12.6	6e-15	221
50	1.384e04	8.846e03	14046.2	8e-08	1.225e04	8.838e03	42.1	9e-15	703	1.225e04	8.835e03	19.7	7e-15	332
100	7.615e03	6.245e03	6607.0	1e-07	7.182e03	6.243e03	32.1	7e-15	470	7.182e03	6.242e03	30.4	7e-15	451
200	6.056e03	5.914e03	517.6	7e-09	9.945e03	5.917e03	102.5	1e-14	1089	9.945e03	5.915e03	56.8	8e-15	611
400	6.045e03	5.912e03	159.9	2e-07	1.637e04	5.916e03	165.1	1e-14	1109	1.637e04	5.913e03	77.4	8e-15	529
Ex. 9, Hereditary bc, $n = 1869$, H is generated by Example 2 in [28]														
5	1.007e05	9.399e04	89093.5	2e-07	1.006e05	9.384e04	192.9	7e-15	1725	1.006e05	9.384e04	33.3	7e-15	276
20	1.580e04	1.381e04	51569.0	9e-07	1.518e04	1.380e04	77.4	8e-15	622	1.518e04	1.379e04	20.8	8e-15	145
50	1.197e04	1.069e04	55899.2	1e-07	1.144e04	1.068e04	57.1	8e-15	437	1.144e04	1.068e04	50.7	8e-15	385
100	1.065e04	1.030e04	25289.8	1e-07	1.200e04	1.029e04	127.9	9e-15	785	1.200e04	1.028e04	67.9	8e-15	409
200	1.032e04	1.022e04	4350.6	5e-07	1.824e04	1.023e04	178.4	1e-14	896	1.824e04	1.022e04	77.8	8e-15	387
400	1.032e04	1.022e04	303.6	1e-07	2.920e04	1.023e04	344.4	1e-14	1135	2.920e04	1.022e04	116.5	9e-15	385

Below we consider a test instance of problem (6.2) with extra fixed constraints.

Ex. 10: The matrices C, H are the same as the ones in Ex. 4. The index set \mathcal{B}_e consists of $\min\{n_e, n - i\}$ randomly generated integers from $\{1, \dots, n\}$ with $n_e = 3$. We set $q_{ij} = 0$ for $(i, j) \in \mathcal{B}_e$.

The numerical results are presented in Table 6.4, where ‘‘const.’’ represents the total constraint violation ν_k . From the table, we can see that the AFBB method is quite promising, which shows its potential to handle some more general constraints beyond the sphere constraints. As the augment Lagrangian method belongs to a different class of methods, however, we shall go further on this topic elsewhere.

6.3 Kohn-Sham total energy minimization

We test in this subsection a class of nonlinear eigenvalue problems known as Kohn-Sham (KS) equations, which arise in electronic structure calculations. The original KS equation or KS energy minimization problem is a continuous nonlinear problem. To solve the problems numerically, we turn them into finite-dimensional problems. Let the unitary matrix $X \in \mathbb{C}^{n \times p}$ be the approximation of the electronic wave functions of p occupied states, where n is the spatial degrees of freedom. Using the planewave basis, we define the finite-

Table 6.4 Numerical results of the nearest low-rank correlation matrix problem with equality requirements: PenCorr, AFBB

r	PenCorr				AFBB				nffe
	residual	time	feasi	const.	residual	time	feasi	const.	
Ex. 10, $n = 943$, $H = \mathbf{1}$									
10	3.533e02	1082.1	2e-08	2e-07	3.529e02	73.1	6e-15	2e-08	2678
50	2.841e02	93.8	4e-08	9e-08	2.841e02	15.1	6e-15	5e-08	446
100	2.827e02	36.3	1e-07	7e-08	2.827e02	16.9	7e-15	6e-09	398
200	2.827e02	23.4	9e-09	6e-09	2.827e02	24.0	7e-15	2e-08	379
250	2.827e02	23.5	9e-09	6e-09	2.827e02	23.6	7e-15	2e-08	355
Ex. 10, $n = 943$, H given by T. Fushiki									
10	8.306e03	5292.7	3e-08	5e-07	8.238e03	200.9	6e-15	1e-08	6221
50	4.171e03	1540.5	2e-08	1e-08	4.165e03	63.5	7e-15	3e-09	1658
100	3.939e03	1012.4	1e-08	9e-09	3.936e03	55.0	7e-15	1e-08	1189
200	3.936e03	905.5	2e-08	1e-08	3.933e03	60.4	7e-15	2e-08	1154
250	3.936e03	917.7	2e-08	1e-08	3.933e03	67.1	8e-15	2e-08	1148

dimensional approximation to the total energy functional as follows:

$$E_{\text{total}}(X) = \text{tr} \left(X^* \left(\frac{1}{2} \widehat{L} + V_{\text{ion}} \right) X \right) + \frac{1}{2} \rho(X)^\top \widehat{L}^\dagger \rho(X) + \rho(X)^\top \epsilon_{\text{xc}}(\rho(X)) + E_{\text{Ewald}} + E_{\text{rep}}, \quad (6.5)$$

where \widehat{L} is a finite-dimensional representation of the Laplacian operator in the planewave basis, V_{ion} denotes the ionic pseudopotentials sampled on the suitably chosen Cartesian grid, $\rho(X) = \text{diag}(XX^*)$ represents the charge density, the matrix \widehat{L}^\dagger means the pseudo-inverse of \widehat{L} , and $\epsilon_{\text{xc}}(\rho(X))$ is the exchange-correlation energy per particle in a uniform electron gas of density $\rho(X)$. The last two terms in (6.5) are constant shifts of the total energy (see [53] for the details). Consequently, the discretized KS energy minimization can be formulated as

$$\min_{X \in \mathbb{C}^{n \times p}} E_{\text{total}}(X), \quad \text{s.t. } X^*X = I_p. \quad (6.6)$$

For the above problem, the KKT conditions; *i.e.*, the KS equations, are

$$H(X)X - X\Lambda_p = 0, \quad X^*X = I_p. \quad (6.7)$$

Here, $H(X) = \frac{1}{2} \widehat{L} + V_{\text{ion}} + \text{Diag}(\widehat{L}^\dagger \rho(X)) + \text{Diag}(\mu_{\text{xc}}(\rho(X)))$, $\mu_{\text{xc}}(\rho(X)) = d\mu_{\text{xc}}(\rho(X))/d\rho(X)$ and Λ_p is a p -by- p symmetric matrix of Lagrangian multipliers.

Generically, it is sophisticated to compute the objective function and its gradient in (6.6). Thus, we use the Matlab Toolbox KSSOLV [53] which is tailored for easily developing new algorithms for solving the KS equations to do so. In order to show the efficiency of our AFBB method, we compared it with the self-consistent field (SCF) iteration which is currently the most widely used approach for the KS equations, this SCF iteration is provided in KSSOLV. We also compared AFBB with OptM [52] for KS problem (6.6) but only the performance of AFBB is reported because they performed similarly. The maximal iteration of SCF was set to be 200 while the other parameters were set to be their default values in KSSOLV. For the sake of fairness, we improved the stopping accuracy of AFBB; *i.e.*, resetting $\epsilon = 10^{-6}$, $\epsilon_x = 10^{-10}$, $\epsilon_f = 10^{-14}$, MaxIter = 1000, to obtain a higher quality solution. The termination rules are not directly comparable due to the different formulations of the problem used by SCF and AFBB. Specifically, SCF focuses on KS equations (6.7) and needs to solve a series of linear eigenvalue problems, while AFBB minimizes the total energy directly. However, as shown later by the numerical results in Table 6.5, we see that on average the chosen stopping criteria for AFBB are tighter than those of SCF in terms of the residual $\|HX - H(X^*HX)\|_F$. For each problem, we ran the two algorithms 10 times from different random initial points generated by the function “genX0” provided in KSSOLV. Note that for each instance, AFBB and SCF use the same initial point.

A summary of the numerical results on 18 standard testing problems is reported in Table 6.5. In this table, “a. E_{total}^0 ” and “a. E_{total} ” represent the average initial and returned total energy function value, respectively. The term “a.iter” denotes the average total number of iterations, “a.resi”, “a.feasi” and “a.time” the average residual $\|HX - H(X^*HX)\|_F$, the average violation of the constraint $X^*X = I_p$ and the average CPU time in seconds, respectively. We use “a.err” to denote the average relative errors between the average total energy \bar{z}_1 given by AFBB or the average total energy \bar{z}_2 given by SCF and the minimal of \bar{z}_1 and \bar{z}_2 , which is computed by $\frac{\bar{z}_1 - \min\{\bar{z}_1, \bar{z}_2\}}{|\min\{\bar{z}_1, \bar{z}_2\}|}$ or $\frac{\bar{z}_2 - \min\{\bar{z}_1, \bar{z}_2\}}{|\min\{\bar{z}_1, \bar{z}_2\}|}$. From the table, we can see that the AFBB method is considerably competitive and it can always take less CPU time than SCF to find the better solutions in

Table 6.5 Numerical results of the Kohn-Sham total energy minimization: SCF, AFBB

solver	$a.E_{\text{total}}^0$	$a.E_{\text{total}}$	a.resi	a.iter	a.feasi	a.err	a.time
alanine, $n = 12671, p = 18$							
SCF	-6.078e01	-6.116e01	3e-06	48.7	2e-14	2e-13	174.5
AFBB	-6.078e01	-6.116e01	4e-07	77.8	5e-15	0e00	137.8
al, $n = 16879, p = 12$							
SCF	-1.576e01	-1.577e01	8e-03	200.0	6e-15	8e-04	1490.6
AFBB	-1.576e01	-1.580e01	7e-05	986.5	6e-13	0e00	1212.1
benzene, $n = 8407, p = 15$							
SCF	-3.693e01	-3.723e01	2e-06	35.1	1e-13	8e-14	70.3
AFBB	-3.693e01	-3.723e01	4e-07	70.4	4e-15	0e00	56.5
c12h26, $n = 5709, p = 37$							
SCF	-8.073e01	-8.154e01	3e-06	69.1	4e-14	2e-13	216.6
AFBB	-8.073e01	-8.154e01	6e-07	78.9	1e-14	0e00	129.7
c2h6, $n = 2103, p = 7$							
SCF	-1.410e01	-1.442e01	2e-06	16.4	2e-14	2e-13	7.7
AFBB	-1.410e01	-1.442e01	4e-07	57.5	2e-15	0e00	8.2
co2, $n = 2103, p = 8$							
SCF	-3.504e01	-3.512e01	1e-06	18.0	7e-15	4e-14	7.6
AFBB	-3.504e01	-3.512e01	2e-07	63.0	3e-15	0e00	8.3
ctube661, $n = 12599, p = 48$							
SCF	-1.340e02	-1.346e02	3e-06	50.9	4e-14	5e-14	535.6
AFBB	-1.340e02	-1.346e02	6e-07	84.6	8e-14	0e00	377.7
glutamine, $n = 16517, p = 29$							
SCF	-9.087e01	-9.184e01	3e-06	49.2	3e-14	8e-14	436.8
AFBB	-9.087e01	-9.184e01	7e-07	96.2	9e-14	0e00	373.4
graphene16, $n = 3071, p = 37$							
SCF	-9.358e01	-9.400e01	6e-03	200.0	2e-14	5e-04	1058.8
AFBB	-9.358e01	-9.405e01	4e-06	219.5	4e-13	0e00	176.2
graphene30, $n = 12279, p = 67$							
SCF	-1.726e+02	-1.735e+02	9e-03	200.0	3e-14	3e-04	9225.4
AFBB	-1.726e+02	-1.736e+02	6e-07	294.2	2e-14	0e00	2007.3
h2o, $n = 2103, p = 4$							
SCF	-1.643e01	-1.644e01	1e-06	14.3	4e-15	7e-14	4.8
AFBB	-1.643e01	-1.644e01	9e-08	68.6	2e-15	0e00	6.2
hnco, $n = 2103, p = 8$							
SCF	-2.830e01	-2.863e01	1e-06	15.0	6e-15	0e00	10.5
AFBB	-2.830e01	-2.863e01	4e-07	104.7	3e-14	9e-14	14.6
nic, $n = 251, p = 7$							
SCF	-2.053e01	-2.354e01	1e-06	14.0	3e-15	0e00	4.0
AFBB	-2.053e01	-2.354e01	1e-06	52.7	1e-14	3e-13	3.5
pentacene, $n = 44791, p = 51$							
SCF	-1.311e+02	-1.319e+02	4e-06	65.9	5e-14	5e-12	3253.1
AFBB	-1.311e+02	-1.319e+02	7e-07	118.7	2e-14	0e00	2046.5
ptnio, $n = 4069, p = 43$							
SCF	-1.983e02	-2.268e02	8e-06	200.0	2e-14	2e-09	946.7
AFBB	-1.983e02	-2.268e02	4e-06	459.6	1e-14	0e00	480.2
qdot, $n = 2103, p = 8$							
SCF	2.850e01	2.771e01	2e-02	200.0	4e-15	2e-04	106.5
AFBB	2.850e01	2.770e01	3e-04	1000.0	3e-15	0e00	81.2
si2h4, $n = 2103, p = 6$							
SCF	-5.874e00	-6.301e00	1e-06	23.9	2e-14	2e-13	9.2
AFBB	-5.874e00	-6.301e00	4e-07	79.8	3e-15	0e00	9.6
sih4, $n = 2103, p = 4$							
SCF	-6.154e00	-6.177e00	1e-06	11.6	4e-15	2e-13	4.9
AFBB	-6.154e00	-6.177e00	8e-08	55.2	3e-15	0e00	6.1

terms of the total energy and the residual, especially for the large molecules. In particular, for the most hard problem “graphene30” in our test, AFBB is not only significantly faster than SCF, but also returns a better solution with smaller total energy and residual.

6.4 Maximization of sums of heterogeneous quadratic functions on the Stiefel manifold from statistics

In [6], Balogh *et al.* gave a test problem with known global optimal solutions as follows:

$$\min_{X \in \mathbb{R}^{n \times p}} \sum_{i=1}^p X_{(i)}^T A_i X_{(i)}, \quad \text{s.t. } X^T X = I_p, \quad (6.8)$$

where for $1 \leq i \leq p$, $A_i = \text{Diag}(n(i-1)+1, \dots, n(i-1)+i-1, l_i, n(i-1)+i+1, \dots, ni)$ and $l_i < 0$. This is a special maximization of sums of heterogeneous quadratic functions on the Stiefel manifold from statistics

Table 6.6 Numerical results of AFBB $D_{1/2}$ and AFBB $D_{1/4}$ for problem (6.8)

p	a.obj ⁰	f^*	AFBB $D_{1/2}$			AFBB $D_{1/4}$			
			a.obj	a.nfe	a.err	a.obj	a.nfe	a.err	a.s.ratio
random l									
2	8.003e03	-1.304e00	-1.304e00	403.9	4e-07	-1.304e00	405.9	4e-07	0.5
10	2.000e05	-5.133e00	-5.133e00	755.1	1e-06	-5.133e00	598.7	4e-07	-20.7
20	7.998e05	-8.902e00	-8.902e00	839.8	7e-07	-8.902e00	615.4	4e-07	-26.7
40	3.199e06	-1.954e01	-1.954e01	905.8	1e-06	-1.954e01	640.7	5e-07	-29.3
60	7.198e06	-3.096e01	-3.096e01	962.8	8e-07	-3.096e01	692.0	4e-07	-28.1
80	1.280e07	-4.275e01	-4.275e01	977.0	8e-07	-4.275e01	688.4	4e-07	-29.5
100	2.000e07	-5.087e01	-5.087e01	1032.5	1e-06	-5.087e01	714.9	4e-07	-30.8
$l_i = -1, i = 1, \dots, p$									
2	7.997e03	-2.000e00	-2.000e00	391.1	3e-07	-2.000e00	397.6	2e-07	1.7
10	2.000e05	-1.000e01	-1.000e01	726.5	7e-07	-1.000e01	553.0	3e-07	-23.9
20	7.998e05	-2.000e01	-2.000e01	822.7	1e-06	-2.000e01	597.2	4e-07	-27.4
40	3.199e06	-4.000e01	-4.000e01	911.5	8e-07	-4.000e01	648.4	3e-07	-28.9
60	7.198e06	-6.000e01	-6.000e01	890.7	4e-06	-6.000e01	645.6	4e-07	-27.5
80	1.280e07	-8.000e01	-8.000e01	920.5	3e-06	-8.000e01	648.5	4e-07	-29.6
100	2.000e07	-1.000e02	-1.000e02	942.0	8e-07	-1.000e02	696.2	4e-07	-26.1

(it was also considered in [9]). By Proposition 1 in [6], we know that $\{(\pm e_1, \pm e_2, \dots, \pm e_p) : \pm e_i \in \{e_i, -e_i\}\}$ is the set of minimum points of problem (6.8) and $\sum_{i=1}^k l_i$ is the optimal function value. It was pointed out in [6] that there were no efficient numerical methods to solve problem (6.8) yet. Nevertheless, our numerical tests show that the AFBB method works well.

In this experiment, we reset $\epsilon = 10^{-6}$, $\epsilon_x = 10^{-6}$, $\epsilon_f = 10^{-10}$ and fixed $n = 4000$. For $1 \leq p \leq n$ and $1 \leq i \leq p$, we generated l_i in two ways, one is that l_i is uniformly distributed in $[0, 1]$, the other is that $l_i = -1$. We ran our AFBB methods 50 times from different random initial points for each test.

Firstly, we investigate the effect of using different descent directions. We call AFBB methods using the descent directions $D_{1/2}$ and $D_{1/4}$ as AFBB $D_{1/2}$ and AFBB $D_{1/4}$, respectively. The numerical results are shown in Table 6.6. In this table, “a.obj⁰” and “a.obj” represent the average initial function value and returned function value by each method, respectively. The terms f^* , “a.nfe” and “a.err” denote the optimal function value, the average total number of function evaluations and the average relative error between the function value given by each method and f^* , respectively. We use “a.s.ratio” to stand for the average saved ratio of AFBB $D_{1/4}$ which is computed as $100(\text{nfe}_{\rho=1/4} - \text{nfe}_{\rho=1/2})/\text{nfe}_{\rho=1/2}$. From this table, we know that the two methods can always find nearly global solutions in acceptable iterations. Averagely, AFBB $D_{1/4}$ can always find a better solution with smaller function value about 25% faster than AFBB $D_{1/2}$ for most of the tests. This may be due to the fact that $D_{1/4}$ is the steepest descent direction corresponding to the *Euclidean metric*, that is,

$$D_{1/4} = \arg \min_{D \in \mathcal{T}_X} -\frac{\langle G, D \rangle}{\|D\|_F}.$$

Secondly, we consider the effect of using different functions $g(\tau)$ in forming $J(\tau)$. Here, we choose $\rho = 0.5$. We tested two choices: $g_1(\tau) = \tau/2$ which is the default in update scheme (3.15) and $g_2(\tau) = \frac{1}{2}\tau e^{-\tau}$. We call AFBB methods using $g_1(\tau)$ and $g_2(\tau)$ as AFBBg1 and AFBBg2, respectively. From Table 6.7, we see that AFBBg2 improves the performance of AFBBg1 by 15% or more for most tests in terms of the average total number of function evaluations. Meanwhile, it can always return a solution with smaller function value. Nevertheless, it remains under investigation how to seek a better $g(\tau)$.

At the end of this subsection, we remark that $X^T G \equiv G^T X$ happens in the nearest low-rank correlation matrix problem and the Kohn-Sham total energy minimization. In this case, the term $X^T D_\rho$ vanishes and $g(\tau)$ will not play a role in forming $J(\tau)$.

7 Conclusion

In this paper, we have proposed a feasible method for optimization on the Stiefel manifold. Our main contributions are twofold. Firstly, we proposed a new framework of constraint preserving update schemes for optimization on the Stiefel manifold by decomposing each feasible point into the range space of X and the null space of X^T . While this new framework can unify many existing schemes, we also investigated a new update scheme with low complexity. Note that our framework can be viewed as a retraction as well.

Table 6.7 Numerical results of AFBBg1 and AFBBg2 for problem (6.8)

p	a.obj ⁰	f^*	AFBBg1			AFBBg2			
			a.obj	a.nfe	a.err	a.obj	a.nfe	a.err	a.s.ratio
random l									
2	8.004e03	-5.653e-01	-5.653e-01	409.1	1e-06	-5.653e-01	436.4	7e-07	6.7
10	2.000e05	-2.599e00	-2.599e00	782.7	9e-07	-2.599e00	670.0	4e-07	-14.4
20	7.998e05	-1.054e01	-1.054e01	839.7	7e-07	-1.054e01	710.3	3e-07	-15.4
40	3.199e06	-2.007e01	-2.007e01	873.4	8e-07	-2.007e01	718.8	3e-07	-17.7
60	7.198e06	-2.790e01	-2.790e01	941.3	8e-07	-2.790e01	789.1	6e-07	-16.2
80	1.280e07	-4.140e01	-4.140e01	967.8	8e-07	-4.140e01	825.7	4e-07	-14.7
100	2.000e07	-4.158e01	-4.158e01	1039.8	8e-07	-4.158e01	856.0	4e-07	-17.7
$l_i = -1, i = 1, \dots, p$									
2	7.998e03	-2.000e00	-2.000e00	401.8	2e-07	-2.000e00	402.2	3e-07	0.1
10	2.000e05	-1.000e01	-1.000e01	707.5	2e-06	-1.000e01	583.9	3e-07	-17.5
20	7.998e05	-2.000e01	-2.000e01	816.5	6e-07	-2.000e01	717.6	3e-07	-12.1
40	3.199e06	-4.000e01	-4.000e01	882.5	9e-07	-4.000e01	698.3	3e-07	-20.9
60	7.198e06	-6.000e01	-6.000e01	931.1	1e-06	-6.000e01	741.4	3e-07	-20.4
80	1.280e07	-8.000e01	-8.000e01	952.3	8e-07	-8.000e01	799.8	4e-07	-16.0
100	2.000e07	-1.000e02	-1.000e02	987.5	2e-06	-1.000e02	869.4	3e-07	-12.0

Secondly, we proposed the adaptive feasible Barzilai-Borwein-like method and proved its global convergence. To our knowledge, this result is the first global convergence result for the feasible method with nonmonotone linesearch for optimization on the Stiefel manifold. Moreover, the corresponding extension to the generalized Stiefel manifold was also considered.

We have tested our AFBB method on a variety of problems to illustrate its efficiency. Particularly, for the nearest low-rank correlation matrix problem, AFBB performs better than the three state-of-the-art algorithms. Note that the PenCorr, one of the three algorithms, can deal with more general problems. For Kohn-Sham total energy minimization, its superiority is obvious especially for large molecules, and hence it is quite promising to use our AFBB for large-scale electronic structure calculations. Since our update scheme can be done by moving along any given tangent direction, we also explore the effect of different descent directions and different $g(\tau)$'s on the performance of AFBB.

As our framework can unify several famous retractions, it is natural and interesting to argue which one can make the AFBB method find the global optimal solution with highest probability and at the fastest speed. One possible approach is to consider the subspace techniques. This remains under investigation.

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