



A Theory of the NEPv Approach for Optimization on the Stiefel Manifold

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Abstract

The NEPv approach has been increasingly used lately for optimization on the Stiefel manifold arising from machine learning. General speaking, the approach first turns the first order optimality condition into a nonlinear eigenvalue problem with eigenvector dependency (NEPv) and then solve the nonlinear problem via some variations of the self-consistent-field (SCF) iteration. The difficulty, however, lies in designing a proper SCF iteration so that a maximizer is found at the end. Currently, each use of the approach is very much individualized, especially in its convergence analysis phase to show that the approach does work or otherwise. Related, the NPDo approach is recently proposed for the sum of coupled traces and it seeks to turn the first order optimality condition into a nonlinear polar decomposition with orthogonal factor dependency (NPDo). In this paper, two unifying frameworks are established, one for each approach. Each framework is built upon a basic assumption, under which globally convergence to a stationary point is guaranteed and during the SCF iterative process that leads to the stationary point, the objective function increases monotonically. Also the notion of atomic function for each approach is proposed, and the atomic functions include commonly used matrix traces of linear and quadratic forms as special ones. It is shown that the basic assumptions of the approaches are satisfied by their respective atomic functions and, more importantly, by convex compositions of their respective atomic functions. Together they provide a large collection of objectives for which either one of approaches or both are guaranteed to work, respectively.

Keywords Nonlinear eigenvalue problem with eigenvector dependency · Nonlinear polar decomposition with orthogonal factor dependency · NEPv · NPDo · Atomic function · Convergence · Self-consistent-field iteration · SCF

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1 Introduction

Optimization on the Stiefel and Grassmann manifold is constrained optimization with orthogonality constraints, and optimization problems as such can be and often are handled by the method of Lagrange multipliers. In a milestone paper, Edelman, Ariasz, and Smith [18] in 1999 advocated to treat orthogonality constraints from the geometrical point of view and established a unifying framework to adapt standard optimization techniques, such as Newton's method and conjugate gradient methods, for better understanding and computational efficiency. Since then, there have been a long list of research articles on optimization on matrix manifolds seeking the benefit of the view and extending most generic optimization techniques such as gradient descent/ascent methods, trusted region methods, and many others, to optimization on matrix manifolds [1]. Most conveniently, there are software toolboxes `manopt` [12] and `STOP` [22, 66] for optimization on manifolds that have been made available online to allow anyone to try out.

By and large, aforementioned progresses, while successful, are about skillful adaptations of classical optimization techniques for optimization on Riemannian manifolds (see [1, 12, 18, 22, 66, 70] and references therein), following the geometrical point of view [18]. Recently, we witnessed several optimization problems on the Stiefel and Grassmann manifolds emerging from data science applications. Prominent examples include the orthogonal linear discriminant analysis (OLDA) and several others that will be listed momentarily in Table 1. In those problems, matrices of large/huge sizes may be involved and objective functions are made from one or more matrix traces to serve various modeling objectives for underlying applications. Apart from the trend of adapting generic optimization techniques, efforts and progresses have been made along a different route of designing customized optimization methods through taking advantage of structures in objective functions and leveraging mature numerical linear algebra (NLA) techniques and software packages so as to gain even more efficiency (see [68, 75–78] and references therein). This new route is the NEPv approach, where NEPv stands for *nonlinear eigenvalue problem with eigenvector dependency* coined by [14], and has been successfully demonstrated on several machine learning applications in these papers, where theoretical analysis seems to be much individualized. The goal of this paper is to establish a unifying framework that streamlines the NEPv approach among these papers and guides new applications of the approach to emerging optimization on Riemannian manifolds from data science and other disciplines. In addition, we will also establish another unifying framework for the NPDo approach, where NPDo stands for *nonlinear polar decomposition with orthogonal polar factor dependency*, along the line of [67].

A maximization problem on the Stiefel manifold in its generality takes the form

$$\max_{P^T P = I_k} f(P), \quad (1.1)$$

Table 1 Objective functions in the literature

- $\text{tr}(P^T A P)$, the symmetric eigenvalue problem (SEP) [17, 24, 52, 57], where $\text{tr}(\cdot)$ is the matrix-trace function;
- $\frac{\text{tr}(P^T A P)}{\text{tr}(P^T B P)}$, the orthogonal linear discriminant analysis (OLDA) [14, 21, 49, 73, 74];
- $\frac{\text{tr}(P^T A P)}{\text{tr}(P^T B P)} + \text{tr}(P^T C P)$, the sum of the trace ratios (SumTR) [76, 77];
- $\frac{\text{tr}(P^T D)}{\sqrt{\text{tr}(P^T B P)}}$, the orthogonal canonical correlation analysis (OCCA) [16, 78];
- $\frac{\text{tr}(P^T A P + P^T D)}{[\text{tr}(P^T B P)]^\theta}$ for $0 \leq \theta \leq 1$, the θ -trace ratio problem (Θ TR) [68];
- $\text{tr}(P^T A P + P^T D)$, the MAXBET subproblem (MBSUB) [46, 62, 64, 67, 68, 75];
- $\sum_{i=1}^N \text{tr}(P_i^T A_i P_i + P_i^T D_i)$, the sum of coupled traces (SumCT) [6, 9, 10, 55, 67], where P is column-partitioned as $[P_1, P_2, \dots, P_N]$;
- $\phi(\mathbf{x})$ with $\mathbf{x} = [\text{tr}(P^T A_1 P), \dots, \text{tr}(P^T A_N P)]^T$, trace composition (TrCP), where $\phi(\mathbf{x})$ is a scalar function in $\mathbf{x} \in \mathbb{R}^n$;
- $\sum_{i=1}^N \|P^T A_i P\|_F^2$, the uniform multidimensional scaling (UMDS) [80];
- $\text{tr}(P^T A P) + \phi(\text{diag}(P P^T))$ [18], the density functional theory (DFT) of Hohenberg and Kohn [27] and Kohn and Sham [34], where $\phi(\mathbf{x})$ is a scalar function in $\mathbf{x} \in \mathbb{R}^n$, and $\text{diag}(P P^T)$ extracts the diagonal entries of $P P^T$ into a vector.

A , B , and all A_i are symmetric and may or may not be positive semidefinite

where $P \in \mathbb{R}^{n \times k}$ with $1 \leq k \leq n$ (usually $k \ll n$), I_k is the $k \times k$ identity matrix, and objective function $f(P)$ is defined on some neighborhood of the Stiefel manifold

$$\text{St}(k, n) := \{P \in \mathbb{R}^{n \times k} : P^T P = I_k\} \subset \mathbb{R}^{n \times k} \quad (1.2)$$

and is differentiable in the neighborhood. Specifically, f is well defined and differentiable on some neighborhood

$$\text{St}_\delta(k, n) := \{P \in \mathbb{R}^{n \times k} : \|P^T P - I_k\| < \delta\} \quad (1.3)$$

of $\text{St}(k, n)$, where $0 < \delta$ is a constant and $\|\cdot\|$ is some matrix norm.

Although in general objective function f can be any differentiable function that is well-defined on $\text{St}_\delta(k, n)$, in practical applications often f is a composition of matrix traces of linear or quadratic forms in P . A partial list of most commonly used ones in the literature is given in Table 1, where A , B , D , all A_i and D_i are constant matrices, and A , B , and all A_i are symmetric and may or may not be positive semidefinite. All but the last two in the table are clearly composed of one or more matrix traces depending on P , and the last two are no exceptions! To see that, we notice

$$\|P^T A_i P\|_F^2 = \text{tr}((P^T A_i P)^2), \quad [\text{diag}(P P^T)]_{(i)} = \text{tr}(\mathbf{e}_i^T P P^T \mathbf{e}_i) = \text{tr}(P^T \mathbf{e}_i \mathbf{e}_i^T P),$$

where $[\text{diag}(P P^T)]_{(i)}$ is the i th entries of vector $\text{diag}(P P^T)$ and $\mathbf{e}_i$ is the i th column of the identity matrix. TrCP is included in Table 1 to represent a broad class of objective functions some of which may have possibly appeared in the past literature, for example,

the monotone nonlinear eigenvector problem (mNEPv) [5]: $\sum_{i=1}^N \psi_i(\mathbf{p}^T A_i \mathbf{p})$ where $\mathbf{p} \in \mathbb{R}^n$ and each $\psi_i(\cdot)$ is a single-variable convex function in $\mathbb{R}$.

Beyond Table 1, there are matrix optimization problems that can be reduced to one alike for numerical purposes. For example, the following least-squared minimization

$$\min_{P \in \text{St}(k, n)} \|CP - B\|_F^2 \quad (1.4)$$

can be reformulated into the MAXBET subproblem in the table with $A = -C^T C$ and $D = C^T B/2$. It can be found in many real world applications including the orthogonal least squares regression (OLSR) for feature extraction [50, 81], the multidimensional similarity structure analysis (SSA) [11, chapter 19], and the unbalanced Procrustes problem [15, 18, 19, 25, 30, 75, 79].

1.1 Review of the NEPv and NPDo Approach

Maximizing trace $\text{tr}(P^T A P)$, at the top of Table 1, has an explicit solution in terms of the eigenvalues and eigenvectors of symmetric matrix A , known as Fan's trace maximization principle [20, 29], p. 248 (see also [43–45] for later extensions). For that reason, it is often regarded indistinguishably as the symmetric eigenvalue problem (SEP) that is ubiquitous throughout mathematics, science, engineering, and especially today's data sciences. It has been well studied theoretically and numerically in NLA [17, 24, 41, 52, 56, 57] and often serves as the most distinguished illustrating example for optimization on the Stiefel and Grassmann manifolds [1, 18]. For the rest of the objective functions, the so-called NEPv approach and NPDo approach have been investigated for numerically solving the associated optimization problems.

The basic idea of the NEPv approach [68, 75, 78] is as follows:

1. Establish an NEPv

$$H(P)P = P\Omega, \quad P \in \text{St}(k, n) \quad (1.5)$$

that either is or can be made equivalent to the first order optimality condition, also known as the KKT condition (see sect. 2 for detail), where $H(P) \in \mathbb{R}^{n \times n}$ is a symmetric matrix-valued function dependent of P ;

2. Solve NEPv (1.5) by the self-consistent-field (SCF) iteration: given P_0 , iteratively

compute partial eigendecomposition $H(P_{i-1})\hat{P}_i = \hat{P}_i\hat{\Omega}_i$ associated with the k largest (or smallest) eigenvalues of $H(P_{i-1})$ for $\hat{P}_i \in \text{St}(k, n)$, and postprocess $\hat{P}_i$ to P_i .

(1.6)

While the idea of SCF seems rather natural, its convergence analysis is not and often has to be done on a case-by-case basis where novelty lies [4, 14, 47, 68, 78]. In particular, it is critical to know what part of the spectrum of $H(P_{i-1})$ whose partial eigendecomposition in (1.6) is about so as to move the objective function f up. The

SCF iteration (1.6) differs from the classical SCF for solving the discretized Kohn-Sham equations in its postprocessing from $\widehat{P}_i$ to P_i , which is not needed in the classical SCF for NEPv that is *right-unitarily invariant* (see Definition 2.1 in the next section). Indiscriminately, we use SCF to refer to both the classical SCF and SCF (1.6) when no confusion arises.

SCF, in connection with the NEPv approach, has been one of the default methods for solving the discretized Kohn-Sham equations in the density function theory [58, 71]. Since then, the same idea has been proven effective in several data science applications (see Table 1): OLDA [73, 74], OCCA [78], MBSUB [67, 68], and Θ TR [68]. Later, we will show that the approach will work on UMDS [80] and TrCP, too.

Related, in [67], the NPDo approach is proposed to numerically maximize SumCT. A similar idea appeared before in [10] where each P_i is a vector and $D_i = 0$. The basic idea of the NPDo approach is as follows:

1. Establish the first order optimality condition, which takes the form

$$\mathcal{H}(P) = P \Lambda, \quad P \in \text{St}(k, n), \quad (1.7)$$

where $\mathcal{H}(P) \in \mathbb{R}^{n \times k}$ is the Euclidean gradient of $f(P)$ and, provably, Λ is positive semidefinite at optimality;

2. Solve NPDo (1.7) by the self-consistent-field iteration: given P_0 , iteratively

compute polar decomposition¹ $\mathcal{H}(P_{i-1}) = \widehat{P}_i \Lambda_i$ of $\mathcal{H}(P_{i-1})$ for $\widehat{P}_i \in \text{St}(k, n)$, and postprocess $\widehat{P}_i$ to P_i .

(1.8)

A key prerequisite of the NPDo approach is that, at an optimality P_* , (1.7) is a polar decomposition of $\mathcal{H}(P_*)$. This is proved in [67] for SumCT under the condition that all A_i are positive semidefinite, and later in this paper, we will prove it for more optimization problems, including those in Table 1 that do not appear in ratio forms. As $\mathcal{H}(P)$ to be decomposed also depends on orthogonal polar factor P , we call it a *nonlinear polar decomposition with orthogonal polar factor dependency*, or NPDo in short. Polar decomposition is often computed via SVD [24] which can be viewed as a special SEP [17]. For that reason, NPDo may also be regarded as another kind of NEPv.

1.2 Contributions

We observe that all objective functions in Table 1 are compositions of some scalar functions, matrix traces such as $\text{tr}(P^T A P)$ and $\text{tr}(P^T D)$ in fact. For example, in

¹ Throughout this paper, a polar decomposition of $B \in \mathbb{R}^{n \times k}$ ($k \leq n$) refers to $B = P \Omega$ with $P \in \text{St}(k, n)$ and positive semidefinite $\Omega \in \mathbb{R}^{k \times k}$. $\Omega = (B^T B)^{1/2}$ is always unique, but $P \in \text{St}(k, n)$ is unique if and only if $\text{rank}(B) = k$ [38]. The matrix P in the decomposition is called an *orthogonal polar factor* of B .

Θ TR [68], $f(P)$ can be expressed as a composition of three functions $\text{tr}(P^T B P)$, $\text{tr}(P^T A P)$, and $\text{tr}(P^T D)$ by ϕ :

$$f(P) = \phi \circ T(P) \quad \text{with } T(P) = \begin{bmatrix} \text{tr}(P^T B P) \\ \text{tr}(P^T A P) \\ \text{tr}(P^T D) \end{bmatrix}, \quad \phi(x_1, x_2, x_3) = \frac{x_2 + x_3}{x_1^\theta}, \quad (1.9)$$

i.e., it is a composition of the 3-variable function ϕ with three matrix traces: $\text{tr}(P^T B P)$, $\text{tr}(P^T A P)$, and $\text{tr}(P^T D)$. Each trace serves as a singleton unit of function in P that does seem to be decomposable into finer units for any benefit of study and numerical computations. For that reason, later in this paper, we shall call such a singleton unit of function in P an *atomic* function. In its generality, an atomic function is defined upon satisfying two basic conditions but may not necessarily be in a matrix trace form.

Unfortunately, ϕ in (1.9) is not convex in $\mathbf{x}$, but ϕ^2 for $0 \leq \theta \leq 1/2$ is (more detail can be found in Remark 8.1 in sect. 8). Except for OLDA and SumTR, all objective functions in Table 1, either themselves or squared (for OCCA and Θ TR with $0 \leq \theta \leq 1/2$), are convex compositions of atomic functions, assuming ϕ for both TrCP and DFT are convex.

Our main contributions of this paper are summarized as follows:

1. Creating two unifying frameworks of the NEPv and NPDo approaches, respectively, to numerically solve (1.1) by their corresponding SCF iterations, with guaranteed convergence to a KKT point that satisfies certain necessary conditions to be established for a maximizer;
2. Introducing the notion of *atomic functions* in P with respect to both approaches, and showing that,

$$[\text{tr}((P^T A P)^m)]^s, \quad [\text{tr}((P^T D)^m)]^s, \quad (1.10)$$

are concrete atomic functions, where $m \geq 1$ is an integer, $s \geq 1$ is a scalar, and A is symmetric but may or may not be a positive semidefinite matrix depending on the circumstances;

3. Showing the NEPv and NPDo approaches work on each individual atomic function for the approach and, more importantly, any convex composition $\phi \circ T$ of their respective atomic functions, where $\phi(\mathbf{x})$ for $\mathbf{x} \in \mathcal{D} \subseteq \mathbb{R}^N$ is convex, each entry of $T(P) \in \mathbb{R}^N$ is an atomic function, and the partial derivative of ϕ with respect to an entry may be required nonnegative, depending on the particular atomic function that occupies the entry.

Although the two approaches look very much parallel to each other in presentation, there are differences in applicabilities and numerical implementations, making them somewhat complementary to each other. A brief comparison of the two approaches is given in sect. 9.

1.3 Organization and Notation

After stating the KKT condition of maximization problem (1.1) in sect. 2, we divide the rest of this paper into two parts. With maximization problem (1.1) in mind, in Part I we focus on the NPDo approach to solve the KKT condition in three sections: sect. 3 creates a unifying NPDo framework, including **the NPDo Ansatz** to guarantee that the KKT condition is an NPDo at optimality of (1.1), the global convergence of the SCF iteration (1.8); sect. 4 develops a general theory that governs atomic functions for NPDo and show that matrix-trace functions, $\text{tr}((P^T D)^m)$ and $\text{tr}((P^T A P)^m)$ and their powers of order higher than 1, are atomic functions; finally in sect. 5, we investigate the NPDo approach for convex compositions $\phi \circ T(P)$ of atomic functions and elaborate on a few $T(P) \in \mathbb{R}^N$ of common matrix-trace functions that include some of those appearing in Table 1. In Part II, we focus on the NEPv approach for the same purpose. It also has three sections to address the corresponding issues: a unifying framework built upon an ansatz – **the NEPv Ansatz**, the global convergence of the SCF iteration (1.6), atomic functions for NEPv, and their convex compositions $\phi \circ T(P)$ along with a few $T(P) \in \mathbb{R}^N$ of common matrix-trace functions. Both frameworks are very similar in appearance, but there are subtle differences in requirements and ease to use, making each have advantages over the other in circumstances. A brief comparison to highlight the major differences between the two approaches is made in sect. 9. Concluding remarks are drawn in sect. 10. There are two appendices at the end to supplement necessary material. Appendix A reviews the canonical angles between subspaces of equal dimensions; appendix B cites a couple of well known inequalities for scalars and establishes a few new ones for matrices to serve the main body of the paper.

For notation, we follow the following convention:

- $\mathbb{R}^{m \times n}$ is the set of $m \times n$ real matrices, $\mathbb{R}^n = \mathbb{R}^{n \times 1}$, and $\mathbb{R} = \mathbb{R}^1$;
- As in [1], $\text{St}(k, n)$ in (1.2) denotes the Stiefel manifold, while $\text{St}_\delta(k, n)$ in (1.3) is some neighborhood of it; In particular, $\text{St}(k, k)$ contains all k -by- k orthogonal matrices; Also frequently, given $D \in \mathbb{R}^{n \times k}$,

$$\text{St}(k, n)_{D+} := \{X \in \text{St}(k, n) : X^T D \succeq 0\};$$

- $I_n \in \mathbb{R}^{n \times n}$ is the identity matrix or simply I if its size is clear from the context, and $\mathbf{e}_j$ is the j th column of I of an apt size;
- B^T stands for the transpose of a matrix/vector B ;
- $\mathcal{R}(B)$ is the column subspace of a matrix B , spanned by its columns, whose dimension is $\text{rank}(B)$, the rank of B ;
- For $B \in \mathbb{R}^{m \times n}$, unless otherwise explicitly stated, its SVD refers to the one $B = U \Sigma V^T$, also known as the *thin* SVD of B , with

$$\Sigma = \text{diag}(\sigma_1(B), \sigma_2(B), \dots, \sigma_s(B)) \in \mathbb{R}^{s \times s}, \quad U \in \text{St}(s, m), \quad V \in \text{St}(s, n),$$

where $s = \min\{m, n\}$, the singular values $\sigma_j(B)$ are always arranged decreasingly as

$$\sigma_1(B) \geq \sigma_2(B) \geq \dots \geq \sigma_s(B) \geq 0,$$

and $\sigma_{\min}(B) = \sigma_s(B)$; Accordingly, $\|B\|_2$, $\|B\|_F$, and $\|B\|_{\text{tr}}$ are the spectral, Frobenius, and trace norms of B :

$$\|B\|_2 = \sigma_1(B), \quad \|B\|_F = \left(\sum_{i=1}^s [\sigma_i(B)]^2 \right)^{1/2}, \quad \|B\|_{\text{tr}} = \sum_{i=1}^s \sigma_i(B),$$

respectively; The trace norm is also known as the nuclear norm;

- For a symmetric matrix $A \in \mathbb{R}^{n \times n}$, $\text{eig}(A) = \{\lambda_i(A)\}_{i=1}^n$ denotes the set of its eigenvalues (counted by multiplicities) arranged in the decreasing order:

$$\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_n(A),$$

and $S_k(A) = \sum_{i=1}^k \lambda_i(A)$ and $s_k(A) = \sum_{i=1}^k \lambda_{n-i+1}(A)$, the sum of the k largest eigenvalues and that of the k smallest eigenvalues of A , respectively;

- A matrix $A > 0$ (≥ 0) means that it is symmetric and positive definite (semi-definite), and accordingly $A < 0$ (≤ 0) if $-A > 0$ (≥ 0).

2 KKT Condition

Consider maximization problem (1.1) on the Stiefel manifold $\text{St}(k, n)$ in its generality. For $P = [p_{ij}] \in \text{St}_\delta(k, n)$ defined in (1.3), denote by

$$\mathcal{H}(P) := \frac{\partial f(P)}{\partial P} \in \mathbb{R}^{n \times k} \quad \text{with its } (i, j)\text{th entry } \frac{\partial f(P)}{\partial p_{ij}}, \quad (2.1)$$

the partial derivative of $f(P)$ with respect to P as a matrix variable in $\mathbb{R}^{n \times k}$, where all entries of P are treated as independent. It is also known as the *Euclidean gradient* in recent literature. Throughout this paper, notation $\mathcal{H}(P)$ is reserved for the Euclidean gradient of objective function f within the context.

As an optimization problem on the Stiefel manifold, the first order optimality condition (1.1), also known as the KKT condition, is given by setting the Riemannian gradient of f with respect to the Stiefel manifold $\text{St}(k, n)$ at P to 0. It is well-known that the Riemannian gradient of a smooth function f with respect to the Stiefel manifold at $P \in \text{St}(k, n)$ can be calculated according to (see, e.g., [1, (3.37)])

$$\text{grad } f|_{\text{St}(k, n)}(P) = \Pi_P(\mathcal{H}(P)) = \mathcal{H}(P) - P \cdot \text{sym}(P^T \mathcal{H}(P)), \quad (2.2)$$

where the projection $\Pi_P(Z) := P - P \text{sym}(P^T Z)$ with $\text{sym}(P^T Z) = (P^T Z + Z^T P)/2$. Setting $\text{grad } f|_{\text{St}(k, n)}(P) = 0$ yields the first-order optimality condition:

$$\mathcal{H}(P) = P \Lambda \quad \text{with } \Lambda^T = \Lambda \in \mathbb{R}^{k \times k}, \quad P \in \text{St}(k, n), \quad (2.3)$$

where $\Lambda = \text{sym}(P^T \mathcal{H}(P))$. The exact form of Λ , however, is not important, but its symmetry is, for example, it implies that $P^T \mathcal{H}(P)$ is symmetric at any KKT

point P . The KKT condition (2.3) can also be inferred from treating $P \in \text{St}(k, n)$ as the orthogonality constraint $P^T P = I_k$ and then using the classical method of Lagrange multipliers for constrained optimization [51]. Geometrically, the condition (2.3) simply asks for that the Euclidean gradient belongs to the normal space to the Stiefel manifold at P .

For simple functions, $f(P) = \text{tr}(P^T D)$ or $\text{tr}(P^T A P)$, the KKT condition (2.3) can be considered as solved. In fact, for the two functions, (2.3) becomes $D = P \Lambda$ or $2AP = P \Lambda$, respectively, which, in consideration of (1.1), tell us that a maximizer can be taken to be an orthogonal polar factor of D [29, 78], or an orthonormal basis matrix of the eigenspace of A associated with its k largest eigenvalues [43–45, 59], respectively. In both cases, the maximizer as described is considered a close form solution to the respective problem because of the numerical maturity by existing NLA techniques and software [2, 3, 17, 24, 41, 52].

In general, equation (2.3) is not an easy equation to solve in searching for a maximizer of (1.1) with guarantee. For example, in the MAXBET subproblem, simply $f(P) = \text{tr}(P^T D) + \text{tr}(P^T A P)$, the sum of the two simple matrix-trace functions and (2.3) becomes $2AP + D = P \Lambda$ for which there is no existing NLA technique that yields a solution to maximize $f(P)$ with guarantee. Having said that, we point out that the eigenvalue-based method [75], which falls into the NEPv approach, has been demonstrated to be numerically efficient [75] and often produces global maximizers. The MAXBET subproblem is a special case of SumCT. As such, in [67], the NPDo approach has also been successfully applied.

We now formally define the notion of a function being right-unitarily invariant, originally introduced in [47]. It is an important concept that we will frequently refer to in the rest of this paper. However, our definition here differs from [47, Definition 2.1] slightly in that we limit the domain to some neighborhood $\text{St}_\delta(k, n)$ of the Stiefel manifold $\text{St}(k, n)$, rather than the entire space $\mathbb{R}^{n \times k}$ used in [47]. Carefully going through [47], one can see that our definition here is actually sufficient for the development in [47] as it is here.

Definition 2.1 A function $F : \text{St}_\delta(k, n) \rightarrow \mathbb{R}^{p \times q}$ is said *right-unitarily invariant* if

$$F(PQ) \equiv F(P) \quad \text{for } P \in \text{St}_\delta(k, n) \text{ and } Q \in \text{St}(k, k).$$

Part I

The NPDo Approach

3 The NPDo Framework

In [67], an NPDo approach is proposed to numerically maximize the sum of coupled traces (SumCT) in Table 1. It is an SCF iterative procedure (1.8) that solves the KKT condition (2.3) for its solution with an eye on maximizing the sum. Our general framework in this section is inspired by and bears similarity to the developments there, but in more abstract terms.

3.1 The NPDo Ansatz

The success of the NPDo approach in [67] rests on a monotonicity lemma which motivates us to formulate the following ansatz to build our framework upon. The key point of the assumption is the ability to generate an improved approximate maximizer $\tilde{P}$ from a given one P , where both the given P and the improved $\tilde{P}$ may have to come out of possibly a strict subset $\mathbb{P}$ of $\text{St}(k, n)$. What $\mathbb{P}$ to use depends on the underlying optimization problem (1.1) at hand, as we will repeatedly demonstrate later by concrete examples.

The NPDo Ansatz. Let function f be defined in some neighborhood $\text{St}_\delta(k, n)$ of $\text{St}(k, n)$, and denote by $\mathcal{H}(P) = \frac{\partial f(P)}{\partial P}$. Given $P \in \mathbb{P} \subseteq \text{St}(k, n)$ and $\hat{P} \in \text{St}(k, n)$, if

$$\text{tr}(\hat{P}^T \mathcal{H}(P)) \geq \text{tr}(P^T \mathcal{H}(P)) + \eta \quad \text{for some } \eta \in \mathbb{R}, \quad (3.1)$$

then there exists $Q \in \text{St}(k, k)$ such that $\tilde{P} = \hat{P}Q \in \mathbb{P}$ and $f(\tilde{P}) \geq f(P) + \omega\eta$, where ω is some positive constant, independent of P and $\hat{P}$.

For any given $P \in \text{St}(k, n)$, by Lemma B.9, there is always $\hat{P} \in \text{St}(k, n)$ such that (3.1) holds with some $\eta > 0$, unless for that given P , (2.3) holds with $\Lambda \geq 0$. In fact, we can take $\hat{P} \in \text{St}(k, n)$ to be an orthogonal polar factor of $\mathcal{H}(P)$, which also maximizes $\text{tr}(X^T \mathcal{H}(P))$ over $X \in \text{St}(k, n)$ to $\|\mathcal{H}(P)\|_{\text{tr}}$ again by Lemma B.9. Hence, for the purpose of solving (1.1), we may relax the ansatz to $\eta \geq 0$. As far as verifying this ansatz is concerned, it is the desirable aim, $f(\tilde{P}) \geq f(P) + \omega\eta$, that needs to be checked. The necessity of also involving $\mathbb{P}$, a subset of $\text{St}(k, n)$, can be best justified by Example 3.1 below.

Example 3.1 Consider $f(P) = \text{tr}(P^T A P) + \text{tr}((P^T D)^2)$ where $0 \leq A \in \mathbb{R}^{n \times n}$ and $D \in \mathbb{R}^{n \times k}$. It can be verified that $\mathcal{H}(P) = 2AP + 2DP^T D$ (see also (4.10) in the next section). Suppose now that (3.1) holds for $P, \hat{P} \in \text{St}(k, n)$, or equivalently,

$$2 \text{tr}(\hat{P}^T A P) + 2 \text{tr}(\hat{P}^T D P^T D) \geq 2 \text{tr}(P^T A P) + 2 \text{tr}((P^T D)^2) + \eta. \quad (3.2)$$

The right-hand side of this inequality seems relatable to $f(P)$, but P and $\hat{P}$ are coupled together in its left-hand side. Somehow we have to separate them in order to establish the desired inequality $f(\tilde{P}) \geq f(P) + \omega\eta$ as demanded by the NPDo Ansatz. Indeed this is what we will do next. Let $X = A^{1/2} \hat{P}$ and $Y = A^{1/2} P$ where $A^{1/2}$ is the unique positive semidefinite square root of A . By Lemma B.7, we get

$$2 \text{tr}(\hat{P}^T A P) = 2 \text{tr}(X^T Y) \leq \text{tr}(X^T X) + \text{tr}(Y^T Y) = \text{tr}(\hat{P}^T A \hat{P}) + \text{tr}(P^T A P), \quad (3.3)$$

successfully separating P and $\hat{P}$ from their coupling by $\text{tr}(\hat{P}^T A P)$. Turning to $\text{tr}(\hat{P}^T D P^T D)$, we assume that $P^T D \geq 0$, i.e., $P \in \mathbb{P} = \text{St}(k, n)_{D+}$, and let $Q \in \text{St}(k, k)$ be an orthogonal polar factor of $\hat{P}^T D$ and hence $Q^T(\hat{P}^T D) \geq 0$, implying $\tilde{P} = \hat{P}Q \in \mathbb{P}$. We get

$$2 \text{tr}(\hat{P}^T D P^T D) \leq 2 \|\hat{P}^T D P^T D\|_{\text{tr}} \quad (\text{by Lemma B.8})$$

$$\begin{aligned} &\leq \operatorname{tr}((Q^T \hat{P}^T D)^2) + \operatorname{tr}((P^T D)^2) \quad (\text{by Lemma B.6}) \\ &= \operatorname{tr}((\tilde{P}^T D)^2) + \operatorname{tr}((P^T D)^2). \end{aligned} \quad (3.4)$$

Combine (3.2), (3.3), and (3.4) to get $f(\tilde{P}) \geq f(P) + \eta$ upon noticing $\operatorname{tr}(\tilde{P}^T A \tilde{P}) = \operatorname{tr}(\hat{P}^T A \hat{P})$. We observe the critical conditions: $P^T D \geq 0$ and $Q^T \hat{P}^T D \geq 0$ that ensure (3.4), which we use to separate P and $\hat{P}$ from their coupling by $\operatorname{tr}(\hat{P}^T D P^T D)$. The first condition $P^T D \geq 0$ can be fulfilled by simply starting with $P \in \mathbb{P}$, while the second condition $Q^T \hat{P}^T D \geq 0$ is made possible by the chosen Q and, as a byproduct, $\tilde{P} \in \mathbb{P}$, too. Besides this role of making $Q^T \hat{P}^T D \geq 0$, Q also increases the objective value as a result of the two inequality signs in the derivation of (3.4). In our later use of (3.1), we begin with some $P \in \mathbb{P} \subseteq \operatorname{St}(k, n)$ and then find some $\hat{P} \in \operatorname{St}(k, n)$ such that $\eta > 0$ in (3.1), and therefore having a flexibility of judiciously choosing a proper Q becomes a logical necessity.

Remark 3.1 A few comments on **the NPDo Ansatz** are in order.

- i. When $f(P)$ is right-unitarily invariant, it suffices to take $Q = I_k$ and $\tilde{P} = \hat{P}$ because $f(\hat{P}) = f(\tilde{P})$ regardless of Q . Introducing subset $\mathbb{P}$ of $\operatorname{St}(k, n)$ and judiciously choosing Q are for generality in order to deal with the case when $f(P)$ is not right-unitarily invariant, e.g., the one in Example 3.1 and those from Table 1 in sect. 1 that involve D or D_i . Throughout this paper, we will assume that $\mathbb{P}$ is as inclusive as necessary to allow our proving arguments to go through. In particular, at the minimum, $\mathbb{P}$ should contain one or more maximizers of the associated optimization problem (1.1).
- ii. For computational purposes, it is necessary to have an efficient way to construct Q in the ansatz. That is often the case when it comes to common concrete objective functions f that are in use today. In our later development, either a proper $\mathbb{P}$ can maximally increase the value of objective function f , e.g., when $\operatorname{tr}((P^T D)^m)$ for $m \geq 1$ is involved, or we have to have it for our theoretical proofs to go through. In fact for $\operatorname{tr}((P^T D)^m)$, we may take $\mathbb{P} = \operatorname{St}(k, n)_{D+}$, and let $Q \in \operatorname{St}(k, k)$ be an orthogonal polar factor of $\hat{P}^T D$ to ensure $\tilde{P}^T D = Q^T (\hat{P}^T D) \geq 0$. As a consequence, $(\tilde{P}^T D)^m \geq 0$ and $\|(\tilde{P}^T D)^m\|_{\operatorname{tr}} = \operatorname{tr}((\tilde{P}^T D)^m)$ by Lemma B.8 and hence an orthogonal polar factor Q of $\hat{P}^T D$ maximizes $\operatorname{tr}[(\hat{P} Z)^T D]^m$ over $Z \in \operatorname{St}(k, k)$. Calculating this Q via the SVD of $\hat{P}^T D \in \mathbb{R}^{k \times k}$ is efficient since k is usually small (in the tens or no more than a couple of hundreds).
- iii. It is tempting to stipulate $f(\hat{P}) \geq f(P) + \omega\eta$, but that is either false or just hard to prove, e.g., for the one in Example 3.1. Often in our algorithms to solve (1.1) iteratively, with P being the current approximate maximizer, assuming **the NPDo Ansatz**, we naturally compute $\hat{P}$ that maximizes $\operatorname{tr}(X^T \mathcal{H}(P))$ over $X \in \operatorname{St}(k, n)$. With that $\hat{P}$, settling whether $f(\hat{P}) \geq f(P) + \omega\eta$ or not can be a hard or even impossible task, for example, in Example 3.1 it is not clear if $f(\hat{P}) \geq f(P) + \omega\eta$ at all.

As to the validity of **the NPDo Ansatz** on the objective functions in Table 1, it holds for all, except for those that involve quotients, under reasonable conditions on the constant matrices and function ϕ . Table 2 details conditions under which **the NPDo Ansatz** holds, where the last column points to the places for justifications. We point

Table 2 The NPDo Ansatz on objective functions in Table 1

	$\mathcal{H}(P)$	Conditions	By
SEP	$2AP$	$A \geq 0$	Theorem 5.2
MBSUB	$2AP + D$	$A \geq 0$	Theorem 5.2, [67]
SumCT	$2[A_1 P_1, \dots, A_N P_N] + D$	$A_i \geq 0 \forall i$	Theorem 5.2, [67]
TrCP	$2 \sum_{i=1}^N \phi_i(\mathbf{x}) A_i P$	$A_i \geq 0, \phi_i \geq 0 \forall i$ convex ϕ	Theorem 5.2
UMDS	$4 \sum_{i=1}^N A_i P P^T A_i P$	$A_i \geq 0 \forall i$	Example 5.2
DFT	$2AP + 2 \sum_{i=1}^n \phi_i(\mathbf{x}) \mathbf{e}_i \mathbf{e}_i^T P$	$A \geq 0, \phi_i \geq 0 \forall i$ convex ϕ	Theorem 5.2

$\phi_i(\mathbf{x}) := \partial \phi(\mathbf{x}) / \partial x_i$ for $\mathbf{x} = [x_i]$

out that we can take $\mathbb{P} = \text{St}(k, n)$, $Q = I_k$, and $\omega = 1$ for all in Table 2 but judicious choices of $\mathbb{P}$ and Q can increase the values of objective functions more than $\omega\eta$ as stipulated by the NPDo Ansatz for MBSUB and SumCT [67, Theorem 5.2].

The first immediate consequence of the NPDo Ansatz is the following theorem that provides a characterization of the maximizers of the associated optimization problem (1.1).

Theorem 3.1 *Let $P_* \in \text{St}(k, n)$ be a maximizer of (1.1). Suppose that the NPDo Ansatz holds and $P_* \in \mathbb{P}$. Then (2.3) holds for $P = P_*$ and $\Lambda = \Lambda_* := P_*^T \mathcal{H}(P_*) \succeq 0$.*

Proof Any maximizer is a KKT point, and hence (2.3) holds for $P = P_*$ and $\Lambda = \Lambda_*$. Assume, to the contrary, that $\Lambda_* = P_*^T \mathcal{H}(P_*) \not\succeq 0$ (which means either Λ_* is not symmetric or it is symmetric but indefinite or even negative semidefinite). Then by Lemma B.9, we have $\text{tr}(\tilde{P}^T \mathcal{H}(P_*)) = \|\mathcal{H}(P_*)\|_{\text{tr}} \geq \text{tr}(P_*^T \mathcal{H}(P_*)) + \eta$ for some $\eta > 0$, where $\tilde{P}$ is an orthogonal polar factor of $\mathcal{H}(P_*)$. By the NPDo Ansatz, we can find $\tilde{P} = \tilde{P}Q \in \mathbb{P}$ such that $f(\tilde{P}) \geq f(P_*) + \omega\eta > f(P_*)$, contradicting that P_* is a maximizer. $\square$

What this theorem says is that at a maximizer P_* , (2.3) is a polar decomposition of $\mathcal{H}(P_*)$. Hence solving (1.1) through its KKT condition is necessarily looking for some P_* so that (2.3) is a polar decomposition. Since the matrix of which we are seeking a polar decomposition is a matrix-valued function that depends on its orthogonal polar factor, we naturally call (2.3) a *nonlinear polar decomposition with orthogonal polar factor dependency* (NPDo) of $\mathcal{H}(\cdot)$.

We note that $\mathcal{H}(P_*)$ has a unique polar decomposition if $\text{rank}(\mathcal{H}(P_*)) = k$ [38]; but it is not unique if $\text{rank}(\mathcal{H}(P_*)) < k$ [26, 37, 40]. However in the latter case, it does not mean that any orthogonal polar factor of $\mathcal{H}(P_*)$, other than P_* , also satisfies (2.3), unless $\mathcal{H}(\cdot)$ is right-unitarily invariant.

Algorithm 3.1 NPDoSCF: NPDo (2.3) solved by SCF

Input: Function $\mathcal{H}(P) \equiv \partial f(P)/\partial P$ satisfying the **NPDo Ansatz**, $P^{(0)} \in \mathbb{P}$;

Output: an approximate maximizer of (1.1).

```

1: for  $i = 0, 1, \dots$  until convergence do
2:   compute  $H_i = \mathcal{H}(P^{(i)}) \in \mathbb{R}^{n \times k}$  and its thin SVD:  $H_i = U_i \Sigma_i V_i^T$ ;
3:    $\hat{P}^{(i)} = U_i V_i^T \in \text{St}(k, n)$ , an orthogonal polar factor of  $\mathcal{H}(P^{(i)})$ ;
4:   calculate  $Q_i \in \text{St}(k, k)$  whose existence is stipulated by the NPDo Ansatz and let  $P^{(i+1)} = \hat{P}^{(i)} Q_i \in \mathbb{P}$ ;
5: end for
6: return the last  $P^{(i)}$ .
```

3.2 SCF Iteration and Convergence

The second immediate consequence of the **NPDo Ansatz** is the global convergence of an SCF iteration for solving optimization problem (1.1) as outlined in Algorithm 3.1.

This algorithm is similar to [67, Algorithm 3.1], but the latter has more details that are dictated by the particularity of objective function f there. We have a few general comments regarding the implementation of Algorithm 3.1 (NPDoSCF):

1. At Line 4 it refers to the **NPDo Ansatz** for the calculation of Q_i . Exactly how it is computed depends on the structure of f at hand. In Remark 3.1(ii), we commented on the issue in the case when $f(P)$ involves and increases with $\text{tr}((P^T D)^m)$, e.g., the one in Example 3.1, Q_i can be taken to be an orthogonal polar factor of $(\hat{P}^{(i)})^T D$. Later in sect. 5 we will elaborate on how to choose Q_i for a few convex compositions of matrix-trace functions.
2. A reasonable stopping criterion at Line 1 is

$$\varepsilon_{\text{KKT}} + \varepsilon_{\text{sym}} := \frac{\|\mathcal{H}(P) - P[P^T \mathcal{H}(P)]\|_F}{\xi} + \frac{\|[P^T \mathcal{H}(P)] - [P^T \mathcal{H}(P)]^T\|_F}{\xi} \leq \epsilon, \quad (3.5)$$

where ϵ is a given tolerance, and ξ is some normalization quantity that should be designed according to the underlying $\mathcal{H}(P)$, but generically, $\xi = \|\mathcal{H}(P)\|_F$, or any reasonable estimate of it, should work well. The significance of both ε_{KKT} and ε_{sym} is rather self-explanatory. In fact, we will call ε_{KKT} and ε_{sym} the *normalized residual for the KKT equation* (2.3) and the *normalized residual for the symmetry* in $\Lambda = P^T \mathcal{H}(P)$, respectively.

3. Let us investigate the computational complexity per iterative step. Since how $H_i = \mathcal{H}(P^{(i)})$ and Q_i are computed is generally problem-dependent, we will only examine the cost for all other operations. At Line 2, the thin SVD of $H_i \in \mathbb{R}^{n \times k}$ is often computed in two steps: compute a thin QR decomposition $H_i = W R$ and then the SVD of $R \in \mathbb{R}^{k \times k}$ followed by the product of W with the left singular vector matrix of R . Hence the overall cost per SCF iterative step, stemming from the SVD of R and three matrix products of an n -by- k matrix with an k -by- k matrix, is about $O(nk^2 + k^3)$ flops [24, p.493] which is linear in n for small k .

Next, we will state our convergence theorems for Algorithm 3.1 under **the NPDo Ansatz**. It is shown that as the SCF iteration progresses, the value of the objective function monotonically increases, any accumulation point of the generated approximation sequence satisfies the necessary conditions in Theorem 3.1 for a global maximizer, and under certain conditions, the accumulation point can be proved to be the limit point of the entire approximation sequence. In short, the NPDo approach is guaranteed to work.

Theorem 3.2 *Suppose that the NPDo Ansatz holds, and let the sequence $\{P^{(i)}\}_{i=0}^{\infty}$ be generated by Algorithm 3.1. The following statements hold.*

- The sequence $\{f(P^{(i)})\}_{i=0}^{\infty}$ is monotonically increasing and convergent;*
- Any accumulation point P_* of the sequence $\{P^{(i)}\}_{i=0}^{\infty}$ satisfies the necessary conditions in Theorem 3.1 for a global maximizer, i.e., (2.3) holds for $P = P_*$ with $\Lambda_* = P_*^T \mathcal{H}(P_*) \succeq 0$;*
- We have two convergent series*

$$\sum_{i=1}^{\infty} \sigma_{\min}(\mathcal{H}(P^{(i)})) \|\sin \Theta(\mathcal{R}(P^{(i+1)}), \mathcal{R}(P^{(i)}))\|_F^2 < \infty, \quad (3.6a)$$

$$\sum_{i=1}^{\infty} \sigma_{\min}(\mathcal{H}(P^{(i)})) \frac{\|\mathcal{H}(P^{(i)}) - P^{(i)}([P^{(i)}]^T \mathcal{H}(P^{(i)}))\|_F^2}{\|\mathcal{H}(P^{(i)})\|_F^2} < \infty, \quad (3.6b)$$

where $\Theta(\cdot, \cdot)$ is the diagonal matrix of the canonical angles between two subspaces (see appendix A).

Proof See [42, Appendix C]. □

Both Theorem 3.2(b,c) have useful consequences. As a corollary of Theorem 3.2(b), we find that **the NPDo Ansatz** is a sufficient condition for NPDo (2.3) to have a solution because there always exists an accumulation point P_* of the sequence $\{P^{(i)}\}_{i=0}^{\infty}$ in $\text{St}(k, n)$.

Corollary 3.1 *Under the NPDo Ansatz, NPDo (2.3) is solvable, i.e., there exists $P \in \text{St}(k, n)$ such that $\Lambda = P^T \mathcal{H}(P) \succeq 0$ and (2.3) holds.*

As a corollary of Theorem 3.2(c), if $\sigma_{\min}(\mathcal{H}(P^{(i)}))$ is eventually bounded below away from 0 uniformly,² then

$$\lim_{i \rightarrow \infty} \frac{\|\mathcal{H}(P^{(i)}) - P^{(i)}([P^{(i)}]^T \mathcal{H}(P^{(i)}))\|_F}{\|\mathcal{H}(P^{(i)})\|_F} = 0,$$

namely, increasingly $\mathcal{H}(P^{(i)}) \approx P^{(i)}([P^{(i)}]^T \mathcal{H}(P^{(i)}))$ towards a polar decomposition of $\mathcal{H}(P^{(i)})$, which means that $P^{(i)}$ becomes a more and more accurate

² By which we mean that there exist a constant $\tau > 0$ and an integer K such that $\sigma_{\min}(\mathcal{H}(P^{(i)})) \geq \tau$ for all $i \geq K$.

approximate solution to NPDo (2.3), even in the absence of knowing whether the entire sequence $\{P^{(i)}\}_{i=0}^{\infty}$ converges or not. The latter does require additional conditions to establish in the next theorem.

Theorem 3.3 *Suppose that the NPDo Ansatz holds, and let the sequence $\{P^{(i)}\}_{i=0}^{\infty}$ be generated by Algorithm 3.1 and P_* be an accumulation point of the sequence. The following statements hold.*

- a. $\mathcal{R}(P_*)$ is an accumulation point of the sequence $\{\mathcal{R}(P^{(i)})\}_{i=0}^{\infty}$.
- b. Suppose that $\mathcal{R}(P_*)$ is an isolated accumulation point of $\{\mathcal{R}(P^{(i)})\}_{i=0}^{\infty}$. If

$$\text{rank}(\mathcal{H}(P_*Q)) = k \quad \text{for any } Q \in \text{St}(k, k), \quad (3.7)$$

then the entire sequence $\{\mathcal{R}(P^{(i)})\}_{i=0}^{\infty}$ converges to $\mathcal{R}(P_*)$;

- c. Suppose that P_* is an isolated accumulation point of $\{P^{(i)}\}_{i=0}^{\infty}$. If

$$\text{rank}(\mathcal{H}(P_*)) = k, \quad (3.8)$$

and if $f(P_*) > f(P)$ for any $P \neq P_*$ and $\mathcal{R}(P) = \mathcal{R}(P_*)$, i.e., $f(P)$ has unique maximizer in the orbit $\{P_*Q : Q \in \text{St}(k, k)\}$, then the entire sequence $\{P^{(i)}\}_{i=0}^{\infty}$ converges to P_* .

Proof See [42, Appendix C]. □

In the case when objective function f is right-unitarily invariant, Theorem 3.3(c) is clearly not applicable. In such a case, computing $\mathcal{R}(P_*)$ is the ultimate goal because each maximizer P_* is really a representative from the orbit $\{P_*Q : Q \in \text{St}(k, k)\}$. Given $Q \in \mathbb{R}^{k \times k}$, let $g(P) = f(PQ)$. It can be verified that

$$\frac{\partial g(P)}{\partial P} = \frac{\partial f(\hat{P})}{\partial \hat{P}} \bigg|_{\hat{P}=PQ} Q^T = \mathcal{H}(PQ) Q^T.$$

Thus if f is right-unitarily invariant, then $g(P) \equiv f(P)$ and thus $\mathcal{H}(P) = \mathcal{H}(PQ) Q^T$; if also $Q \in \text{St}(k, k)$, then we get $\mathcal{H}(PQ) = \mathcal{H}(P) Q$ and as a result, condition (3.7) is equivalently to $\text{rank}(\mathcal{H}(P_*)) = k$.

3.3 Acceleration by LOCG and Convergence

Although Algorithm 3.1, an SCF iteration for solving NPDo (2.3), is proved always convergent to KKT points under the NPDo Ansatz, it may take many SCF iterations to converge to a solution with desired accuracy and that can be costly for large scale problems, even though the complexity per SCF iterative step is linear in n . In fact, for $f(P) = \text{tr}(P^T A P)$ with $A \geq 0$, Algorithm 3.1 is simply the subspace iteration which converges linearly at the rate of $\lambda_{k+1}(A)/\lambda_k(A)$. This rate is 1 if $\lambda_{k+1}(A) = \lambda_k(A)$, indicating possible divergence, but strictly less than 1 otherwise. In the latter case, although the convergence is guaranteed, it can be slow when $\lambda_{k+1}(A) < \lambda_k(A)$ only slightly such that $\lambda_{k+1}(A)/\lambda_k(A) \approx 1$ [17, 24]. In [67], acceleration by a locally

optimal conjugate gradient technique (LOCG) was demonstrated to be rather helpful to speed things up for maximizing SumCT. The same idea can be used to speed up Algorithm 3.1, too. In this subsection, we will explain the idea, which draws inspiration from optimization [53, 61] and has been increasingly used in NLA for linear systems and eigenvalue problems [7, 31, 33, 41, 72].

A Variant of LOCG for Acceleration

Without loss of generality, let $P^{(-1)} \in \text{St}(k, n)$ be the approximate maximizer of (1.1) from the very previous iterative step, and $P \in \text{St}(k, n)$ the current approximate maximizer. We are now looking for the next approximate maximizer $P^{(1)}$, along the line of LOCG, according to

$$P^{(1)} = \arg \max_{Y \in \text{St}(k, n)} f(Y), \text{ s.t. } \mathcal{R}(Y) \subseteq \mathcal{R}([P, \mathcal{R}(P), P^{(-1)}]), \quad (3.9)$$

where

$$\mathcal{R}(P) := \text{grad } f|_{\text{St}(k, n)}(P) = \mathcal{H}(P) - P \cdot \frac{1}{2} [P^T \mathcal{H}(P) + \mathcal{H}(P)^T P] \quad (3.10)$$

by (2.2). Initially for the first iteration, we don't have $P^{(-1)}$ and it is understood that $P^{(-1)}$ is absent from (3.9), i.e., simply $\mathcal{R}(Y) \subseteq \mathcal{R}([P, \mathcal{R}(P)])$.

We still have to numerically solve (3.9). For that purpose, let $W \in \text{St}(m, n)$ be an orthonormal basis matrix of subspace $\mathcal{R}([P, \mathcal{R}(P), P^{(-1)}])$. Generically, $m = 3k$ but $m < 3k$ can happen. It can be implemented by the Gram-Schmidt orthogonalization process, starting with orthogonalizing the columns of $\mathcal{R}(P)$ against P since $P \in \text{St}(k, n)$ already. In MATLAB, to fully take advantage of its optimized functions, we simply set $W = [\mathcal{R}(P), P^{(-1)}]$ (or $W = \mathcal{R}(P)$ for the first iteration) and then do

$$\begin{aligned} W &= W - P * (P' * W); \quad W = \text{orth}(W); \quad W = W - P * (P' * W); \quad W = \text{orth}(W); \\ W &= [P, W]; \end{aligned}$$

where the first line performs the classical Gram-Schmidt orthogonalization twice to almost ensure that the resulting columns of W are fully orthogonal to the columns of P at the end of the first line, and `orth` is a MATLAB function for orthogonalization. It is important to note that the first k columns of the final W are the same as those of P .

Now it follows from $\mathcal{R}(Y) \subseteq \mathcal{R}([P, \mathcal{R}(P), P^{(-1)}]) = \mathcal{R}(W)$ that in (3.9)

$$Y = WZ \quad \text{for } Z \in \text{St}(k, m). \quad (3.11a)$$

Problem (3.9) becomes

$$Z_{\text{opt}} = \arg \max_{Z \in \text{St}(k, m)} \tilde{f}(Z) \quad \text{with} \quad \tilde{f}(Z) := f(WZ), \quad (3.11b)$$

Algorithm 3.2 NPDoLOC: NPDo (2.3) solved by LOCG

Input: Function $\mathcal{H}(P) \equiv \partial f(P)/\partial P$ satisfying the NPDo Ansatz, $P^{(0)} \in \mathbb{P}$;

Output: an approximate maximizer of (1.1).

```

1:  $P^{(-1)} = []$ ; % null matrix
2: for  $i = 0, 1, \dots$  until convergence do
3:   compute  $W \in \text{St}(m, n)$  such that  $\mathcal{R}(W) = \mathcal{R}([P^{(i)}, \mathcal{R}(P^{(i)}), P^{(i-1)}])$  and  $P^{(i)}$  occupies the first
       $k$  columns of  $W$ ;
4:   solve (3.11b) via NPDo (3.12) for  $Z_{\text{opt}}$  by Algorithm 3.1 with initially  $Z^{(0)}$  being the first  $k$  columns
      of  $I_m$ , or approximately such that  $\tilde{f}(Z_{\text{opt}}) \geq \tilde{f}(Z^{(0)}) + \omega\eta$  for some  $\eta > 0$ ;
5:    $P^{(i+1)} = WZ_{\text{opt}}$ ;
6: end for
7: return the last  $P^{(i)}$ .
```

and $P^{(1)} = WZ_{\text{opt}}$ for (3.9). It can be verified that

$$\tilde{\mathcal{H}}(Z) := \frac{\partial \tilde{f}(Z)}{\partial Z} = W^T \frac{\partial f(P)}{\partial P} \Big|_{P=WZ} = W^T \mathcal{H}(WZ), \quad (3.12a)$$

and the first order optimality condition for (3.11b) is

$$\tilde{\mathcal{H}}(Z) = Z\tilde{\Lambda} \quad \text{with} \quad \tilde{\Lambda}^T = \tilde{\Lambda} \in \mathbb{R}^{k \times k}, \quad Z \in \text{St}(k, m). \quad (3.12b)$$

Lemma 3.1 Suppose that the NPDo Ansatz holds for f , and let $\mathbb{Z} := W^T \mathbb{P} \subseteq \text{St}(k, m)$. If $W\mathbb{Z} \subseteq \mathbb{P}$, then the NPDo Ansatz holds for $\tilde{f}$ defined in (3.11b).

Proof Let $Z \in \mathbb{Z}$ and $\hat{Z} \in \text{St}(k, m)$ such that

$$\text{tr}(\hat{Z}^T \tilde{\mathcal{H}}(Z)) \geq \text{tr}(Z^T \tilde{\mathcal{H}}(Z)) + \eta \quad \text{for some } \eta \in \mathbb{R}. \quad (3.13)$$

Set $P = WZ \in \mathbb{P}$ (because of $W\mathbb{Z} \subseteq \mathbb{P}$) and $\hat{P} = W\hat{Z} \in \text{St}(k, n)$. Noticing that $\tilde{\mathcal{H}}(Z) = W^T \mathcal{H}(WZ)$, we have (3.1) from (3.13). By the NPDo Ansatz for f , there exists $Q \in \text{St}(k, k)$ such that $\tilde{P} = \hat{P}Q = W(\hat{Z}Q) =: W\tilde{Z} \in \mathbb{P}$ and $f(\tilde{P}) \geq f(P) + \omega\eta$. Hence,

$$\tilde{f}(\tilde{Z}) = \tilde{f}(\hat{Z}Q) = f(\tilde{P}) \geq f(P) + \omega\eta = f(WZ) + \omega\eta = \tilde{f}(Z) + \omega\eta.$$

Note also $\tilde{Z} = W^T \tilde{P} \in \mathbb{Z}$. Hence the NPDo Ansatz holds for $\tilde{f}$. $\square$

As a consequence of this lemma and the results in subsections 3.1 and 3.2, Algorithm 3.1 is applicable to compute Z_{opt} of (3.11b) via NPDo (3.12b). We outline the resulting method in Algorithm 3.2, which is an inner-outer iterative scheme for (1.1), where at Line 4 any other method, if known, can also be inserted to replace Algorithm 3.1 to solve (3.11b).

Remark 3.2 A few comments regarding Algorithm 3.2 are in order.

- It is important to compute W at Line 4 in such a way, as explained moments ago, that its first k columns are exactly the same as those of $P^{(i)}$. As $P^{(i)}$ converges,

- conceivably $P^{(i+1)}$ changes little from $P^{(i)}$ and hence Z_{opt} is increasingly close to the first k columns of I_m . This explains the choice of $Z^{(0)}$ at Line 4.
- ii. Another area of improvement is to solve (3.11b) with an accuracy, comparable but fractionally better than the current $P^{(i)}$ as an approximate solution of (1.1). Specifically, if we use (3.5) at Line 2 to stop the for-loop: Lines 2–6 of Algorithm 3.2, with tolerance ϵ , then instead of using the same ϵ for Algorithm 3.1 at its line 1, we can use a fraction, say $1/4$, of $\epsilon_{\text{KKT}} + \epsilon_{\text{sym}}$ evaluated at the current approximation $P = P^{(i)}$ as stopping tolerance, when Algorithm 3.1 is called upon at Line 4 of Algorithm 3.2.

Whether Algorithm 3.2 speeds up Algorithm 3.1 depends on two factors at the runtime: 1) it takes significantly fewer the number of outer iterative steps than the number of SCF iterative steps by Algorithm 3.1 as it does without acceleration, and 2) the cost per SCF step on NPDo (3.12) is significantly less than that on NPDo (2.3). Both factors are materialized for SumCT (see [67, Example 4.1]).

Convergence Analysis

We will perform a convergence analysis for Algorithm 3.2, considering an ideal situation that at its Line 4, Z_{opt} is computed to be an exact maximizer of (3.11) for simplicity. We point out that the seemingly ideal situation is not completely unrealistic. In actual computation, as we explained in Remark 3.2(ii), the computed Z_{opt} should be sufficiently more accurate as an approximate solution for (3.11) than $P^{(i)}$ as an approximate solution for the original problem (1.1) at that moment.

Theorem 3.4 *Suppose that the NPDo Ansatz holds, and let sequence $\{P^{(i)}\}_{i=0}^{\infty}$ be generated by Algorithm 3.2 in which, it is assumed that Z_{opt} is an exact maximizer of (3.11) in each outer iterative step. The following statements hold.*

- $(P^{(i)})^T \mathcal{H}(P^{(i)}) \geq 0$ for $i \geq 1$;
- The sequence $\{f(P^{(i)})\}_{i=0}^{\infty}$ is monotonically increasing and convergent;
- Any accumulation point P_* of the sequence $\{P^{(i)}\}_{i=0}^{\infty}$ is a KKT point of (1.1) and satisfies the necessary conditions in Theorem 3.1 for a global maximizer, i.e., (2.3) holds for $P = P_*$ and $\Lambda = \Lambda_* := P_*^T \mathcal{H}(P_*) \succeq 0$.

Proof Consider iterative step i . By the assumption that Z_{opt} is an exact maximizer of (3.11), we have at the end of Line 4

$$0 \leq Z_{\text{opt}}^T \widetilde{\mathcal{H}}(Z_{\text{opt}}) = Z_{\text{opt}}^T W^T \mathcal{H}(W Z_{\text{opt}}) = (P^{(i+1)})^T \mathcal{H}(P^{(i+1)}),$$

proving item (a). Let Z be the first k columns of I_m . Then $\widetilde{f}(Z) = f(P^{(i)})$ in (3.11), and thus

$$f(P^{(i+1)}) = f(W Z_{\text{opt}}) = \widetilde{f}(Z_{\text{opt}}) \geq \widetilde{f}(Z) = f(P^{(i)}).$$

This proves item (b).

Next, we prove item (c). Let $\{P^{(i)}\}_{i \in \mathbb{I}}$ be a subsequence that converges to P_* . Letting $\mathbb{I} \ni i \rightarrow \infty$ in the inequalities in item (a) immediately yields $P_*^T \mathcal{H}(P_*) \succeq 0$. It remains to show $\mathcal{H}(P_*) = P_* \Lambda_*$, where $\Lambda_* = P_*^T \mathcal{H}(P_*)$. The proof of [67, Theorem 4.1(c)] essentially works here. $\square$

4 Atomic Functions for NPDo

Armed with the general theoretical framework for the NPDo approach in sect. 3, in this section, we introduce the notion of atomic functions for NPDo, which serves as a singleton unit of function on $\text{St}_\delta(k, n)$ for which **the NPDo Ansatz** holds and thus the NPDo approach is guaranteed to work for solving (1.1), and more importantly, the NPDo approach works on any convex composition of atomic functions.

In what follows, we will first formulate two conditions that define atomic functions and explain why the NPDo approach will work on the atomic functions, and then we give concrete examples of atomic functions that encompass nearly all practical ones that are in use today. We leave the investigation of how the NPDo approach works on convex compositions of atomic functions to sect. 5, along with a few convex compositions of our concrete atomic functions to guide the use of the general result.

Combining the results in this section and the next section will yield a large collection of objective functions, including those in Table 2, for which **the NPDo Ansatz** holds and therefore the NPDo framework as laid out in sect. 3 works on them.

4.1 Conditions on Atomic Functions

We are interested in functions f defined on some neighborhood $\text{St}_\delta(k, n)$ of the Stiefel manifold $\text{St}(k, n)$ that satisfy

$$\text{tr} \left(P^T \frac{\partial f(P)}{\partial P} \right) = \gamma f(P) \quad \text{for } P \in \mathbb{P} \subseteq \text{St}(k, n), \quad (4.1a)$$

and given $P \in \mathbb{P}$ and $\hat{P} \in \text{St}(k, n)$, there exists $Q \in \text{St}(k, k)$ such that $\tilde{P} = \hat{P}Q \in \mathbb{P}$ and

$$\text{tr} \left(\hat{P}^T \frac{\partial f(P)}{\partial P} \right) \leq \alpha f(\tilde{P}) + \beta f(P), \quad (4.1b)$$

where $\alpha > 0$, $\beta \geq 0$, and $\gamma = \alpha + \beta$ are constants that are dependent of f . Some subset $\mathbb{P}$ of $\text{St}(k, n)$ is also involved and, as we commented in Remark 3.1(i) for **the NPDo Ansatz**, $\mathbb{P}$ should be sufficiently inclusive to serve the purpose of solving (1.1) with the function as objective, and for the case of $\mathbb{P} = \text{St}(k, n)$, Q can be taken to be I_k . More comments on this are in Remark 4.1(ii) below.

Definition 4.1 A function f defined on some neighborhood $\text{St}_\delta(k, n)$ of $\text{St}(k, n)$ is an *atomic function* for NPDo if there are constants $\alpha > 0$, $\beta \geq 0$, and $\gamma = \alpha + \beta$ such that both conditions in (4.1) hold.

The constants in the definition may vary with the atomic function in question. The descriptive word “*atomic*” is used here to loosely suggest that such a function is somehow “*unbreakable*”, such as the concrete ones in the next subsection. Having said that, we also find that *for two atomic functions f_1 and f_2 , if they share the same $\mathbb{P}$, the same constants α , β , γ , and the same Q for (4.1b), then any linear combination $f := c_1 f_1 + c_2 f_2$ with $c_1, c_2 \geq 0$ but $c_1 + c_2 > 0$ also satisfies (4.1), and hence an atomic function as well.* Evidently, $f = c_1 f_1 + c_2 f_2$ is “*breakable*”. Nonetheless, “*atomic*” still seems to be suitably descriptive despite of what we just discussed.

Throughout this paper, we actually define two types of atomic functions. One type is what we just defined in Definition 4.1. It is for the NPDo approach. The other type will come in Part II later for the NEPv approach.

Remark 4.1 There are two comments regarding Definition 4.1.

- i. Theoretically, each of the two conditions in (4.1) has interest of its own. For example, equation (4.1a) is a partial differential equation (PDE) in its own right. In that regard, a natural question arises: does it have a close form solution, given $\gamma \in \mathbb{R}$ (that is not necessarily nonnegative)? In this paper, we group the two together because later we need both to show that together they imply **the NPDo Ansatz** for an atomic function and thus the NPDo approach works. Also importantly, we need $\gamma = \alpha + \beta$.
- ii. How inclusive should $\mathbb{P}$ as a subset of $\text{St}(k, n)$ be? Often certain necessary conditions for the maximizers of (1.1) with given atomic function as objective can be derived to limit the extent of searching. For example, as has been extensively exploited in [47, 67, 68, 75, 78], any maximizer P_* must satisfy $P_*^T D \geq 0$ in the case where $f(P)$ contains $\text{tr}(P^T D)$ and increases as $\text{tr}(P^T D)$ does. In such a case, searching a maximizer can be naturally limited among those $P \in \text{St}(k, n)$ such that $P^T D \geq 0$, i.e., $P \in \mathbb{P} = \text{St}(k, n)_{D+}$. As a result, it suffices to just require that the equality and inequality in (4.1) hold for all $P, \tilde{P} \in \mathbb{P} = \text{St}(k, n)_{D+}$. In our later concrete examples in subsect. 4.2, equation (4.1a) even holds for all $P \in \mathbb{R}^{n \times k}$ for some atomic functions.

The next theorem shows that if f is an atomic function for NPDo, then so is any of its positive powers of order higher than 1, if well-defined, and moreover the α -constant does not change but the β -constant will.

Theorem 4.1 *Given function f satisfying (4.1), suppose that $f(P) \geq 0$ for $P \in \mathbb{P}$. Let $g(P) = c[f(P)]^s$ where $c > 0$ and $s > 1$. Then*

$$\text{tr} \left(P^T \frac{\partial g(P)}{\partial P} \right) = s\gamma g(P) \quad \text{for } P \in \mathbb{P} \subseteq \text{St}(k, n), \quad (4.2a)$$

and given $P \in \mathbb{P}$ and $\hat{P} \in \text{St}(k, n)$, there exists $Q \in \text{St}(k, k)$ such that $\tilde{P} = \hat{P}Q \in \mathbb{P}$ and

$$\text{tr} \left(\tilde{P}^T \frac{\partial g(P)}{\partial P} \right) \leq \alpha g(\tilde{P}) + (s\gamma - \alpha)g(P). \quad (4.2b)$$

Proof It can be seen that $\frac{\partial g(P)}{\partial P} = c s [f(P)]^{s-1} \frac{\partial f(P)}{\partial P}$, and thus

$$\operatorname{tr} \left(P^T \frac{\partial g(P)}{\partial P} \right) = c s [f(P)]^{s-1} \operatorname{tr} \left(P^T \frac{\partial f(P)}{\partial P} \right) = c s [f(P)]^{s-1} \gamma f(P) = s \gamma g(P),$$

yielding (4.2a). On the other hand, for $P \in \mathbb{P}$ and $\hat{P} \in \operatorname{St}(k, n)$, we have

$$\begin{aligned} \operatorname{tr} \left(\hat{P}^T \frac{\partial g(P)}{\partial P} \right) &= c s [f(P)]^{s-1} \operatorname{tr} \left(\hat{P}^T \frac{\partial f(P)}{\partial P} \right) \\ &\leq c s [f(P)]^{s-1} \left\{ \alpha [f(\tilde{P})] + \beta [f(P)] \right\} \quad (\text{by (4.1b)}) \\ &= c s \alpha [f(\tilde{P})] [f(P)]^{s-1} + \beta s c [f(P)]^s \\ &\leq c s \alpha \left\{ \frac{1}{s} [f(\tilde{P})]^s + \frac{s-1}{s} [f(P)]^s \right\} + \beta s g(P) \\ &= \alpha g(\tilde{P}) + \alpha (s-1) g(P) + \beta s g(P) \\ &= \alpha g(\tilde{P}) + [\alpha (s-1) + \beta s] g(P), \end{aligned} \quad (4.3)$$

yielding (4.2b), where we have used Lemma B.2 on $[f(\tilde{P})][f(P)]^{s-1}$ to get (4.3). $\square$

In Theorem 4.1, $g(P) = h(f(P))$ where $h(t) = ct^s$, i.e., $g = h \circ f$ is a composition function. It turns out that this is the only composition function that satisfies the same type of PDE as f does in (4.1a) [42, Remark 4.2].

Theorem 4.2 *The NPDo Ansatz holds with $\omega = 1/\alpha$ for atomic function f that satisfies the conditions in (4.1).*

Proof Given $P \in \mathbb{P} \subseteq \operatorname{St}(k, n)$ and $\hat{P} \in \operatorname{St}(k, n)$, suppose that (3.1) holds, i.e., $\operatorname{tr}(\hat{P}^T \mathcal{H}(P)) \geq \operatorname{tr}(P^T \mathcal{H}(P)) + \eta$. We have by (4.1)

$$\eta + \gamma f(P) = \eta + \operatorname{tr}(P^T \mathcal{H}(P)) \leq \operatorname{tr}(\hat{P}^T \mathcal{H}(P)) \leq \alpha f(\tilde{P}) + \beta f(P)$$

yielding $\eta/\alpha + f(P) \leq f(\tilde{P})$, as was to be shown. $\square$

As a corollary of Theorem 4.2, the NPDo approach as laid out in sect. 3 works on any atomic function for NPDo.

4.2 Concrete Atomic Functions

We will show that

$$[\operatorname{tr}((P^T D)^m)]^s, \quad [\operatorname{tr}((P^T A P)^m)]^s \quad \text{for integer } m \geq 1, s \geq 1, \text{ and } A \geq 0 \quad (4.4)$$

satisfy (4.1) and hence are atomic functions for NPDo. Therefore, by Theorem 4.2, the NPDo Ansatz holds for them. We point out that the results we will prove in this subsection are actually for more general P , $\hat{P}$ and $\tilde{P}$ than required in Definition 4.1.

We start by considering $\operatorname{tr}((P^T D)^m)$ and its power.

Theorem 4.3 Let $D \in \mathbb{R}^{n \times k}$, and let $m \geq 1$ be an integer.

a. For $P \in \mathbb{R}^{n \times k}$, we have

$$\operatorname{tr} \left(P^T \frac{\partial \operatorname{tr}((P^T D)^m)}{\partial P} \right) = m \operatorname{tr}((P^T D)^m). \quad (4.5)$$

b. Let $P, \hat{P} \in \mathbb{R}^{n \times k}$.

i. For $m = 1$, we have

$$\operatorname{tr} \left(\hat{P}^T \frac{\partial \operatorname{tr}(P^T D)}{\partial P} \right) = \operatorname{tr}(\hat{P}^T D); \quad (4.6)$$

ii. For $m > 1$, if $P^T D \succeq 0$, then

$$\operatorname{tr} \left(\hat{P}^T \frac{\partial \operatorname{tr}((P^T D)^m)}{\partial P} \right) \leq \operatorname{tr}((\tilde{P}^T D)^m) + (m-1) \operatorname{tr}((P^T D)^m), \quad (4.7)$$

where $\tilde{P} = \hat{P}Q$ for $Q \in \operatorname{St}(k, k)$ such that $\tilde{P}^T D \succeq 0$.

In particular, the conditions in (4.1) hold with $\mathbb{P} = \operatorname{St}(k, n)_{D^+}$, $\alpha = 1$ and $\beta = m-1$, and thus $\operatorname{tr}((P^T D)^m)$ is an atomic function for NPDo.

Just for the case $m = 1$, we can also take $\mathbb{P} = \operatorname{St}(k, n)$ and $\tilde{P} = \hat{P}$ in (4.1), and then (4.1b) becomes an equality. Therefore, $\operatorname{tr}(P^T D)$ is also an atomic function for NPDo with $\mathbb{P} = \operatorname{St}(k, n)$ and $Q = I_k$ in the definition.

Proof Consider perturbing $P \in \mathbb{R}^{n \times k}$ to $P + E$ where $E \in \mathbb{R}^{n \times k}$ with $\|E\|$ sufficiently tiny. We have

$$\begin{aligned} [(P + E)^T D]^m &= [P^T D + E^T D]^m \\ &= (P^T D)^m + \sum_{i=0}^{m-1} (P^T D)^i E^T D (P^T D)^{m-1-i} + O(\|E\|^2), \end{aligned} \quad (4.8)$$

$$\operatorname{tr}([(P + E)^T D]^m) = \operatorname{tr}((P^T D)^m) + m \operatorname{tr}(E^T D (P^T D)^{m-1}) + O(\|E\|^2). \quad (4.9)$$

Immediately, it follows from (4.9) that

$$\frac{\partial \operatorname{tr}((P^T D)^m)}{\partial P} = m D (P^T D)^{m-1}. \quad (4.10)$$

Equation (4.5) is a direct consequence of (4.10). This proves item (a).

Now, we prove item (b). Equation (4.6) which is for $m = 1$ is easily verified. In general, for $m > 1$, noticing the assumption $P^T D \succeq 0$ and $\tilde{P}^T D = Q^T (\hat{P}^T D) \succeq 0$

for the case, we have, by Lemma B.6,

$$\begin{aligned} \operatorname{tr} \left(\widehat{P}^T \frac{\partial \operatorname{tr}((P^T D)^m)}{\partial P} \right) &= m \operatorname{tr}(\widehat{P}^T D (P^T D)^{m-1}) \\ &\leq \operatorname{tr}((\widetilde{P}^T D)^m) + (m-1) \operatorname{tr}((P^T D)^m), \end{aligned} \quad (4.11)$$

which is (4.7). $\square$

Remark 4.2 In obtaining (4.11) by Lemma B.6, it is needed that $P^T D \succeq 0$ and $\widetilde{P}^T D = Q^T (\widehat{P}^T D) \succeq 0$. This explains the necessity of having a strict subset $\mathbb{P}$ of $\operatorname{St}(k, n)$ and aligning $\widehat{P}$ to $\widetilde{P} \in \mathbb{P}$ by some Q in (4.1) for defining atomic function for NPDo in general. For the purpose of maximizing $\operatorname{tr}((P^T D)^m)$, given $P \in \mathbb{P} = \operatorname{St}(k, n)_{D+}$ being the current approximation, to compute the next and hopefully improved approximation, the NPDo approach will seek $\widehat{P}$ to maximize $\operatorname{tr} \left(X^T \frac{\partial \operatorname{tr}((P^T D)^m)}{\partial P} \right)$, or equivalently, $\operatorname{tr}(X^T D (P^T D)^{m-1})$, over $X \in \operatorname{St}(k, n)$, and hence $\widehat{P}$ is taken to be an orthogonal polar factor of $D (P^T D)^{m-1}$. For that $\widehat{P}$, likely $\widehat{P}^T D \not\geq 0$, and hence necessarily $\widehat{P}$ needs to be aligned to $\widetilde{P} = \widehat{P} Q \in \mathbb{P}$ so that $\widetilde{P}^T D \succeq 0$.

For any $s > 1$, $f(P) = [\operatorname{tr}((P^T D)^m)]^s$ is well-defined for any $P \in \mathbb{R}^{n \times k}$ such that $\operatorname{tr}((P^T D)^m) \geq 0$. In particular, $[\operatorname{tr}((P^T D)^m)]^s$ is well-defined for

$$P \in \mathbb{R}_{D+}^{n \times k} := \{X \in \mathbb{R}^{n \times k} : X^T D \succeq 0\}.$$

With Theorem 4.3, a minor modification to the proof of Theorem 4.1 leads to

Corollary 4.1 Let $D \in \mathbb{R}^{n \times k}$, integer $m \geq 1$, $s > 1$, $g(P) = [\operatorname{tr}((P^T D)^m)]^s$.

a. For $P \in \mathbb{R}^{n \times k}$ at which $g(P)$ is well defined, we have

$$\operatorname{tr} \left(P^T \frac{\partial [\operatorname{tr}((P^T D)^m)]^s}{\partial P} \right) = sm [\operatorname{tr}((P^T D)^m)]^s; \quad (4.12a)$$

b. Let $P \in \mathbb{R}_{D+}^{n \times k}$, $\widehat{P} \in \mathbb{R}^{n \times k}$, and let $\widetilde{P} = \widehat{P} Q$, where $Q \in \operatorname{St}(k, k)$ is an orthogonal polar factor of $\widehat{P}^T D$. We have $\widetilde{P} \in \mathbb{R}_{D+}^{n \times k}$ and

$$\operatorname{tr} \left(\widehat{P}^T \frac{\partial [\operatorname{tr}((P^T D)^m)]^s}{\partial P} \right) \leq [\operatorname{tr}((\widetilde{P}^T D)^m)]^s + (sm-1) [\operatorname{tr}((P^T D)^m)]^s. \quad (4.12b)$$

In particular, the conditions in (4.1) hold with $\mathbb{P} = \operatorname{St}(k, n)_{D+}$, $\alpha = 1$ and $\beta = sm-1$, and thus $[\operatorname{tr}((P^T D)^m)]^s$ for $s > 1$ is an atomic function for NPDo.

Next we consider $\operatorname{tr}((P^T A P)^m)$ and its power.

Theorem 4.4 Let symmetric $A \in \mathbb{R}^{n \times n}$, and let $m \geq 1$ be an integer.

a. For $P \in \mathbb{R}^{n \times k}$, we have

$$\operatorname{tr} \left(P^T \frac{\partial \operatorname{tr}((P^T A P)^m)}{\partial P} \right) = 2m \operatorname{tr}((P^T A P)^m). \quad (4.13)$$

b. For P , $\widehat{P} \in \mathbb{R}^{n \times k}$, if $A \succeq 0$, then

$$\operatorname{tr} \left(\widehat{P}^T \frac{\partial \operatorname{tr}((P^T A P)^m)}{\partial P} \right) \leq \operatorname{tr}((\widehat{P}^T A \widehat{P})^m) + (2m - 1) \operatorname{tr}((P^T A P)^m). \quad (4.14)$$

In particular, the conditions in (4.1) hold with $\mathbb{P} = \operatorname{St}(k, n)$, $Q = I_k$ and $\widetilde{P} = \widehat{P}$, $\alpha = 1$ and $\beta = 2m - 1$, and thus $\operatorname{tr}((P^T A P)^m)$ is an atomic function for NPDo.

Proof Consider perturbing $P \in \mathbb{R}^{n \times k}$ to $P + E$ where $E \in \mathbb{R}^{n \times k}$ with $\|E\|$ sufficiently tiny. We have

$$\begin{aligned} [(P + E)^T A (P + E)]^m &= [P^T A P + E^T A P + P^T A E + E^T A E]^m \\ &= (P^T A P)^m + \sum_{i=0}^{m-1} (P^T A P)^i (E^T A P + P^T A E) (P^T A P)^{m-1-i} \\ &\quad + O(\|E\|^2), \end{aligned} \quad (4.15)$$

$$\begin{aligned} \operatorname{tr}([(P + E)^T A (P + E)]^m) &= \operatorname{tr}((P^T A P)^m) + m \operatorname{tr}(E^T A P (P^T A P)^{m-1}) \\ &\quad + m \operatorname{tr}((P^T A P)^{m-1} P^T A E) + O(\|E\|^2) \\ &= \operatorname{tr}((P^T A P)^m) + 2m \operatorname{tr}(E^T A P (P^T A P)^{m-1}) + O(\|E\|^2). \end{aligned} \quad (4.16)$$

Immediately, it follows from (4.16) that

$$\frac{\partial \operatorname{tr}((P^T A P)^m)}{\partial P} = 2m A P (P^T A P)^{m-1}. \quad (4.17)$$

Equation (4.13) is a direct consequence of (4.17). This proves item (a).

Next we prove item (b). Let $X = A^{1/2} \widehat{P}$ and $Y = A^{1/2} P$, where $A^{1/2}$ is the unique positive semidefinite square root of A . We have

$$\begin{aligned} \operatorname{tr} \left(\widehat{P}^T \frac{\partial \operatorname{tr}((P^T A P)^m)}{\partial P} \right) &= 2m \operatorname{tr}(\widehat{P}^T A P (P^T A P)^{m-1}) \\ &= 2m \operatorname{tr}(X^T Y (Y^T Y)^{m-1}) \\ &\leq \operatorname{tr}((X^T X)^m) + (2m - 1) \operatorname{tr}((Y^T Y)^m) \quad (\text{by Lemma B.7}) \\ &= \operatorname{tr}((\widehat{P}^T A \widehat{P})^m) + (2m - 1) \operatorname{tr}((P^T A P)^m), \end{aligned}$$

which is (4.14). $\square$

With Theorem 4.4, a minor modification to the proof of Theorem 4.1 leads to

Corollary 4.2 *Let symmetric $A \in \mathbb{R}^{n \times n}$, and let $m \geq 1$ be an integer and $s > 1$. For $P, \tilde{P} \in \mathbb{R}^{n \times k}$, if $A \geq 0$, then*

$$\operatorname{tr} \left(P^T \frac{\partial [\operatorname{tr}((P^T A P)^m)]^s}{\partial P} \right) = 2sm [\operatorname{tr}((P^T A P)^m)]^s, \quad (4.18a)$$

$$\operatorname{tr} \left(\tilde{P}^T \frac{\partial [\operatorname{tr}((P^T A P)^m)]^s}{\partial P} \right) \leq [\operatorname{tr}((\tilde{P}^T A \tilde{P})^m)]^s + (2sm - 1) [\operatorname{tr}((P^T A P)^m)]^s. \quad (4.18b)$$

In particular, the conditions in (4.1) hold with $\mathbb{P} = \operatorname{St}(k, n)$, $Q = I_k$, $\alpha = 1$ and $\beta = 2sm - 1$, and thus $[\operatorname{tr}((P^T A P)^m)]^s$ for $s > 1$ is an atomic function for NPDo.

5 Convex Composition

The concrete atomic functions for NPDo in (4.4) provides a limited collection of objective functions for which the NPDo approach provably works. In this section, we will vastly expand the collection to include any convex composition of atomic functions, provided that some of the partial derivatives of the composing convex function are nonnegative.

Specifically, we are interested in a special case of optimization problem (1.1) on the Stiefel manifold $\operatorname{St}(k, n)$ where f is a convex composition of atomic functions for NPDo, namely,

$$\max_{P \in \operatorname{St}(k, n)} f(P) \quad \text{with} \quad f(P) := (\phi \circ T)(P) \equiv \phi(T(P)), \quad (5.1)$$

where $T : P \in \operatorname{St}(k, n) \rightarrow T(P) \in \mathfrak{D} \subseteq \mathbb{R}^N$ whose components are atomic functions dependent of just a few or all columns of P , and $\phi : \mathfrak{D} \rightarrow \mathbb{R}$ is convex and differentiable. Denote the partial derivatives of ϕ with respect to $\mathbf{x} = [x_1, x_2, \dots, x_N]^T \in \mathfrak{D} \subseteq \mathbb{R}^N$ by

$$\phi_i(\mathbf{x}) = \frac{\partial \phi(\mathbf{x})}{\partial x_i} \quad \text{for } 1 \leq i \leq N. \quad (5.2)$$

Our goal is to solve (5.1) by Algorithm 3.1 and its accelerating variation in Algorithm 3.2 with convergence guarantee. To that end, we will have to place consistency conditions upon all components of $T(P)$. Let

$$T(P) = \begin{bmatrix} f_1(P_1) \\ f_2(P_2) \\ \vdots \\ f_N(P_N) \end{bmatrix}, \quad (5.3)$$

where each P_i is a submatrix of P , consisting of a few or all columns of P . We point out that it is possible that some of P_i may share common column(s) of P , different

from the situation in SumCT in Table 1. Alternatively, we can write $P_i = P J_i$ where $J_i \in \mathbb{R}^{k \times k_i}$ is submatrices of I_k , taking the columns of I_k with the same column indices as P_i to P . Each J_i acts as a column selector.

The KKT condition (2.3) for (5.1) becomes

$$\mathcal{H}(P) := \frac{\partial f(P)}{\partial P} = \sum_{i=1}^N \phi_i(T(P)) \frac{\partial f_i(P_i)}{\partial P_i} J_i^T = P \Lambda, \quad (5.4a)$$

$$\text{with } \Lambda^T = \Lambda \in \mathbb{R}^{k \times k}, \quad P \in \text{St}(k, n). \quad (5.4b)$$

The consistency conditions on atomic functions $f_i(P_i)$ for $1 \leq i \leq N$ are

$$\text{tr} \left(P_i^T \frac{\partial f_i(P_i)}{\partial P_i} \right) = \gamma_i f_i(P_i) \quad \text{for } P \in \mathbb{P} \subseteq \text{St}(k, n), \quad (5.5a)$$

and given $P \in \mathbb{P}$ and $\hat{P} \in \text{St}(k, n)$, there exists $Q \in \text{St}(k, k)$ such that $\tilde{P} = \hat{P}Q \in \mathbb{P}$ and

$$\text{tr} \left(\hat{P}_i^T \frac{\partial f_i(P_i)}{\partial P_i} \right) \leq \alpha f_i(\tilde{P}_i) + \beta_i f_i(P_i), \quad (5.5b)$$

where $\alpha > 0$, $\beta_i \geq 0$, and $\gamma_i = \alpha + \beta_i$ are constants, $\hat{P}_i$ and $\tilde{P}_i$ are the submatrices of $\hat{P}$ and $\tilde{P}$, respectively, with the same column indices as P_i to P . It is important to keep in mind that some of the inequalities in (5.5b) may actually be equalities, e.g., for $f_i(P_i) = \text{tr}(P_i^T D_i)$ it is an equality by Theorem 4.3.

On the surface, it looks like that each f_i is simply an atomic function for NPDo, but there are three built-in consistency requirements in (5.5) among all components $f_i(P_i)$: 1) the same $\mathbb{P}$ for all; 2) the same α for all, and 3) the same Q to give $\tilde{P} = \hat{P}Q$ for all.

Theorem 5.1 Consider $f = \phi \circ T$, where $T(\cdot)$ takes the form in (5.3) satisfying (5.5) and ϕ is convex and differentiable with partial derivatives denoted by ϕ_i as in (5.2). If $\phi_i(\mathbf{x}) \geq 0$ for those i for which (5.5b) does not become an equality, then the NPDo Ansatz holds with $\omega = 1/\alpha$.

Proof Given $P \in \mathbb{P} \subseteq \text{St}(k, n)$ and $\hat{P} \in \text{St}(k, n)$, suppose that (3.1) holds, i.e., $\text{tr}(\hat{P}^T \mathcal{H}(P)) \geq \text{tr}(P^T \mathcal{H}(P)) + \eta$. Write

$$\mathbf{x} = T(P) \equiv [x_1, x_2, \dots, x_N]^T, \quad \tilde{\mathbf{x}} = T(\tilde{P}) \equiv [\tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_N]^T,$$

i.e., $x_i = f_i(P_i)$ and $\tilde{x}_i = f_i(\tilde{P}_i)$. Noticing $\mathcal{H}(P)$ in (5.4), we have

$$\begin{aligned} \text{tr}(P^T \mathcal{H}(P)) &= \sum_{i=1}^N \phi_i(\mathbf{x}) \text{tr} \left(P^T \frac{\partial f_i(P_i)}{\partial P_i} J_i^T \right) \\ &= \sum_{i=1}^N \phi_i(\mathbf{x}) \text{tr} \left(P_i^T \frac{\partial f_i(P_i)}{\partial P_i} \right) \end{aligned}$$

$$\begin{aligned}
 &= \sum_{i=1}^N \gamma_i \phi_i(\mathbf{x}) x_i, \quad (\text{by (5.5a)}) \\
 \text{tr}(\widehat{P}^T \mathcal{H}(P)) &= \sum_{i=1}^N \phi_i(\mathbf{x}) \text{tr} \left(\widehat{P}_i^T \frac{\partial f_i(P_i)}{\partial P_i} \right) \\
 &\leq \sum_{i=1}^N \phi_i(\mathbf{x}) (\alpha \widetilde{x}_i + \beta_i x_i),
 \end{aligned}$$

where the last inequality is due to $\phi_i \geq 0$ when the corresponding (5.5b) does not become an equality. Plug them into (3.1) and simplify the resulting inequality with the help of $\gamma_i = \alpha + \beta_i$ to get

$$\eta/\alpha + \nabla \phi(\mathbf{x})^T \mathbf{x} = \eta/\alpha + \sum_{i=1}^N \phi_i(\mathbf{x}) x_i \leq \sum_{i=1}^N \phi_i(\mathbf{x}) \widetilde{x}_i = \nabla \phi(\mathbf{x})^T \widetilde{\mathbf{x}}.$$

Finally apply Lemma B.3 to yield $f(\widetilde{P}) \geq f(P) + \eta/\alpha$. $\square$

With Theorem 5.1 come the general results established in sect. 3. In particular, Algorithm 3.1 (NPDoSCF) and its accelerating variation in Algorithm 3.2 can be applied to find a maximizer of (5.1), except that the calculation of Q_i at Line 4 of Algorithm 3.1 remains to be specified. This missing detail is in general dependent of the particularity of the mapping T and the convex function ϕ , to which we shall return after we showcase a few concrete mappings of T , where $A_i \in \mathbb{R}^{n \times n}$ for $1 \leq i \leq \ell$ are at least symmetric and $D_i \in \mathbb{R}^{n \times k_i}$ with $1 \leq k_i \leq k$ for $1 \leq i \leq t$.

Example 5.1 Consider the **first** concrete mapping of T :

$$T_1 : P \in \text{St}(k, n) \rightarrow T_1(P) := \begin{bmatrix} \text{tr}(P_1^T A_1 P_1) \\ \vdots \\ \text{tr}(P_\ell^T A_\ell P_\ell) \\ \text{tr}(P_{\ell+1}^T D_1) \\ \vdots \\ \text{tr}(P_{\ell+t}^T D_t) \end{bmatrix} \in \mathbb{R}^{\ell+t}. \quad (5.6)$$

Either $\ell = 0$ or $t = 0$ (i.e., TrCP in Table 1) is allowed. If all $A_i \succeq 0$, then the consistency conditions in (5.5) are satisfied with $\mathbb{P} = \text{St}(k, n)$, $Q = I_k$, $\alpha = 1$, $\beta_i = 1$ for $1 \leq i \leq \ell$ and $\beta_{\ell+j} = 0$ for $1 \leq j \leq t$, by Theorems 4.3 and 4.4. In particular, now (5.5b) for $\ell + 1 \leq i \leq \ell + t$ are equalities. Thus Theorem 5.1 applies, assuming $\phi_j(\mathbf{x}) \geq 0$ for $1 \leq j \leq \ell$. Two existing special cases of T_1 are

1. $\ell = t$, $P_i = P_{\ell+i}$ for $1 \leq i \leq \ell$, $P = [P_1, P_2, \dots, P_\ell]$, and $\phi(\mathbf{x}) = \sum_{i=1}^{\ell+t} x_i$, which gives SumCT investigated by [67] (see also Table 1), and

2. $t = 0, k = 1, P_i = \mathbf{p}$ (a unit vector) for $1 \leq i \leq \ell$, which gives the main problem of [5] (in the paper, $\phi(\mathbf{x}) = \sum_{i=1}^{\ell} \psi_i(x_i)$ for $\mathbf{x} = [x_1, x_2, \dots, x_{\ell}]^T$ with each ψ_i being a convex function of a single-variable).

Despite that we can take $\mathbb{P} = \text{St}(k, n)$ and $Q = I_k$ here, with favorable compositions of P_i as submatrices of P , we can find a better Q , other than I_k , so that the objective value increases more than **the NPDo Ansatz** suggests. Here are two of them:

- a. $J_{\ell+i}^T J_{\ell+j} = 0$ for $i \neq j$, which means that $P_{\ell+i}$ and $P_{\ell+j}$ share no common column of P ;

b. For $1 \leq i \leq \ell, 1 \leq j \leq t$, either $J_{\ell+j}^T J_i = 0$ or no row of $J_{\ell+j}^T J_i$ is 0, which means either P_i and $P_{\ell+j}$ share no common column of P or $P_{\ell+j}$ is a submatrix of P_i .
- (5.7)

- a. either $J_{\ell+i}^T J_{\ell+j} = 0$ or $J_{\ell+i}^T J_{\ell+j} = I$ for any $i \neq j$, which means that $P_{\ell+i}$ and $P_{\ell+j}$ either share no common column of P , or $P_{\ell+i} = P_{\ell+j}$, i.e., the same submatrix of P ;

b. the same as item (b) in (5.7).
- (5.8)

For (5.7), we determine Q implicitly by $\tilde{P}_{\ell+j} = \hat{P}_{\ell+j} S_j$ where S_j is an orthogonal polar factor of $\phi_{\ell+j}(T_1(P)) \hat{P}_{\ell+j}^T D_j$ for $1 \leq j \leq t$. In the case of (5.8), $J_{\ell+j}$ for $1 \leq j \leq t$ can be divided into no more than t groups, and within each group all $J_{\ell+j}$ are the same and two $J_{\ell+j}$ from different groups share no common column of P at all. For ease of presentation, let us say the set of indices $\{1, 2, \dots, t\}$ is divided into τ exclusive subsets $\mathbb{I}_q$ for $1 \leq q \leq \tau$ such that

$$\cup_{j=1}^{\tau} \mathbb{I}_j = \{1, 2, \dots, t\}, \quad \mathbb{I}_i \cap \mathbb{I}_j = \emptyset \text{ for } i \neq j, \text{ and } J_{\ell+i} = J_{\ell+j} \text{ if } i, j \text{ belong to the same } \mathbb{I}_q \text{ but } J_{\ell+i}^T J_{\ell+j} = 0 \text{ otherwise.}$$

Now determine Q implicitly by taking just one index j from each $\mathbb{I}_q$ for $1 \leq q \leq \tau$ and letting $\tilde{P}_{\ell+j} = \hat{P}_{\ell+j} S_q$ where S_q is an orthogonal polar factor of

$$\hat{P}_{\ell+j}^T \left[\sum_{i \in \mathbb{I}_q} \phi_{\ell+i}(T_1(P)) D_i \right]. \quad (5.9)$$

Example 5.2 The **second** concrete mapping of T is

$$T_2 : P \in \text{St}(k, n) \rightarrow T_2(P) := \begin{bmatrix} \|P_1^T A_1 P_1\|_{\text{F}}^2 \\ \vdots \\ \|P_{\ell}^T A_{\ell} P_{\ell}\|_{\text{F}}^2 \\ \|P_{\ell+1}^T D_1\|_{\text{F}}^2 \\ \vdots \\ \|P_{\ell+t}^T D_t\|_{\text{F}}^2 \end{bmatrix} \in \mathbb{R}^{\ell+t}. \quad (5.10)$$

Either $\ell = 0$ or $t = 0$ is allowed. To use Theorem 4.4, we notice that

$$\|P_i^T A_i P_i\|_F^2 = \text{tr}((P_i^T A_i P_i)^2), \quad \|P_{\ell+j}^T D_j\|_F^2 = \text{tr}(P_{\ell+j}^T D_j D_j^T P_{\ell+j}).$$

Hence if all $A_i \geq 0$, then the consistency conditions in (5.5) are satisfied with $\mathbb{P} = \text{St}(k, n)$, $Q = I_k$, $\alpha = 1$, $\beta_i = 3$ for $1 \leq i \leq \ell$, and $\beta_{\ell+j} = 1$ for $1 \leq j \leq t$. Theorem 5.1 applies, assuming $\phi_j(\mathbf{x}) \geq 0$ for $1 \leq j \leq \ell + t$.

A special case of T_2 is $t = 0$ and $P_i = P$ for $1 \leq i \leq \ell$, for which (5.1) with $T = T_2$ gives the key optimization problem in the uniform multidimensional scaling (UMDS) [80] (see also Table 1).

Example 5.3 More generally, the **third** concrete mapping of T is

$$T_3 : P \in \text{St}(k, n) \rightarrow T_3(P) := \begin{bmatrix} \text{tr}((P_1^T A_1 P_1)^{m_1}) \\ \vdots \\ \text{tr}((P_\ell^T A_\ell P_\ell)^{m_\ell}) \\ \text{tr}((P_{\ell+1}^T D_1)^{m_{\ell+1}}) \\ \vdots \\ \text{tr}((P_{\ell+t}^T D_t)^{m_{\ell+t}}) \end{bmatrix} \in \mathbb{R}^{\ell+t}, \quad (5.11)$$

where integer $m_i \geq 1$ for all $1 \leq i \leq \ell + t$. It reduces to Example 5.1 if $m_i = 1$ for all $1 \leq i \leq \ell + t$. Either $\ell = 0$ or $t = 0$ is allowed. Suppose all $A_i \geq 0$. Suppose all P_i together have the properties in (5.7). Then the consistency conditions in (5.5) are satisfied with

$$\mathbb{P} = \{P \in \text{St}(k, n) : P_{\ell+j}^T D_j \geq 0 \text{ for } 1 \leq j \leq t\}, \quad (5.12)$$

$\alpha = 1$, $\beta_i = 2m_i - 1$ for $1 \leq i \leq \ell$ and $\beta_{\ell+j} = m_{\ell+j} - 1$ for $1 \leq j \leq t$, by Theorems 4.3 and 4.4. Theorem 5.1 applies, assuming $\phi_j(\mathbf{x}) \geq 0$ for $1 \leq j \leq \ell$ and for each $j \in \{\ell + 1, \dots, \ell + t\}$ with $m_j \geq 2$. Q is implicitly determined by $\tilde{P}_{\ell+j} = \hat{P}_{\ell+j} S_j$ where S_j is an orthogonal polar factor of $\hat{P}_{\ell+j}^T D_j$ for $1 \leq j \leq t$.

We pointed out in Example 5.1 that judiciously choosing Q to go from $\hat{P}$ to $\tilde{P}$ in (5.5) can increase the objective function value more than Theorem 5.1 suggests. To further strengthen this point, we consider a special case of T_1 : $P_i = P$ for $1 \leq i \leq \ell + t$. For ease of future reference, denote the special T_1 by

$$T_{1a} : P \in \text{St}(k, n) \rightarrow T_{1a}(P) := \begin{bmatrix} \text{tr}(P^T A_1 P) \\ \vdots \\ \text{tr}(P^T A_\ell P) \\ \text{tr}(P^T D_1) \\ \vdots \\ \text{tr}(P^T D_t) \end{bmatrix} \in \mathbb{R}^{\ell+t}. \quad (5.13)$$

Theorem 5.2 Consider $f = \phi \circ T_{1a}$ where ϕ is convex and differentiable with $\phi_j(\mathbf{x}) \geq 0$ for $1 \leq j \leq \ell$, and suppose $A_i \geq 0$ for $1 \leq i \leq \ell$. Given $\hat{P} \in \text{St}(k, n)$, $P \in \text{St}(k, n)$, let $\tilde{P} = \hat{P}Q$ where Q is an orthogonal polar factor of $\hat{P}^T \mathcal{D}(P)$ with

$$\mathcal{D}(P) = \sum_{j=1}^t \phi_{\ell+j}(T_{1a}(P)) D_j. \quad (5.14)$$

If $\text{tr}(\hat{P}^T \mathcal{H}(P)) \geq \text{tr}(P^T \mathcal{H}(P)) + \eta$, then $f(\tilde{P}) \geq f(P) + \eta + \delta$, where $\delta = \|\hat{P}^T \mathcal{D}(P)\|_{\text{tr}} - \text{tr}(\hat{P}^T \mathcal{D}(P))$. In particular, the **NPD Ansatz** holds with $\omega = 1$.

Proof Along the lines in the proof of Theorem 5.1, here we will have

$$\begin{aligned} \text{tr}(P^T \mathcal{H}(P)) &= 2 \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) x_i + \sum_{j=1}^t \phi_{\ell+j}(\mathbf{x}) x_{\ell+j}, \\ \|\hat{P}^T \mathcal{D}(P)\|_{\text{tr}} &= \text{tr}(\tilde{P}^T \mathcal{D}(P)) \quad (\text{since } \tilde{P}^T \mathcal{D}(P) = Q^T [\hat{P}^T \mathcal{D}(P)] \geq 0) \\ &= \sum_{j=1}^t \phi_{\ell+j}(\mathbf{x}) \tilde{x}_{\ell+j}, \\ \text{tr}(\hat{P}^T \mathcal{H}(P)) &= 2 \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) \text{tr}(\hat{P}^T A_i P) + \sum_{j=1}^t \phi_{\ell+j}(\mathbf{x}) \text{tr}(\hat{P}^T D_j) \\ &\leq \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) \left[\text{tr}(\hat{P}^T A_i \hat{P}) + \text{tr}(P^T A_i P) \right] + \text{tr}(\hat{P}^T \mathcal{D}(P)) \\ &= \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) \left[\tilde{x}_i + x_i \right] + \|\hat{P}^T \mathcal{D}(P)\|_{\text{tr}} - \delta \\ &= \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) \left[\tilde{x}_i + x_i \right] + \sum_{j=1}^t \phi_{\ell+j}(\mathbf{x}) \tilde{x}_{\ell+j} - \delta. \end{aligned}$$

Plug them into $\eta + \text{tr}(P^T \mathcal{H}(P)) \leq \text{tr}(\hat{P}^T \mathcal{H}(P))$ and simplify the resulting inequality to get $\eta + \delta + \nabla \phi(\mathbf{x})^T \mathbf{x} \leq \nabla \phi(\mathbf{x})^T \tilde{\mathbf{x}}$, and then apply Lemma B.3 to conclude the proof. $\square$

Theorem 5.2 improves Theorem 5.1 when it comes to $T = T_{1a}$: the objective value increases additional δ more. We notice, by Lemma B.9, that $\delta \geq 0$ always and it is strict unless $\hat{P}^T \mathcal{D}(P) \geq 0$. Also note $\tilde{P}$ satisfies $\tilde{P}^T \mathcal{D}(P) \geq 0$. As a result of Theorem 5.2, along the same line of the proof of Theorem 3.1, we have another necessary condition on a maximizer P_* of (5.1) with $T = T_{1a}$ in Corollary 5.1, beyond the ones in Theorem 3.1.

Corollary 5.1 Suppose $A_i \geq 0$ for $1 \leq i \leq \ell$ and that ϕ is convex and differentiable with $\phi_j(\mathbf{x}) \geq 0$ for $1 \leq j \leq \ell$. If P_* is a maximizer of (5.1) with $T = T_{1a}$, then we have not only (2.3) for $P = P_*$ with $\Lambda = \Lambda_* := P_*^T \mathcal{H}(P_*) \geq 0$ but also $P_*^T \mathcal{D}(P_*) \geq 0$.

Table 3 Condition on ϕ_j and choice of Q_i at Line 4 of Algorithm 3.1

T_1 and T_{1a}	$\phi_j \geq 0$ for $1 \leq j \leq \ell$, $Q_i = I_k$.
T_1 with (5.7) and $t \geq 1$	$\phi_j \geq 0$ for $1 \leq j \leq \ell$, Q_i is implicitly determined by $\tilde{P}_{\ell+j}^{(i+1)} = \tilde{P}_{\ell+j}^{(i)} S_j$ where S_j is an orthogonal polar factor of $\phi_{\ell+j}(T_1(P)) [\hat{P}_{\ell+j}^{(i)}]^T D_j$ for $1 \leq j \leq t$.
T_1 with (5.8) and $t \geq 1$	$\phi_j \geq 0$ for $1 \leq j \leq \ell$, Q_i is implicitly determined by: for just one element j from each $\mathbb{I}_q$ ($1 \leq q \leq \tau$), $\tilde{P}_{\ell+j}^{(i+1)} = \tilde{P}_{\ell+j}^{(i)} S_q$ where S_q is an orthogonal polar factor of $[\hat{P}_{\ell+j}^{(i)}]^T [\sum_{p \in \mathbb{I}_q} \phi_{\ell+p}(T_1(P)) D_p]$ for $1 \leq q \leq \tau$.
T_{1a} with $t \geq 1$	$\phi_j \geq 0$ for $1 \leq j \leq \ell$, Q_i is an orthogonal polar factor of $[\hat{P}^{(i)}]^T \mathcal{D}(P^{(i)})$.
T_2	$\phi_j \geq 0$ for $1 \leq j \leq \ell + t$, $Q_i = I_k$.
T_3 with $t = 0$	$\phi_j \geq 0$ for $1 \leq j \leq \ell$, $Q_i = I_k$.
T_3 with (5.7) and $t \geq 1$	$\phi_j \geq 0$ for $1 \leq j \leq \ell$ and for each $j \in \{\ell + 1, \dots, \ell + t\}$ with $m_j \geq 2$, Q_i is implicitly determined by $\tilde{P}_{\ell+j}^{(i+1)} = \tilde{P}_{\ell+j}^{(i)} S_j$ where S_j is an orthogonal polar factor of $[\hat{P}_{\ell+j}^{(i)}]^T D_j$ for $1 \leq j \leq t$.

$$\phi_j(\mathbf{x}) := \partial \phi(\mathbf{x}) / \partial x_j \text{ for } \mathbf{x} = [x_j]$$

In Table 3, we list conditions on partial derivatives ϕ_j and the best choices of Q_i at Line 4 of Algorithm 3.1 that, when it is not I_k , can increase the objective value even more per SCF iterative step than **the NPDo Ansatz** suggests. Having said that, we notice that $P^{(i)}$ as i varies may belong to different subsets $\mathbb{P}$ of $\text{St}(k, n)$. For example, with $T = T_{1a}$, if Q_i is calculated according to Theorem 5.2, i.e., Q_i is an orthogonal polar factor of $[\hat{P}^{(i)}]^T \mathcal{D}(P^{(i)})$, then $P^{(i+1)} \in \mathbb{P}_i := \{X \in \text{St}(k, n) : X^T \mathcal{D}(P^{(i)}) \succeq 0\}$ that varies from one iterative step to the next. Eventually, $\mathbb{P}_i$ approaches $\mathbb{P}_* := \{X \in \text{St}(k, n) : X^T \mathcal{D}(P_*) \succeq 0\}$ by Corollary 5.1. Similar comments can be said about T_1 with (5.7) or (5.8) that we discussed towards the end of Example 5.1. Numerically, such variations in $\mathbb{P}$ does not pose any problem for Algorithm 3.1 to compute an approximate maximizer for the maximization problem (5.1).

Remark 5.1 We conclude this section by commenting on the applicability of the results of this section to the objective functions in Table 1 via convex compositions of atomic functions for NPDo. Essentially our results are applicable to all of those that are not in the quotient form, i.e., SEP, MBSUB, SumCT, TrCP, UMDS, and DFT, assuming that matrices A and A_i are positive semidefinite. SEP is simply about the atomic function $\text{tr}(P^T A P)$. For OLDA and SumTR, the corresponding composing functions ϕ are x_2/x_1 and $x_2/x_1 + x_3$, respectively, but both are non-convex. The composing function for OCCA is $\phi_0(\mathbf{x}) = x_2/\sqrt{x_1}$ where $\mathbf{x} = [x_1, x_2]^T$, which is not convex but whose square $\phi(\mathbf{x}) := [\phi_0(\mathbf{x})]^2 = x_2^2/x_1$ is convex for $x_2 \geq 0$ and $x_1 > 0$. Unfortunately, the atomic function associated with x_1 is $\text{tr}(P^T B P)$, for which $\phi_1(\mathbf{x}) := \partial \phi(\mathbf{x}) / \partial x_1 = -(x_2/x_1)^2 \leq 0$, violating the conditions of Theorems 5.1 and 5.2. A similar argument

applies to Θ TR. So the NPDo approach does not work for OLDA, OCCA, and Θ TR. But, fortunately, the NEPv approach next will.

Part II

The NEPv Approach

6 The NEPv Framework

There are cases for which

$$\mathcal{H}(P) := \frac{\partial f(P)}{\partial P} \equiv H(P)P \quad (6.1)$$

for $P \in \text{St}(k, n)$ (or even $\mathbb{R}^{n \times k}$), where $H(P) \in \mathbb{R}^{n \times n}$ is a symmetric matrix-valued function dependent of P , e.g., for $f(P) = \frac{\text{tr}(P^T A P)}{\text{tr}(P^T B P)} + \text{tr}(P^T C P)$ from the sum of trace ratios (SumTR) [76, 77], which includes SEP and OLDA as special cases,

$$\mathcal{H}(P) = 2 \left[\frac{1}{\text{tr}(P^T B P)} \left(A - \frac{\text{tr}(P^T A P)}{\text{tr}(P^T B P)} B \right) + C \right] P \equiv H(P)P \quad (6.2)$$

for $P \in \mathbb{R}^{n \times k}$, where $H(P)$ is easily identified. In fact, Lu and Li [47, Lemma 2.1] show that (6.1) always hold for some symmetric and right-unitarily invariant $H(P)$ if f is right-unitarily invariant. As a result of (6.1), the KKT condition (2.3) is an NEPv:

$$H(P)P = P\Omega, \quad P \in \text{St}(k, n). \quad (6.3)$$

Necessarily $\Omega = P^T H(P)P \in \mathbb{R}^{k \times k}$ is symmetric.

But not all $\mathcal{H}(P) = \partial f(P)/\partial P$ take the form $H(P)P$, and in the latter, we can still construct some $H(P)$ to turn the KKT condition (2.3) equivalently into an NEPv in the form of (6.3) under some mild condition. For example, for $f(P) = \frac{\text{tr}(P^T A P + P^T D)}{[\text{tr}(P^T B P)]^\theta}$ of the θ -trace ratio problem (Θ TR) which includes OCCA and the MAXBET subproblem as special cases, the authors of [68] used

$$H(P) = \frac{2}{[\text{tr}(P^T B P)]^\theta} \left(A + \frac{D P^T + P D^T}{2} - \theta \frac{\text{tr}(P^T A P + P^T D)}{\text{tr}(P^T B P)} B \right). \quad (6.4)$$

In general, we can always take

$$H(P) := [\mathcal{H}(P)]P^T + P[\mathcal{H}(P)]^T = \left[\frac{\partial f(P)}{\partial P} \right] P^T + P \left[\frac{\partial f(P)}{\partial P} \right]^T. \quad (6.5)$$

In the case when $\mathcal{H}(P) \equiv H_0(P)P$, this $H(P)$ becomes $2 H_0(P)$ for $P \in \text{St}(k, n)$.

Why $H(P)$ in (6.4) and (6.5) work for Θ TR and in general, respectively, can be best explained by the next theorem.

Theorem 6.1 Let $H(P) \in \mathbb{R}^{n \times n}$ be a symmetric matrix-valued function satisfying

$$H(P)P - \frac{\partial f(P)}{\partial P} = P \mathcal{M}(P) \text{ for } P \in \text{St}(k, n), \quad (6.6)$$

where $\mathcal{M}(P) \in \mathbb{R}^{k \times k}$ is some matrix-valued function. $P \in \text{St}(k, n)$ is a solution to the KKT condition (2.3) if and only if it is a solution to NEPv (6.3) and $\mathcal{M}(P)$ is symmetric.

Proof If P is a solution to the KKT condition (2.3), i.e., $\mathcal{H}(P) = P\Lambda$, $P \in \text{St}(k, n)$, and $\Lambda = \Lambda^T$. Then, by (6.6),

$$H(P)P = P\Lambda + P\mathcal{M}(P) = P(\Lambda + \mathcal{M}(P)) =: P\Omega,$$

where $\Omega = \Lambda + \mathcal{M}(P)$ is symmetric because alternatively $\Omega = P^T H(P)P$ which is symmetric, and hence $\mathcal{M}(P) = \Omega - \Lambda$ is also symmetric. On the other hand, if P is a solution to NEPv (6.3) such that $\mathcal{M}(P)$ is symmetric, then again by (6.6)

$$\mathcal{H}(P) = P\Omega - P\mathcal{M}(P) = P(\Omega - \mathcal{M}(P)) =: P\Lambda,$$

where $\Lambda = \Omega - \mathcal{M}(P)$ is symmetric because $\mathcal{M}(P)$ is assumed symmetric. $\square$

According to Theorem 6.1, to solve the KKT condition (2.3) via solving NEPv (6.3) with an $H(P)$ that satisfies (6.6), we need to limit the solutions to those of the NEPv such that $\mathcal{M}(P)$ is symmetric. Return to the concrete $H(P)$ given by (6.4) and (6.5). It can be verified that, for $H(P)$ in (6.4) for ΘTR ,

$$H(P)P - \mathcal{H}(P) = P \left(\frac{1}{[\text{tr}(P^T B P)]^\theta} D^T P \right),$$

and hence any solution to the resulting NEPv (6.3) such that $D^T P$ is symmetric is a KKT point of ΘTR and vice versa. Similarly, for $H(P)$ in (6.5) in general,

$$H(P)P - \mathcal{H}(P) = P([\mathcal{H}(P)]^T P)$$

and hence any solution to the resulting NEPv (6.3) such that $[\mathcal{H}(P)]^T P$ is symmetric is a KKT point and vice versa.

We note that (6.6) is a guiding equation for $H(P)$, and satisfying (6.6) yields a candidate $H(P)$ and the resulting NEPv (6.3). In general, given $\mathcal{H}(P)$, there are infinitely many $H(P)$ that satisfy (6.6).

Our goal in this part is still the same as in Part I, namely establishing conditions under which SCF (1.6) on NEPv (6.3) is provably convergent, except that the conditions will be imposed on $H(P)$, instead of $\mathcal{H}(P)$ earlier. The developments in this section follow the lines of [68, 78], but in more abstract terms.

6.1 The NEPv Ansatz

The successes of the NEPv approach used in [68, 78] for solving OCCA and Θ TR relies on certain monotonicity lemmas which inspire us to make the following ansatz to build our framework upon. It also requires a sufficiently inclusive subset $\mathbb{P}$ of $\text{St}(k, n)$ as in the NPDo framework in Part I.

The NEPv Ansatz. For function f defined in some neighborhood $\text{St}_\delta(k, n)$ of the Stiefel manifold $\text{St}(k, n)$, there is a symmetric matrix-valued function $H(P) \in \mathbb{R}^{n \times n}$ such that for $\hat{P} \in \text{St}(k, n)$, $P \in \mathbb{P} \subseteq \text{St}(k, n)$, if

$$\text{tr}(\hat{P}^T H(P) \hat{P}) \geq \text{tr}(P^T H(P) P) + \eta \quad \text{for some } \eta \in \mathbb{R}, \quad (6.7)$$

then there exists $Q \in \text{St}(k, k)$ such that $\tilde{P} = \hat{P}Q \in \mathbb{P}$ and $f(\tilde{P}) \geq f(P) + \omega\eta$, where ω is some positive constant, independent of P and $\hat{P}$.

For any $P \in \text{St}(k, n)$, there is always $\hat{P} \in \text{St}(k, n)$ such that (6.7) holds with some $\eta > 0$, unless for that given P , $H(P)P = P\Omega$ holds and the eigenvalues of Ω consist of the k largest eigenvalues of $H(P)$. In fact, we can take $\hat{P} \in \text{St}(k, n)$ to be an orthonormal basis matrix of the eigenspace of $H(P)$ associated with its k largest eigenvalues, which also maximizes $\text{tr}(X^T H(P) X)$ over $X \in \text{St}(k, n)$ [20]. For the purpose of solving (1.1), we may relax the ansatz to $\eta \geq 0$ only. In general, it is the desirable aim, $f(\tilde{P}) \geq f(P) + \omega\eta$, in the NEPv Ansatz that needs to be verified before the general theory of this section can be applied. Below we will use the same objective function in Example 3.1 to rationalize this ansatz.

Example 6.1 Consider $f(P) = \text{tr}(P^T A P) + \text{tr}((P^T D)^2)$ where $A \in \mathbb{R}^{n \times n}$ is symmetric and $D \in \mathbb{R}^{n \times k}$. Note now no longer A is required to be positive semidefinite as it had to be in Example 3.1. Since $\mathcal{H}(P) = 2AP + 2DP^T D$, no longer there exists a symmetric $H(P)$ such that (6.1) holds. Our discussion above leads us to use $H(P) = 2A + 2(DP^T D P^T + P D^T P D^T)$ for which

$$H(P)P - \mathcal{H}(P) = P[2(D^T P)^2] \quad \text{for } P \in \text{St}(k, n),$$

satisfying (6.6). To achieve equivalency between the KKT condition (2.3) and NEPv (6.3), according to Theorem 6.1 we should limit the scope to those $P \in \text{St}(k, n)$ such that $(D^T P)^2$ is symmetric. Actually we will further limit the scope to $P \in \mathbb{P} = \text{St}(k, n)_{D+}$. Suppose now that (6.7) holds for $P \in \text{St}(k, n)_{D+}$ and $\hat{P} \in \text{St}(k, n)$, or equivalently,

$$2\text{tr}(\hat{P}^T A \hat{P}) + 4\text{tr}(\hat{P}^T D P^T D P^T \hat{P}) \geq 2\text{tr}(P^T A P) + 4\text{tr}((P^T D)^2) + \eta. \quad (6.8)$$

Next let $Q \in \text{St}(k, k)$ be an orthogonal polar factor of $\hat{P}^T D$ and let $\tilde{P} = \hat{P}Q \in \mathbb{P}$. We find that $\text{tr}(\tilde{P}^T A \tilde{P}) = \text{tr}(\hat{P}^T A \hat{P})$, but it remains to break the second term in the left-hand side of (6.8) apart so that P and $\hat{P}$ are detached. For that purpose, we note

$$\begin{aligned} 2\text{tr}(\hat{P}^T D P^T D P^T \hat{P}) &\leq 2\|\hat{P}^T D P^T D P^T \hat{P}\|_{\text{tr}} \quad (\text{by Lemma B.8}) \\ &\leq 2\|\hat{P}^T D P^T D\|_{\text{tr}} \|P^T \hat{P}\|_2 \end{aligned}$$

$$\begin{aligned}
 &\leq 2\|\widehat{P}^T D P^T D\|_{\text{tr}} \quad (\text{since } \|P^T \widehat{P}\|_2 \leq 1) \\
 &\leq \text{tr}((Q^T \widehat{P}^T D)^2) + \text{tr}((P^T D)^2) \quad (\text{by Lemma B.6}) \\
 &= \text{tr}((\widetilde{P}^T D)^2) + \text{tr}((P^T D)^2). \quad (6.9)
 \end{aligned}$$

Combine (6.8) and (6.9) to get $f(\widetilde{P}) \geq f(P) + \eta/2$ upon noticing $\text{tr}(\widetilde{P}^T A \widetilde{P}) = \text{tr}(\widehat{P}^T A \widehat{P})$. As in Example 3.1, we observe the critical conditions: $P^T D \succeq 0$ and $\widetilde{P}^T D \succeq 0$ (i.e., $P, \widetilde{P} \in \mathbb{P}$), that we used to derive (6.9), where $\widetilde{P}^T D = Q^T \widehat{P}^T D \succeq 0$ is again made possible by the chosen Q .

Remark 6.1 A few comments on the **NEPv Ansatz** are in order.

- i. **The NEPv Ansatz** critically involves a symmetric matrix-valued function $H(P) \in \mathbb{R}^{n \times n}$ that has to be constructed. In Theorem 6.1, we provide a guiding equation (6.6) for the purpose so that the KKT condition (2.3) and NEPv (6.3) are equivalent as far as solving the associated optimization problem (1.1) is concerned. It is fulfilled naturally when $\mathcal{H}(P) \equiv H(P)P$ for $P \in \text{St}(k, n)$ exactly (e.g., for OLDA, SumTR, TrCP, UMDS, and DFT), but at other times, we will have to construct $H(P)$ individually based on the particularity of $\mathcal{H}$ as in [78] for OCCA, [68] for Θ TR, [75] for MAXBET and Example 6.1, or we simply use the generic (6.5). The ansatz does not demand any explicit association of $H(P)$ with $\mathcal{H}(P)$, but conceivably they should be highly related, such as the relation imposed by (6.6).
- ii. One may argue that the ansatz might be made unnecessarily complicated. After all $\text{tr}(\widehat{P}^T H(P) \widehat{P}) = \text{tr}(\widetilde{P}^T H(P) \widetilde{P})$. Should we get rid of $\widehat{P}$ in the ansatz altogether? One possibility is to require that

$$\boxed{\text{tr}(\widetilde{P}^T H(P) \widetilde{P}) \geq \text{tr}(P^T H(P) P) + \eta \text{ for } P, \widetilde{P} \in \mathbb{P} \text{ implies } f(\widetilde{P}) \geq f(P) + \omega\eta.} \quad (6.10)$$

This is a stronger version, however, assuming that for any $\widehat{P} \in \text{St}(k, n)$, there exists $Q \in \text{St}(k, k)$ such that $\widetilde{P} = \widehat{P}Q \in \mathbb{P}$. Here is why. Suppose that (6.10) holds. Given $\widehat{P} \in \text{St}(k, n)$, $P \in \mathbb{P} \subseteq \text{St}(k, n)$, let $\widetilde{P} = \widehat{P}Q \in \mathbb{P}$ for some $Q \in \text{St}(k, k)$. If (6.7) holds, then

$$\text{tr}(\widetilde{P}^T H(P) \widetilde{P}) = \text{tr}(\widehat{P}^T H(P) \widehat{P}) \geq \text{tr}(P^T H(P) P) + \eta,$$

which, under (6.10), yields $f(\widetilde{P}) \geq f(P) + \omega\eta$, proving the desired inequality of **the NEPv Ansatz**.

- iii. When $f(P)$ is right-unitarily invariant, $H(P)$ always exists such that (6.1) holds and can be taken to be right-unitarily invariant, too [47, Lemma 2.1]. In such a case, the ansatz can be simplified to: $Q = I_k$ and $\widetilde{P} = \widehat{P}$ always because $f(\widehat{P}) = f(\widetilde{P})$ regardless of Q . Also often $\mathbb{P} = \text{St}(k, n)$.
- iv. Introducing a subset $\mathbb{P}$ of $\text{St}(k, n)$ and judiciously choosing Q are for generality to deal with the case when $f(P)$ is not right-unitarily invariant, e.g., the one in Example 6.1 and those in Table 1 in sect. 1 that involve D or D_i . Suitable Q can

also increase the objective value more than $\omega\eta$. For example, for Θ TR with $H(P)$ given by (6.4), the **NEPv Ansatz** holds with taking Q to be an orthogonal polar factor of $\widehat{P}^T D$. In fact, along the line of the proof of [68, Lemma 2.1], assuming $B \geq 0$, $\text{rank}(B) > n - k$, and $\text{tr}(P^T A P + P^T D) \geq 0$ in the case of $0 < \theta < 1$ but otherwise no need to impose nonnegativity on $\text{tr}(P^T A P + P^T D)$ for $\theta \in \{0, 1\}$, we can improve the conclusion of [68, Theorem 2.2] to (in the current notation): if $\text{tr}(\widehat{P}^T H(P) \widehat{P}) - \text{tr}(P^T H(P) P) \geq 0$, then

$$f(\tilde{P}) \geq f(P) + \frac{1}{2} \left(\frac{s_k(B)}{S_k(B)} \right)^\theta \left[\text{tr}(\widehat{P}^T H(P) \widehat{P}) - \text{tr}(P^T H(P) P) \right] + [S_k(B)]^{-\theta} \left[\|\widehat{P}^T D\|_{\text{tr}} - \text{tr}(\widehat{P}^T D P^T \widehat{P}) \right], \quad (6.11)$$

where $0 \leq \theta \leq 1$. The last term is contributed by the selection of Q as described. A proof of (6.11) can be found in [42, appendix F].

The comments in Remark 3.1(ii) on $\mathbb{P}$ apply here, too.

- v. It is tempting to stipulate $f(\widehat{P}) \geq f(P) + \omega\eta$, but that is either false or just hard to prove for the one in Example 6.1 and some of those in Table 1 that involve D . Often in our algorithms to solve (1.1) iteratively, with P being the current approximate maximizer, assuming the **NEPv Ansatz**, we naturally compute $\widehat{P}$ that maximizes $\text{tr}(X^T H(P) X)$ over $X \in \text{St}(k, n)$. With that $\widehat{P}$, settling whether $f(\widehat{P}) \geq f(P) + \omega\eta$ or not can be a hard task, as in Example 6.1 where the objective function involves $\text{tr}((P^T D)^2)$.

As to the validity of the **NEPv Ansatz** on the objective functions in Table 1, it holds for all, except SumTR, under mild conditions on the constant matrices and function ϕ . Table 4 provides the details on $H(P)$ and conditions under which the **NEPv Ansatz** holds, where the last column refers to places for justifications. We leave $\mathbb{P}$ unspecified for SumCT but refer it to [67] because it is more complicated to fit the space in the table. In fact, it is required that each P_i falls in $\{X \in \text{St}(k_i, n) : X^T D_i \geq 0\}$. In [42, sect. 8.2], it is argued that for SumCT it would be more efficient to go for the NPDo approach in Part I. For SumTR with $H(P)$ given by (6.2), $\mathbb{P} = \text{St}(k, n)$ and $Q = I_k$ and the **NEPv Ansatz** does not hold. This can be drawn from the counterexample, [77, Example 4.1], for which SCF diverges, but later we will show, under the **NEPv Ansatz**, SCF is guaranteed to converge!

Comparing Table 2 for NPDo with Table 4 for NEPv here, we find that, among those in Table 1, the **NEPv Ansatz** provably holds for three more of them, which are OLDA, OCCA, and Θ TR (all involving ratios), than the **NPDo Ansatz** does. This observation that the **NEPv Ansatz** is satisfied more often than the **NPDo Ansatz** among those in Table 1 is not an accident. In fact the **NPDo Ansatz** is stronger than the **NEPv Ansatz** with the generic $H(P)$ in (6.5), as shown by the next theorem.

Theorem 6.2 *Let function f be defined on some neighborhood $\text{St}_\delta(k, n)$ of $\text{St}(k, n)$ and let $H(P)$ be as in (6.5). Then the **NPDo Ansatz** implies the **NEPv Ansatz**.*

Proof Suppose that the **NPDo Ansatz** holds. Given $\widehat{P} \in \text{St}(k, n)$, $P \in \mathbb{P} \subseteq \text{St}(k, n)$ such that (6.7) holds, let $W \in \text{St}(k, k)$ be an orthogonal polar factor of $\widehat{P}^T \mathcal{H}(P)$, and

Table 4 The NEPv Ansatz on objective functions in Table 1

	$H(P)$	conditions	$\mathbb{P}$	by
SEP	A	none	$\text{St}(k, n)$	[20], [29, p.248]
OLDA	(6.4) with $\theta = 1, D = 0$	$B \succeq 0, s_k(B) > 0$	$\text{St}(k, n)$	(6.11)
OCCA	(6.4) with $\theta = 1/2, A = 0$	$B \succeq 0, s_k(B) > 0$	$\text{St}(k, n)_{D+}$	(6.11)
$\varnothing\text{TR}$	(6.4) for case $0 < \theta < 1$	$B \succeq, s_k(B) > 0$ $\text{tr}(P^T A P + P^T D) \geq 0$	$\text{St}(k, n)_{D+}$	(6.11)
MBSub	(6.4) for case $\theta = 1$	$B \succeq 0, s_k(B) > 0$	$\text{St}(k, n)_{D+}$	(6.11)
SumCT	(6.4) with $\theta = 0$	none	$\text{St}(k, n)_{D+}$	(6.11)
TrCP	(6.5)	$A_i \succeq 0 \forall i$	[67]	[42, sec. 8.2]
UMDS	$2 \sum_{i=1}^N \phi_i(\mathbf{x}) A_i$	convex ϕ	$\text{St}(k, n)$	Example 8.1
DFT	$4 \sum_{i=1}^N A_i P P^T A_i$	$A_i \succeq 0 \forall i$	$\text{St}(k, n)$	Example 8.2
	$2A + 2 \sum_{i=1}^n \phi_i(\mathbf{x}) \mathbf{e}_i \mathbf{e}_i^T$	convex ϕ	$\text{St}(k, n)$	Example 8.1

$\phi_i(\mathbf{x}) := \partial \phi(\mathbf{x}) / \partial x_i$ for $\mathbf{x} = [x_i]$. $\varnothing\text{TR}$ for $\theta = 0$ becomes MBSub

set $\check{P} = \widehat{P}W_1$. Then $\check{P}^T \mathcal{H}(P) = W_1^T [\widehat{P}^T \mathcal{H}(P)] \succeq 0$, and thus by Lemma B.8

$$\mathrm{tr}(\check{P}^T \mathcal{H}(P)) = \|\check{P}^T \mathcal{H}(P)\|_{\mathrm{tr}} = \|\widehat{P}^T \mathcal{H}(P)\|_{\mathrm{tr}} \geq \mathrm{tr}(\widehat{P}^T \mathcal{H}(P)). \quad (6.12)$$

Recalling (6.5), we have

$$\begin{aligned} \mathrm{tr}(\widehat{P}^T H(P) \widehat{P}) &= 2 \mathrm{tr}(\widehat{P}^T \mathcal{H}(P) P^T \widehat{P}) \\ &\leq 2 \|\widehat{P}^T \mathcal{H}(P) P^T \widehat{P}\|_{\mathrm{tr}} \quad (\text{by Lemma B.8}) \\ &\leq 2 \|\widehat{P}^T \mathcal{H}(P)\|_{\mathrm{tr}} \|P^T \widehat{P}\|_2 \\ &\leq 2 \|\widehat{P}^T \mathcal{H}(P)\|_{\mathrm{tr}} \quad (\text{since } \|P^T \widehat{P}\|_2 \leq 1) \\ &\leq 2 \mathrm{tr}(\check{P}^T \mathcal{H}(P)). \quad (\text{by (6.12)}) \end{aligned}$$

Now noticing that $\mathrm{tr}(P^T H(P) P) = 2 \mathrm{tr}(P^T \mathcal{H}(P))$, we get from inequality (6.7) that

$$\mathrm{tr}(\check{P}^T \mathcal{H}(P)) \geq \mathrm{tr}(P^T \mathcal{H}(P)) + \eta/2.$$

By the **NPDo Ansatz**, there exists $W_2 \in \mathrm{St}(k, k)$ such that $\widetilde{P} = P\check{W}_2 = \widehat{P}(W_1 W_2) \in \mathbb{P}$ and $f(\widetilde{P}) \geq f(P) + (\omega/2)\eta$, verifying the **NEPv Ansatz**. $\square$

The first immediate consequence of the **NEPv Ansatz** is the following theorem that provides a characterization of the maximizers of the associated optimization problem (1.1).

Theorem 6.3 *Let $P_* \in \mathrm{St}(k, n)$ be a maximizer of (1.1). Suppose that the **NEPv Ansatz** holds and $P_* \in \mathbb{P}$. Then NEPv (6.3) holds for $P = P_*$ and the eigenvalues of $\Omega = \Omega_* := P_*^T H(P_*) P_*$ consist of the first k largest eigenvalues of $H(P_*)$.*

Proof Consider

$$\max_{P \in \mathrm{St}(k, n)} \mathrm{tr}(P^T H(P_*) P). \quad (6.13)$$

We claim P_* is a maximizer of (6.13); otherwise there would be some $\widehat{P} \in \mathrm{St}(k, n)$ such that

$$\mathrm{tr}(\widehat{P}^T H(P_*) \widehat{P}) \geq \mathrm{tr}(P_*^T H(P_*) P_*) + \eta$$

for some $\eta > 0$. Invoking the **NEPv Ansatz**, we can find $\widetilde{P} = \widehat{P}Q \in \mathbb{P}$ such that $f(\widetilde{P}) \geq f(P_*) + \omega\eta > f(P_*)$, contradicting that P_* is a maximizer. Thus P_* is a maximizer of (6.13) whose KKT condition is $H(P_*)P = P\Omega$ which P_* will have to satisfy, i.e., $H(P_*)P_* = P_*\Omega_*$, where $\Omega_* = P_*^T H(P_*) P_*$ whose eigenvalues consists of the k largest ones of $H(P_*)$. $\square$

Algorithm 6.1 NEPvSCF: NEPv (6.3) solved by SCF

Input: Symmetric matrix-valued function $H(P)$ satisfying the **NEPv Ansatz**, $P^{(0)} \in \mathbb{P}$;

Output: an approximate maximizer of (1.1).

```

1: for  $i = 0, 1, \dots$  until convergence do
2:   compute  $H_i = H(P^{(i)}) \in \mathbb{R}^{n \times n}$ ;
3:   solve SEP  $H_i \hat{P}^{(i)} = \hat{P}^{(i)} \Omega_i$  for  $\hat{P}^{(i)} \in \text{St}(k, n)$ , an orthonormal basis matrix of the eigenspace
      associated with the first  $k$  largest eigenvalues of  $H_i$ ;
4:   calculate  $Q_i \in \text{St}(k, k)$  and let  $P^{(i+1)} = \hat{P}^{(i)} Q_i \in \mathbb{P}$ , according to the NEPv Ansatz;
5: end for
6: return the last  $P^{(i)}$ .

```

6.2 SCF Iteration and Convergence

The second immediate consequence of the **NEPv Ansatz** is the global convergence of an SCF iteration for solving optimization problem (1.1) as outlined in Algorithm 6.1.

This algorithm is similar to [78, Algorithm 2], [68, Algorithm 4.1], but the latter two have more details that are dictated by the particularity of f there. A reasonable stopping criterion at Line 1 is

$$\varepsilon_{\text{NEPv}} := \frac{\|H(P)P - P[P^T H(P)P]\|_F}{\xi} \leq \epsilon, \quad (6.14)$$

where ϵ is a given tolerance, and ξ is some normalization quantity that should be designed according to the underlying $H(P)$, but generically, $\xi = \|H(P)\|_F$, or any reasonable estimate of it, should work well.

The cost of a full eigendecomposition of H_i at Line 3 is $4n^3/3$ flops [24, p.463] which is too expensive for large or even modest n , since we have to do it at every SCF iterative step. Fortunately, we do not need the full eigendecomposition but the top k eigenvalues and their associate eigenvectors. Since k is usually small such as a few tens or smaller, a better option is some iterative methods geared for extreme eigenpairs [23, 33, 41, 54]. Furthermore, as far as always moving the objective value up is concerned, it suffices to calculate $\hat{P}^{(i)}$ just well enough such that $\text{tr}([\hat{P}^{(i)}]^T H_i \hat{P}^{(i)}) > \text{tr}([P^{(i)}]^T H_i P^{(i)})$. This observation can become very useful when the k th and $(k+1)$ st eigenvalues of H_i are very close, in which case convergence to the k th eigenvector by an iterative method is often very slow.

At Line 4 it refers to the **NEPv Ansatz** for the calculation of Q_i . Exactly how it is computed depends on the structure of f at hand. We commented on the similar issue for Algorithm 3.1 earlier. In the case of Example 6.1, Q_i is taken to be an orthogonal polar factor of $(\hat{P}^{(i)})^T D$ to make $P^{(i+1)} \in \text{St}(k, n)_{D+}$.

In Algorithm 6.1, we explicitly state that it is for $H(P)$ that satisfies the **NEPv Ansatz**, without which we cannot guarantee convergence as stated in the theorems in the rest of this section, but numerically the body of the algorithm can still be implemented. There is a level-shifting technique that can help achieve local convergence [4, 47].

Theorem 6.4 Suppose that the **NEPv Ansatz** holds, and let the sequence $\{P^{(i)}\}_{i=0}^{\infty}$ be generated by Algorithm 6.1. The following statements hold.

- The sequence $\{f(P^{(i)})\}_{i=0}^{\infty}$ is monotonically increasing and convergent.
- Any accumulation point P_* of the sequence $\{P^{(i)}\}_{i=0}^{\infty}$ satisfies the necessary conditions in Theorem 6.3 for a global maximizer, i.e., (6.3) holds for $P = P_*$ and the eigenvalues of $\Omega_* = P_*^T H(P_*) P_*$ consist of the first k largest eigenvalues of $H(P_*)$. Furthermore in the case when $H(P)$ satisfies (6.6), if $\mathcal{M}(P_*)$ is symmetric, then P_* is a KKT point.
- We have two convergent series

$$\sum_{i=1}^{\infty} \delta_i \|\sin \Theta(\mathcal{R}(P^{(i+1)}), \mathcal{R}(P^{(i)}))\|_F^2 < \infty, \quad (6.15a)$$

$$\sum_{i=1}^{\infty} \delta_i \frac{\|H(P^{(i)})P^{(i)} - P^{(i)}\Lambda_i\|_F^2}{\|H(P^{(i)})\|_F^2} < \infty, \quad (6.15b)$$

where $\delta_i = \lambda_k(H(P^{(i)})) - \lambda_{k+1}(H(P^{(i)}))$ and $\Lambda_i = [P^{(i)}]^T H(P^{(i)}) P^{(i)}$.

Proof See [42, Appendix D]. □

As a corollary of Theorem 6.4(b), we establish a sufficient condition for NEPv (6.3) to have a solution.

Corollary 6.1 *Under the NEPv Ansatz, NEPv (6.3) is solvable, i.e., there exists $P \in \text{St}(k, n)$ such that (6.3) holds and the eigenvalues of $\Omega = P^T H(P) P$ are the k largest ones of $H(P)$.*

As a corollary of Theorem 6.4(c), if $\delta_i = \lambda_k(H(P^{(i)})) - \lambda_{k+1}(H(P^{(i)}))$ is eventually bounded below away from 0 uniformly, then

$$\lim_{i \rightarrow \infty} \frac{\|H(P^{(i)})P^{(i)} - P^{(i)}\Lambda_i\|_F}{\|H(P^{(i)})\|_F} = 0,$$

namely, increasingly $H(P^{(i)})P^{(i)} \approx P^{(i)}\Lambda_i = P^{(i)}([P^{(i)}]^T H(P^{(i)}) P^{(i)})$, which means that $P^{(i)}$ becomes a more and more accurate approximate solution to NEPv (6.3), even in the absence of knowing whether the entire sequence $\{P^{(i)}\}_{i=0}^{\infty}$ converges or not. The latter does require additional condition to establish in the next theorem.

Theorem 6.5 *Suppose that the NEPv Ansatz holds, and let the sequence $\{P^{(i)}\}_{i=0}^{\infty}$ be generated by Algorithm 6.1 and P_* be an accumulation point of the sequence.*

- $\mathcal{R}(P_*)$ is an accumulation point of the sequence $\{\mathcal{R}(P^{(i)})\}_{i=0}^{\infty}$.
- Suppose that $\mathcal{R}(P_*)$ is an isolated accumulation point of $\{\mathcal{R}(P^{(i)})\}_{i=0}^{\infty}$. If

$$\lambda_k(H(P_*Q)) - \lambda_{k+1}(H(P_*Q)) > 0 \quad \text{for any } Q \in \text{St}(k, k), \quad (6.16)$$

then the entire sequence $\{\mathcal{R}(P^{(i)})\}_{i=0}^{\infty}$ converges to $\mathcal{R}(P_*)$.

c. Suppose that P_* is an isolated accumulation point of $\{P^{(i)}\}_{i=0}^\infty$. If

$$\lambda_k(H(P_*)) - \lambda_{k+1}(H(P_*)) > 0 \quad (6.17)$$

and if $f(P_*) > f(P)$ for any $P \neq P_*$ and $\mathcal{R}(P) = \mathcal{R}(P_*)$, i.e., $f(P)$ has unique maximizer in the orbit $\{P_*Q : Q \in \text{St}(k, k)\}$, then the entire sequence $\{P^{(i)}\}_{i=0}^\infty$ converges to P_* .

Proof See [42, Appendix D]. $\square$

6.3 Acceleration by LOCG

At Line 3 of Algorithm 6.1, an $n \times n$ SEP is involved and that can be expensive for large/huge n . As in subsect. 3.3, the same idea for acceleration can be applied here to speed things up. It has in fact been partially demonstrated in [67, sect. 5] on MBSUB.

With the same setup at the beginning of subsect. 3.3 up to (3.12), here we will need a symmetric matrix-valued function $\tilde{H}(Z)$ for the dimensionally reduced maximization problem (3.11) so that the NEPv Ansatz can be passed on from f with H to $\tilde{f}$ with $\tilde{H}$. It turns out that the right choice is

$$\tilde{H}(Z) = W^T H(WZ)W. \quad (6.18)$$

Built upon this $\tilde{H}(Z)$, a variant of LOCG acceleration over Algorithm 6.1 can be obtained along the line of subsect. 3.3. The reader is referred to [42, subsect. 6.3] for more detail.

7 Atomic Functions for NEPv

In this section, we introduce the notion of atomic functions for NEPv, which serves as a singleton unit of function on $\text{St}_\delta(k, n)$ for which the NEPv approach is guaranteed to work for solving (1.1), and more importantly, the NEPv approach works on any convex composition of atomic functions, provided that some of the partial derivatives of the composing convex function are nonnegative.

In what follows, we first formulate two conditions that define atomic function and prove why the NEPv approach will work on the atomic functions, and then we give concrete examples of atomic functions that encompass nearly all practical ones that are in use today, and we leave investigating how the NEPv approach will work on convex compositions of these atomic functions to sect. 8.

Combining the results in this section and the next section will yield a large collection of objective functions, including those in Table 4, for which the NEPv Ansatz holds.

7.1 Conditions on Atomic Functions

Suppose that, for function f defined on some neighborhood $\text{St}_\delta(k, n)$ of the Stiefel manifold $\text{St}(k, n)$, we have already constructed an associated symmetric matrix-valued

function $H(P) \in \mathbb{R}^{n \times n}$. We are interested in those that satisfy

$$\operatorname{tr}(P^T H(P) P) = \underline{\gamma} f(P) \quad \text{for } P \in \mathbb{P} \subseteq \operatorname{St}(k, n), \quad (7.1a)$$

and given $P \in \mathbb{P}$ and $\widehat{P} \in \operatorname{St}(k, n)$, there exists $Q \in \operatorname{St}(k, k)$ such that $\widetilde{P} = \widehat{P}Q \in \mathbb{P}$ and

$$\operatorname{tr}(\widehat{P}^T H(P) \widehat{P}) \leq \underline{\alpha} f(\widetilde{P}) + \underline{\beta} f(P), \quad (7.1b)$$

where $\underline{\alpha} > 0$, $\underline{\beta} \geq 0$, and $\underline{\gamma} = \underline{\alpha} + \underline{\beta}$ are constants. Here a subset $\mathbb{P} \subseteq \operatorname{St}(k, n)$ is also involved.

Definition 7.1 A function f defined on some neighborhood $\operatorname{St}_\delta(k, n)$ of $\operatorname{St}(k, n)$ is an *atomic function* for NEPv if there are a symmetric matrix-valued function $H(P) \in \mathbb{R}^{n \times n}$ for $P \in \operatorname{St}(k, n)$ and constants $\underline{\alpha} > 0$, $\underline{\beta} \geq 0$, and $\underline{\gamma} = \underline{\alpha} + \underline{\beta}$ such that both conditions in (7.1) hold.

An atomic function according to Definition 7.1 is of the second type in this paper and is for the NEPv approach, in contrast to the first type that is defined in subsect. 4.1 of Part I for the NPDo approach. As in subsect. 4.1, here it also can be verified that for two atomic functions f_1 and f_2 with H_1 and H_2 , respectively, that share the same $\mathbb{P}$, the same constants $\underline{\alpha}$, $\underline{\beta}$, $\underline{\gamma}$, and the same Q for (7.1b), any linear combination $f := c_1 f_1 + c_2 f_2$ with $c_1 H_1 + c_2 H_2$ for $c_1, c_2 > 0$ satisfies (7.1), and hence is an atomic function for NEPv as well.

Remark 7.1 An alternative to (7.1b) is

$$\operatorname{tr}(\widetilde{P}^T H(P) \widetilde{P}) \leq \underline{\alpha} f(\widetilde{P}) + \underline{\beta} f(P) \quad \text{for } P, \widetilde{P} \in \mathbb{P} \subseteq \operatorname{St}(k, n), \quad (7.1b')$$

without referring to an intermediate $\widehat{P}$. We claim that (7.1b') is stronger than (7.1b), assuming for any $\widehat{P} \in \operatorname{St}(k, n)$, there exists $Q \in \operatorname{St}(k, k)$ such that $\widetilde{P} = \widehat{P}Q \in \mathbb{P}$. Here is why. Suppose (7.1b') holds. Given any $\widehat{P} \in \operatorname{St}(k, n)$, let $\widetilde{P} = \widehat{P}Q \in \mathbb{P}$ for some $Q \in \operatorname{St}(k, k)$. Then by (7.1b') we have for any $P \in \mathbb{P}$

$$\operatorname{tr}(\widehat{P}^T H(P) \widehat{P}) = \operatorname{tr}(\widetilde{P}^T H(P) \widetilde{P}) \leq \underline{\alpha} f(\widetilde{P}) + \underline{\beta} f(P),$$

yielding (7.1b). In view of this observation, in our later developments, we may verify (7.1b') directly if it can be verified.

In relating $\mathcal{H}(P)$ to $H(P)$ via, e.g., (6.6) when (6.1) does not hold, $H(P)$ in general is not unique [47]. As a result, satisfying (7.1) may depend on both f and the choice of $H(P)$. In other words, it is possible that the conditions in (7.1) are satisfied for one choice of $H(P)$ but may not for another.

Remark 7.2 Previously, (4.1a) appears explicitly as a partial differential equation (PDE), but (7.1a) here does not. Nonetheless, it is likely a PDE in disguise, especially when $H(P)P$ is related to $\mathcal{H}(P) := \partial f(P)/\partial P$ through condition (6.6).

The next theorem basically says that the conditions in (4.1) that define the atomic function for NPDo are stronger than the ones in (7.1) for NEPv with the generic $H(P)$ given by (6.5).

Theorem 7.1 *Let $H(P)$ be as in (6.5).*

- a. *Equation (4.1a) implies (7.1a) with $\underline{\gamma} = 2\gamma$.*
- b. *Inequality (4.1b) implies (7.1b) with $\underline{\alpha} = 2\alpha$, $\underline{\beta} = 2\beta$, and $\underline{\gamma} = \underline{\alpha} + \underline{\beta} = 2\gamma$.*

Proof Assuming (4.1a), for $H(P)$ as given in (6.5), we have for $P \in \mathbb{P} \subseteq \text{St}(k, n)$

$$\text{tr}(P^T H(P) P) = 2 \text{tr} \left(P^T \mathcal{H}(P) \right) = 2\gamma f(P),$$

as was to be shown. Assume (4.1b). Let $\widehat{P} \in \text{St}(k, n)$, $P \in \mathbb{P}$ and let $W_1 \in \text{St}(k, k)$ be an orthogonal polar factor of $\widehat{P}^T \mathcal{H}(P)$ and $\check{P} = \widehat{P} W_1$. Then we again have (6.12) and

$$\begin{aligned} \text{tr}(\widehat{P}^T H(P) \widehat{P}) &= 2 \text{tr} \left(\widehat{P}^T \mathcal{H}(P) P^T \widehat{P} \right) \\ &\leq 2 \left\| \widehat{P}^T \mathcal{H}(P) P^T \widehat{P} \right\|_{\text{tr}} \quad (\text{by Lemma B.8}) \\ &\leq 2 \left\| \widehat{P}^T \mathcal{H}(P) \right\|_{\text{tr}} \|P^T \widehat{P}\|_2 \\ &\leq 2 \left\| \widehat{P}^T \mathcal{H}(P) \right\|_{\text{tr}} \quad (\text{since } \|P^T \widehat{P}\|_2 \leq 1) \\ &= 2 \text{tr} \left(\check{P}^T \mathcal{H}(P) \right) \quad (\text{by (6.12)}). \end{aligned} \quad (7.2)$$

Now use (4.1b) to conclude that there is $W_2 \in \text{St}(k, k)$ such that $\widetilde{P} = P \check{W}_2 = \widehat{P}(W_1 W_2) \in \mathbb{P}$ and

$$2 \text{tr} \left(\check{P}^T \mathcal{H}(P) \right) \leq 2\alpha f(\widetilde{P}) + 2\beta f(P). \quad (7.3)$$

Combine (7.2) and (7.3) to get (7.1b) with $\underline{\alpha} = 2\alpha$, $\underline{\beta} = 2\beta$, and $\underline{\gamma} = \underline{\alpha} + \underline{\beta} = 2\gamma$. $\square$

Theorem 7.2 *Given function f defined on $\text{St}_\delta(k, n)$ and its associated symmetric $H(P)$ that satisfy (7.1), suppose $f(P) \geq 0$ for $P \in \mathbb{P}$. Let $g(P) = c[f(P)]^s$ where $c > 0$, $s > 1$, and let its associated symmetric matrix-valued function be $H_g(P) = cs[f(P)]^{s-1} H(P)$. Then*

$$\text{tr}(P^T H_g(P) P) = s\gamma g(P) \quad \text{for } P \in \mathbb{P} \subseteq \text{St}(k, n), \quad (7.4a)$$

and given $P \in \mathbb{P}$ and $\widehat{P} \in \text{St}(k, n)$, there exists $Q \in \text{St}(k, k)$ such that $\widetilde{P} = \widehat{P} Q \in \mathbb{P}$ and

$$\text{tr}(\widehat{P}^T H_g(P) \widehat{P}) \leq \underline{\alpha} g(\widetilde{P}) + (s\gamma - \underline{\alpha}) g(P), \quad (7.4b)$$

where $\underline{\alpha}$, $\underline{\beta}$ and $\underline{\gamma} = \underline{\alpha} + \underline{\beta}$ are as in (7.1b).

Proof We have

$$\begin{aligned}
 \operatorname{tr}(P^T H_g(P) P) &= c s [f(P)]^{s-1} \operatorname{tr}(P^T H(P) P) \\
 &= c s [f(P)]^{s-1} \underline{\gamma} f(P) \quad (\text{by (7.1a)}) \\
 &= s \underline{\gamma} g(P), \\
 \operatorname{tr}(\widehat{P}^T H_g(P) \widehat{P}) &= c s [f(P)]^{s-1} \operatorname{tr}(\widehat{P}^T H(P) \widehat{P}) \\
 &\leq c s [f(P)]^{s-1} \left[\underline{\alpha} f(\widetilde{P}) + \underline{\beta} [f(P)] \right] \quad (\text{by (7.1b)}) \\
 &= c s \underline{\alpha} f(\widetilde{P}) [f(P)]^{s-1} + \underline{\beta} s c [f(P)]^s \\
 &\leq c s \underline{\alpha} \left\{ \frac{1}{s} [f(\widetilde{P})]^s + \frac{s-1}{s} [f(P)]^s \right\} + \underline{\beta} s g(P) \quad (\text{by Lemma B.2}) \\
 &= \underline{\alpha} g(\widetilde{P}) + \underline{\alpha} (s-1) g(P) + \underline{\beta} s g(P) \\
 &= \underline{\alpha} g(\widetilde{P}) + [\underline{\alpha} (s-1) + \underline{\beta} s] g(P),
 \end{aligned}$$

as expected. $\square$

Finally, we show that **the NEPv Ansatz** holds for atomic functions for NEPv. As a corollary, the NEPv approach as laid out in sect. 6 works on any atomic function for NEPv.

Theorem 7.3 *The NEPv Ansatz holds with $\omega = 1/\underline{\alpha}$ for atomic function f with a symmetric matrix-valued function $H(P) \in \mathbb{R}^{n \times n}$ satisfying the conditions in (7.1).*

Proof Given $P \in \mathbb{P} \subseteq \operatorname{St}(k, n)$ and $\widehat{P} \in \operatorname{St}(k, n)$, suppose that (6.7) holds, i.e., $\operatorname{tr}(\widehat{P}^T H(P) \widehat{P}) \geq \operatorname{tr}(P^T H(P) P) + \eta$. We have by (7.1)

$$\eta + \underline{\gamma} f(P) = \eta + \operatorname{tr}(P^T H(P) P) \leq \operatorname{tr}(\widehat{P}^T H(P) \widehat{P}) \leq \underline{\alpha} f(\widetilde{P}) + \underline{\beta} f(P)$$

yielding $\eta/\underline{\alpha} + f(P) \leq f(\widetilde{P})$, as was to be shown. $\square$

7.2 Concrete Atomic Functions

We will show that

$$\boxed{\operatorname{tr}((P^T D)^m)^s, \operatorname{tr}((P^T A P)^m)^s \text{ for integer } m \geq 1, s \geq 1, \text{ and also } A \succeq 0 \text{ in the case of } m \geq 2 \text{ or } s > 1,} \quad (7.5)$$

with proper symmetric $H(P)$ to be given in the theorems and corollaries below, satisfy (7.1) and hence are atomic functions for NEPv. Therefore, by Theorem 7.3, **the NEPv Ansatz** holds for them. These atomic functions are the same in form as the ones in subject. 4.2 but there are differences as detailed in Table 5. When inequality (4.1b) or (7.1b) become an equality, there is an important implication when it comes to verify the corresponding ansatz for the composition of atomic functions by a convex function ϕ , namely, for equality (4.1b) or (7.1b), the corresponding partial derivative

$\phi_j(\mathbf{x}) := \partial\phi(\mathbf{x})/\partial x_j$ can be of any sign but in general is required to be nonnegative otherwise. We have seen this in Theorem 5.1 and will see it again in Theorem 8.1 later.

Theorem 7.4 *Let $D \in \mathbb{R}^{n \times k}$, integer $m \geq 1$ and $f(P) = \text{tr}((P^T D)^m)$ for which we use*

$$H(P) = m \left[D(P^T D)^{m-1} P^T + P(D^T P)^{m-1} D^T \right], \quad (7.6)$$

and thus $H(P)P - \mathcal{H}(P) \equiv P[m(D^T P)^m]$ for $P \in \text{St}(k, n)$. Then we have

$$\text{tr}(P^T H(P)P) = 2m \text{tr}((P^T D)^m) \quad \text{for } P \in \text{St}(k, n); \quad (7.7a)$$

$$\text{tr}(\tilde{P}^T H(P)\tilde{P}) \leq 2 \text{tr}((\tilde{P}^T D)^m) + 2(m-1) \text{tr}((P^T D)^m) \quad \text{for } P, \tilde{P} \in \mathbb{P}, \quad (7.7b)$$

where $\mathbb{P} = \text{St}(k, n)_{D+}$. They, as argued in Remark 7.1, imply that (7.1) holds with $\alpha = 2$ and $\beta = 2(m-1)$, and thus $f(P) = \text{tr}((P^T D)^m)$ is an atomic function for NEPv. Furthermore, any solution P to NEPv (6.3) with $H(P)$ in (7.6) such that $(P^T D)^m$ is symmetric is a solution to the KKT condition (2.3) and vice versa.

Proof $H(P)$ in the theorem is in fact the generic one in (6.5) for the case and in the notation of Theorem 6.1, $\mathcal{M}(P) = m(P^T D)^m$. Hence any solution P to NEPv (6.3) such that $(P^T D)^m$ is symmetric is a solution to the KKT condition (2.3) and vice versa.

Equation (7.7a) can be straightforwardly verified. Now we prove (7.7b). Inequality (7.7b) for $m = 1$ in fact holds for all $P \in \text{St}(k, n)$. To see this, for $m = 1$ and $P \in \text{St}(k, n)$, since $\tilde{P}^T D \geq 0$,

$$\text{tr}(\tilde{P}^T H(P)\tilde{P}) = 2 \text{tr}(\tilde{P}^T D P^T \tilde{P}) \leq 2 \|\tilde{P}^T D P^T \tilde{P}\|_{\text{tr}} \leq 2 \|\tilde{P}^T D\|_{\text{tr}} = 2 \text{tr}(\tilde{P}^T D)$$

by Lemma B.8, as expected. In general for $m > 1$, suppose both $P^T D \geq 0$ and $\tilde{P}^T D \geq 0$. Then

$$\begin{aligned} \text{tr}(\tilde{P}^T H(P)\tilde{P}) &= 2m \text{tr}(\tilde{P}^T D (P^T D)^{m-1} P^T \tilde{P}) \\ &\leq 2m \left\| \tilde{P}^T D (P^T D)^{m-1} P^T \tilde{P} \right\|_{\text{tr}} \quad (\text{by Lemma B.8}) \\ &\leq 2m \left\| \tilde{P}^T D (P^T D)^{m-1} \right\|_{\text{tr}} \|P^T \tilde{P}\|_2 \\ &\leq 2m \left\| \tilde{P}^T D (P^T D)^{m-1} \right\|_{\text{tr}} \quad (\text{since } \|P^T \tilde{P}\|_2 \leq 1) \\ &\leq 2 \text{tr}((\tilde{P}^T D)^m) + 2(m-1) \text{tr}((P^T D)^m), \end{aligned}$$

where the last inequality is due to Lemma B.5.

Finally (7.7) implies (7.1), as argued in Remark 7.1. $\square$

For any $s > 1$, $[\text{tr}((P^T D)^m)]^s$ is well-defined for any $P \in \mathbb{R}^{n \times k}$ such that $\text{tr}((P^T D)^m) \geq 0$. In particular, $[\text{tr}((P^T D)^m)]^s$ is well-defined for $P \in \text{St}(k, n)_{D+}$. Combining Theorems 7.2 and 7.4, we obtain the following corollary.

Table 5 Concrete atomic functions for NPDo and NEPv

$[\text{tr}((P^T D)^m)]^s$		$[\text{tr}((P^T A P)^m)]^s$
NPDo	$m = s = 1$ (4.1b) an equality, $\mathbb{P} = \text{St}(k, n)_{D+}$, or $\mathbb{P} = \text{St}(k, n)$ (4.1b) an inequality, $\mathbb{P} = \text{St}(k, n)_{D+}$	$m \geq 2$ or $s > 1$ $A \succeq 0$, (4.1b) an inequality, $\mathbb{P} = \text{St}(k, n)$.
NEPv	(7.1b) an inequality, $\mathbb{P} = \text{St}(k, n)_{D+}$.	$m = s = 1$ (7.1b) an equality, $\mathbb{P} = \text{St}(k, n)$ (7.1b) an inequality, $A \succeq 0$, $\mathbb{P} = \text{St}(k, n)$

Integer $m \geq 1$, scalar $s \geq 1$ and A is symmetric

Corollary 7.1 Let $D \in \mathbb{R}^{n \times k}$, integer $m \geq 1$, $s > 1$, $g(P) = [\text{tr}((P^T D)^m)]^s$, and $\mathbb{P} = \text{St}(k, n)_{D+}$. Let $H(P)$ be as in (7.6) and $H_g(P) = s [\text{tr}((P^T D)^m)]^{s-1} H(P)$ for which $H_g(P)P - \partial g(P)/\partial P \equiv P[sm [\text{tr}((P^T D)^m)]^{s-1} (D^T P)^m]$. Then

$$\text{tr}(P^T H_g(P)P) = 2sm [\text{tr}((P^T D)^m)]^s \quad \text{for } P \in \mathbb{P}, \quad (7.8a)$$

$$\text{tr}(\tilde{P}^T H_g(P)\tilde{P}) \leq 2[\text{tr}((\tilde{P}^T D)^m)]^s + 2(sm - 1)[\text{tr}((P^T D)^m)]^s \quad \text{for } P, \tilde{P} \in \mathbb{P}. \quad (7.8b)$$

They, as argued in Remark 7.1, imply that (7.1) holds with $\alpha = 2$ and $\beta = 2(sm - 1)$, and thus $g(P) = [\text{tr}((P^T D)^m)]^s$ for $s > 1$ is an atomic function for NEPv.

Next we consider $\text{tr}((P^T A P)^m)$ and its power.

Theorem 7.5 Let symmetric $A \in \mathbb{R}^{n \times n}$, integer $m \geq 1$, and $f(P) = \text{tr}((P^T A P)^m)$ for which we use

$$H(P) := 2m A(P P^T A)^{m-1} \quad (7.9)$$

and thus $\mathcal{H}(P) \equiv H(P)P$ for $P \in \mathbb{R}^{n \times k}$.

a. For $P \in \mathbb{R}^{n \times k}$, we have

$$\text{tr}(P^T H(P)P) = 2m f(P) \equiv 2m \text{tr}((P^T A P)^m). \quad (7.10a)$$

b. Let $P, \tilde{P} \in \mathbb{R}^{n \times k}$.

i. For $m = 1$, we always have

$$\text{tr}(\tilde{P}^T H(P)\tilde{P}) = 2\text{tr}(\tilde{P}^T A \tilde{P}); \quad (7.10b)$$

ii. For $m > 1$, if $A \succeq 0$, then

$$\text{tr}(\tilde{P}^T H(P)\tilde{P}) \leq 2\text{tr}((\tilde{P}^T A \tilde{P})^m) + 2(m - 1) \text{tr}((P^T A P)^m). \quad (7.10c)$$

They, as argued in Remark 7.1, imply that (7.1) holds with $\alpha = 2$ and $\beta = 2(m - 1)$, and $\mathbb{P} = \text{St}(k, n)$, and thus $f(P) = \text{tr}((P^T A P)^m)$ is an atomic function for NEPv.

Proof With $H(P)$ as in (7.9), equation (7.10a) is straightforwardly verified.

For $m = 1$, $H(P) = 2A$ and hence immediately we have (7.10b).

Consider $m > 1$ and suppose $A \succeq 0$. Let $X = A^{1/2} \tilde{P}$ and $Y = A^{1/2} P$, where $A^{1/2}$ is the positive semidefinite square root of A . We have

$$\begin{aligned} \tilde{P}^T H(P)\tilde{P} &= 2m \tilde{P}^T A P (P^T A P)^{m-2} P^T A \tilde{P} \\ &= 2m X^T Y (Y^T Y)^{m-2} Y^T X \\ &= 2m X^T (Y Y^T)^{m-1} X, \\ \text{tr}(\tilde{P}^T H(P)\tilde{P}) &= 2m \text{tr}(X^T (Y Y^T)^{m-1} X) \end{aligned}$$

$$\begin{aligned}
 &= 2m \operatorname{tr}(XX^T(YY^T)^{m-1}) \\
 &\leq 2 \operatorname{tr}((XX^T)^m) + 2(m-1) \operatorname{tr}((YY^T)^m) \quad (\text{by Lemma B.5}) \\
 &= 2 \operatorname{tr}((X^T X)^m) + 2(m-1) \operatorname{tr}((Y^T Y)^m) \\
 &= 2 \operatorname{tr}((\tilde{P}^T A \tilde{P})^m) + 2(m-1) \operatorname{tr}((P^T A P)^m),
 \end{aligned}$$

which is (7.10c). $\square$

We emphasize that (7.10a), (7.10b), and (7.10c) actually holds for any $P, \tilde{P} \in \mathbb{R}^{n \times k}$, broader than what the conditions in (7.1) entail. With Theorem 7.5 and using a similar proof to that of Theorem 7.2, we get the following corollary that is valid for all $P, \tilde{P} \in \mathbb{R}^{n \times k}$, broader than simply combining Theorems 7.2 with 7.5.

Corollary 7.2 *Let symmetric $A \in \mathbb{R}^{n \times n}$ be positive semidefinite, integer $m \geq 1, s > 1$, $g(P) = [\operatorname{tr}((P^T A P)^m)]^s$, and let $H_g(P) = s [\operatorname{tr}((P^T A P)^m)]^{s-1} H(P)$ for which $\partial g(P)/\partial P \equiv H_g(P)P$ for $P \in \mathbb{R}^{n \times k}$, where $H(P)$ is as in (7.9). For $P, \tilde{P} \in \mathbb{R}^{n \times k}$, we have*

$$\operatorname{tr}(P^T H_g(P) P) = 2sm [\operatorname{tr}((P^T A P)^m)]^s, \quad (7.11a)$$

$$\operatorname{tr}(\tilde{P}^T H_g(P) \tilde{P}) \leq 2[\operatorname{tr}((\tilde{P}^T A \tilde{P})^m)]^s + 2(sm-1)[\operatorname{tr}((P^T A P)^m)]^s. \quad (7.11b)$$

They, as argued in Remark 7.1, imply that (7.1) holds with $\alpha = 2$ and $\beta = 2(sm-1)$, and $\mathbb{P} = \operatorname{St}(k, n)$, and thus $g(P) = [\operatorname{tr}((P^T A P)^m)]^s$ for $s > 1$ is an atomic function for NEPv.

8 Convex Composition

We are interested in solving the same optimization problem on the Stiefel manifold $\operatorname{St}(k, n)$ as in (5.1) by Algorithm 6.1 and its accelerating variation [42, Algorithm 6.2] with convergence guarantee. In that regard, we stick to the initial setup at the beginning of sect. 5 up to the paragraph containing (5.3). We then go along a different path – the path of the NEPv approach. To that end, we will have to specify what $H(P)$, a symmetric matrix-valued function, to use for a given objective function $f = \phi \circ T$ in (5.1), assuming that a symmetric matrix-valued function has already been constructed for each component of $T(P)$.

In its generality, each component $f_i(P_i)$ of $T(P)$ in (5.3) may involve a few but not necessarily all columns of P . It turns out that, for the case when not all $P_i = P$, we do not have a feasible way to construct a symmetric matrix-valued function $H(P)$ for $f(P) = \phi \circ T(P)$ out of those for the components of $T(P)$. That leaves us the only option of using the generic $H(P)$ in (6.5):

$$H(P) := [\mathcal{H}(P)]P^T + P[\mathcal{H}(P)]^T \equiv \left[\frac{\partial f(P)}{\partial P} \right] P^T + P \left[\frac{\partial f(P)}{\partial P} \right]^T,$$

completely ignoring the symmetric matrix-valued functions for the components of $T(P)$ already known. Furthermore, with this generic $H(P)$, in order to fulfill the

NEPv Ansatz, we will have to assume the components of $T(P)$ are atomic functions for NPDo satisfying (5.5), which means that **the NPDo Ansatz** will hold for f . Consequently, our previous NPDo approach in Part I will work on such function f in the first place, making it unnecessary resort to the NEPv approach for solving the optimization problem (5.1). More detail can be found in [42, sect. 8.2]. Besides explaining the extra complexity that not all $P_i = P$ may bring, in [42, sect. 8.2] it is also demonstrated that the NEPv approach can still be made to work with the generic $H(P)$, just that the approach may not be as effective as the NPDo approach in Part I.

Our primary focus is on the case when all $P_i = P$, i.e., each component $f_i(P_i) = f_i(P)$. Specifically, we will consider a special case of $T(P)$ in (5.3):

$$T_0(P) = \begin{bmatrix} f_1(P) \\ f_2(P) \\ \vdots \\ f_N(P) \end{bmatrix}, \quad (8.1)$$

where f_i for $1 \leq i \leq N$ are atomic functions for NEPv, whose associated symmetric matrix-valued functions are $H_i(P) \in \mathbb{R}^{n \times n}$ for $1 \leq i \leq N$, respectively.

Our first task is to create a proper symmetric matrix-valued function $H(P) \in \mathbb{R}^{n \times n}$ to go with $f = \phi \circ T_0$ from $H_i(P)$ for $1 \leq i \leq N$. As we commented in Remark 6.1(i), **the NEPv Ansatz** does not impose any explicit relation between $\mathcal{H}(P)$ and $H(P)P$, e.g., through condition (6.6), but in order to figure out what $H(P)$ should be for the circumstance, let us assume (6.6) holds for each f_i with H_i , namely,

$$H_i(P)P - \frac{\partial f_i(P)}{\partial P} = P \mathcal{M}_i(P) \quad \text{for } 1 \leq i \leq N, \quad (8.2)$$

and then show that the newly created $H(P)$ can serve the purpose for us as far as inheriting **the NEPv Ansatz** from f_i with H_i for $1 \leq i \leq N$ is concerned, without the need to assume (8.2) anymore. Recall notation $\phi_i(\mathbf{x})$ in (5.2) for the i th partial derivative of $\phi(\mathbf{x})$. For $f = \phi \circ T_0$, we have

$$\mathcal{H}(P) := \frac{\partial f(P)}{\partial P} = \sum_{i=1}^N \phi_i(T_0(P)) \frac{\partial f_i(P)}{\partial P},$$

and hence naturally, we may choose

$$H(P) = \sum_{i=1}^N \phi_i(T_0(P)) H_i(P), \quad (8.3)$$

for which, with (8.2), we find

$$H(P)P - \frac{\partial f(P)}{\partial P} = \sum_{i=1}^N \phi_i(T_0(P)) \left(H_i(P)P - \frac{\partial f_i(P)}{\partial P} \right)$$

$$\begin{aligned}
 &= P \sum_{i=1}^N \phi_i(T_0(P)) \mathcal{M}_i(P) \\
 &=: P \mathcal{M}(P).
 \end{aligned} \tag{8.4}$$

Therefore the symmetric $H(P) \in \mathbb{R}^{n \times n}$ in (8.3) fits the one suggested by Theorem 6.1. In particular, any solution P_* to NEPv (6.3) with $H(P)$ given by (8.3) satisfies the KKT condition (2.3) if $\mathcal{M}(P_*)$ defined in (8.4) is symmetric and vice versa, as guaranteed by Theorem 6.1.

Next we will show that $f = \phi \circ T_0$ with $H(P)$ in (8.3) inherits **the NEPv Ansatz** from f_i with H_i for $1 \leq i \leq N$ without assuming (8.2). To that end, we place some consistency conditions upon all components of $T_0(P)$ in (8.1) as follows: for $1 \leq i \leq N$

$$\text{tr}(P^T H_i(P) P) = \gamma_i f_i(P) \quad \text{for } P \in \mathbb{P} \subseteq \text{St}(k, n), \tag{8.5a}$$

and given $\hat{P} \in \text{St}(k, n)$ and $P \in \mathbb{P}$, there exists $Q \in \text{St}(k, k)$ such that $\tilde{P} = \hat{P} Q \in \mathbb{P}$ and

$$\text{tr}(\hat{P}^T H_i(P) \hat{P}) \leq \alpha f_i(\tilde{P}) + \beta_i f_i(P), \tag{8.5b}$$

where $\alpha > 0$, $\beta_i \geq 0$, and $\gamma_i = \alpha + \beta_i$ are constants. It is important to keep in mind that some of the inequalities in (8.5b) may actually be equalities, e.g., for $f_i(P) = \text{tr}(P^T A_i P)$ it is an equality by Theorem 4.3.

On the surface, it looks like that each f_i is simply an atomic function for NEPv, but there are three built-in consistency requirements in (8.5) among all f_i : 1) the same $\mathbb{P}$ for all; 2) the same α for all, and 3) the same Q to give $\tilde{P} = \hat{P} Q$ for all.

Theorem 8.1 Consider $f = \phi \circ T_0$, where $T_0(\cdot)$ takes the form in (8.1) and ϕ is convex and differentiable with partial derivatives denoted by ϕ_i as in (5.2). Let $H(P)$ be given by (8.3) with $H_i(P)$ for $1 \leq i \leq N$ satisfying (8.5). If $\phi_i(\mathbf{x}) \geq 0$ for those i for which (8.5b) does not become an equality, then **the NEPv Ansatz** with $\omega = 1/\alpha$ holds for $f = \phi \circ T_0$ with H .

Proof Given $P \in \mathbb{P} \subseteq \text{St}(k, n)$ and $\hat{P} \in \text{St}(k, n)$, suppose that (6.7) holds, i.e., $\text{tr}(\hat{P}^T H(P) \hat{P}) \geq \text{tr}(P^T H(P) P) + \eta$. Write

$$\mathbf{x} = T_0(P) \equiv [x_1, x_2, \dots, x_N]^T, \quad \tilde{\mathbf{x}} = T_0(\tilde{P}) \equiv [\tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_N]^T,$$

i.e., $x_i = f_i(P)$ and $\tilde{x}_i = f_i(\tilde{P})$. Noticing $H(P)$ in (8.3), we have by (8.5)

$$\begin{aligned}
 \text{tr}(P^T H(P) P) &= \sum_{i=1}^N \phi_i(\mathbf{x}) \text{tr}(P^T H_i(P) P) \\
 &= \sum_{i=1}^N \gamma_i \phi_i(\mathbf{x}) x_i, \quad (\text{by (8.5a)})
 \end{aligned}$$

$$\begin{aligned} \operatorname{tr}(\widehat{P}^T H(P) \widehat{P}) &= \sum_{i=1}^N \phi_i(\mathbf{x}) \operatorname{tr}(\widehat{P}^T H_i(P) \widehat{P}) \\ &\leq \sum_{i=1}^N \phi_i(\mathbf{x}) (\underline{\alpha} \widetilde{x}_i + \underline{\beta}_i x_i), \end{aligned}$$

where the last inequality is due to $\phi_i \geq 0$ when the corresponding (8.5b) does not become an equality. Plug them into $\eta + \operatorname{tr}(P^T H(P) P) \leq \operatorname{tr}(\widehat{P}^T H(P) \widehat{P})$ and simplify the resulting inequality with the help of $\underline{\gamma}_i = \underline{\alpha} + \underline{\beta}_i$ to get

$$\eta/\underline{\alpha} + \nabla \phi(\mathbf{x})^T \mathbf{x} = \eta/\underline{\alpha} + \sum_{i=1}^N \phi_i(\mathbf{x}) x_i \leq \sum_{i=1}^N \phi_i(\mathbf{x}) \widetilde{x}_i = \nabla \phi(\mathbf{x})^T \widetilde{\mathbf{x}}.$$

Finally apply Lemma B.3 to yield $f(\widetilde{P}) \geq f(P) + \eta/\underline{\alpha}$. $\square$

With Theorem 8.1 come the general results established in sect. 6. In particular, Algorithm 6.1 (NEPvSCF) and its accelerating variation [42, Algorithm 6.2] can be applied to find a maximizer of (5.1), except that the calculation of Q_i at Line 4 of Algorithm 6.1 remains to be specified. This missing detail is in general dependent of the particularity of the mapping T_0 and the convex function ϕ . What we will do in Examples 8.1 and 8.3 below provides some ideas on this matter.

In the rest of this section, $A_i \in \mathbb{R}^{n \times n}$ for $1 \leq i \leq \ell$ are at least symmetric and $D_i \in \mathbb{R}^{n \times k}$ for $1 \leq i \leq t$.

Example 8.1 Consider T_{1a} in (5.13), as a special case of T_0 , and optimization problem (5.1) with $f = \phi \circ T_{1a}$. For this example, we will use

$$H(P) = \sum_{i=1}^{\ell} \phi_i(T_{1a}(P)) \underbrace{2A_i}_{=: H_i(P)} + \sum_{j=1}^t \phi_{\ell+j}(T_{1a}(P)) \underbrace{(D_j P^T + P D_j^T)}_{=: H_{\ell+j}(P)}, \quad (8.6)$$

for which $H(P)P - \mathcal{H}(P) \equiv P[\mathcal{D}(P)^T P]$ for $P \in \operatorname{St}(k, n)$, where, as in (5.14),

$$\mathcal{D}(P) = \sum_{j=1}^t \phi_{\ell+j}(T_{1a}(P)) D_j.$$

Any solution P to NEPv (6.3) with $H(P)$ in (8.6) such that $[\mathcal{D}(P)]^T P$ is symmetric is a solution to the KKT condition (2.3) and vice versa. It can be seen that (8.5b) is an equality for $1 \leq i \leq \ell$ and hence it does not need to require $\phi_i \geq 0$ for $1 \leq i \leq \ell$. In addition to this, instead of treating each $H_{\ell+j}(P)$ separately, we can treat $H_{\ell+j}(P)$ for $1 \leq j \leq t$ collectively all at once through $\mathcal{D}(P)$, as we did in (5.2), making all $\phi_{\ell+j} \geq 0$ unnecessary as well. A much more improved version of Theorem 8.1 is stated as Theorem 8.2 below, according to which, the best Q_i at Line 4 of Algorithm 6.1 when applied to $\phi \circ T_{1a}$ is an orthogonal polar factor of $[\widehat{P}^{(i)}]^T \mathcal{D}(P^{(i)})$. A special

case of T_{1a} is: $t = 0, k = 1, P_i = \mathbf{p}$ (a unit vector) for $1 \leq i \leq \ell$, which gives the main problem of [5] (in the paper, $\phi(\mathbf{x}) = \sum_{i=1}^{\ell} \psi_i(x_i)$ for $\mathbf{x} = [x_1, x_2, \dots, x_{\ell}]^T$ with each ψ_i being a convex function of a single-variable).

Theorem 8.2 Consider $f = \phi \circ T_{1a}$, and let $\mathcal{D}(P)$ be as in (5.14) and $H(P)$ as in (8.6). Given $\hat{P} \in \text{St}(k, n)$, $P \in \text{St}(k, n)$, let $\tilde{P} = \hat{P}Q$ where Q is an orthogonal polar factor of $\hat{P}^T \mathcal{D}(P)$. If

$$\text{tr}(\hat{P}^T H(P) \hat{P}) \geq \text{tr}(P^T H(P) P) + \eta,$$

then $f(\tilde{P}) \geq f(P) + \frac{1}{2}\eta + \delta$, where $\delta = \|\hat{P}^T \mathcal{D}(P)\|_{\text{tr}} - \text{tr}(\hat{P}^T \mathcal{D}(P) P^T \hat{P})$. In particular, the NEPv Ansatz holds with $\omega = 1/2$.

Proof Along the lines of the proof of Theorem 8.1, here we will have

$$\begin{aligned} \text{tr}(P^T H(P) P) &= 2 \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) x_i + 2 \sum_{i=1}^t \phi_{\ell+i}(\mathbf{x}) x_{\ell+i}, \\ \|\hat{P}^T \mathcal{D}(P)\|_{\text{tr}} &= \text{tr}(\tilde{P}^T \mathcal{D}(P)) \quad (\text{since } \tilde{P}^T \mathcal{D}(P) = Q^T [\hat{P}^T \mathcal{D}(P)] \succeq 0) \\ &= \sum_{i=1}^t \phi_{\ell+i}(\mathbf{x}) \tilde{x}_{\ell+i}, \\ \text{tr}(\hat{P}^T H(P) \hat{P}) &= 2 \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) \text{tr}(\hat{P}^T A_i \hat{P}) + 2 \sum_{i=1}^t \phi_{\ell+i}(\mathbf{x}) \text{tr}(\hat{P}^T D_i P^T \hat{P}) \\ &= 2 \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) \text{tr}(\tilde{P}^T A_i \tilde{P}) + 2 \text{tr}(\hat{P}^T \mathcal{D}(P) P^T \hat{P}) \\ &= 2 \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) \tilde{x}_i + 2 \|\hat{P}^T \mathcal{D}(P)\|_{\text{tr}} - 2\delta \\ &= 2 \sum_{i=1}^{\ell} \phi_i(\mathbf{x}) \tilde{x}_i + 2 \sum_{i=1}^t \phi_{\ell+i}(\mathbf{x}) \tilde{x}_{\ell+i} - 2\delta, \end{aligned} \quad (8.7)$$

where the last equality is due to (8.7). Plug them into $\eta + \text{tr}(P^T H(P) P) \leq \text{tr}(\hat{P}^T H(P) \hat{P})$ and simplify the resulting inequality to get $\frac{1}{2}\eta + \delta + \nabla \phi(\mathbf{x})^T \mathbf{x} \leq \nabla \phi(\mathbf{x})^T \tilde{\mathbf{x}}$, and then apply Lemma B.3 to conclude the proof. $\square$

Theorem 8.2 improves Theorem 8.1 in that the objective value increases additional δ more. We notice, by Lemma B.8, that

$$\text{tr}(\hat{P}^T \mathcal{D}(P) P^T \hat{P}) \leq \|\hat{P}^T \mathcal{D}(P) P^T \hat{P}\|_{\text{tr}} \leq \|\hat{P}^T \mathcal{D}(P)\|_{\text{tr}} \|P^T \hat{P}\|_2 \leq \|\hat{P}^T \mathcal{D}(P)\|_{\text{tr}}$$

and hence $\delta \geq 0$ and it is strict when any one of the inequalities above is strict. Theorem 8.2 compares favorably against Theorem 5.2. Both are about mapping T_{1a} ,

but Theorem 8.2 puts no condition on symmetric matrices A_i and no condition on the partial derivatives, whereas Theorem 5.2 requires all $A_i \geq 0$ and $\phi_i \geq 0$ for $1 \leq i \leq \ell$.

Also note that, in Theorem 8.2, $\tilde{P}$ satisfies $\tilde{P}^T \mathcal{D}(P) \geq 0$. Along the same line of the proof of Theorem 6.3, we establish another necessary condition in Corollary 8.1 for any maximizer P_* of (5.1) with $T = T_{1a}$, besides the ones in Theorem 6.3.

Corollary 8.1 *Consider (5.1) with $T = T_{1a}$ and let $H(P)$ be as in (8.6). If P_* is a maximizer of (5.1), then we have not only NEPv (6.3) satisfied by $P = P_*$ and $\Omega = \Omega_* := P_*^T H(P_*) P_*$ whose eigenvalues consist of the k largest ones of $H(P_*)$, but also $P_*^T \mathcal{D}(P_*) \geq 0$.*

Example 8.2 Consider T_{2a} , a special case of T_2 in (5.10),

$$T_{2a} : P \in \text{St}(k, n) \rightarrow T_{2a}(P) := \begin{bmatrix} \|P^T A_1 P\|_F^2 \\ \vdots \\ \|P^T A_\ell P\|_F^2 \\ \|P^T D_1\|_F^2 \\ \vdots \\ \|P^T D_t\|_F^2 \end{bmatrix} \in \mathbb{R}^{\ell+t}. \quad (8.8)$$

Either $\ell = 0$ or $t = 0$ is allowed. Notice that

$$\|P^T A_i P\|_F^2 = \text{tr}((P^T A_i P)^2), \quad \|P^T D_j\|_F^2 = \text{tr}(P^T D_j D_j^T P).$$

For optimization problem (5.1) with $f = \phi \circ T_{2a}$, we will use

$$H(P) = \sum_{i=1}^{\ell} \phi_i(T_{2a}(P)) \underbrace{4A_i P P^T A_i}_{=: H_i(P)} + \sum_{j=1}^t \phi_{\ell+j}(T_{2a}(P)) \underbrace{D_j D_j^T}_{=: H_{\ell+j}(P)}, \quad (8.9)$$

for which $\mathcal{H}(P) \equiv H(P)P$ for $P \in \mathbb{R}^{n \times k}$. If all $A_i \geq 0$, then, by Theorem 7.5, the consistency conditions in (8.5) are satisfied with $\mathbb{P} = \text{St}(k, n)$, $Q = I_k$, $\alpha = 2$, $\beta_i = 2$ for $1 \leq i \leq \ell$ and $\beta_{\ell+j} = 0$ for $1 \leq j \leq t$. Note, for the example, (8.5b) for $\ell+1 \leq i \leq \ell+t$ are equalities and hence Theorem 8.1 requires $\phi_i \geq 0$ for $1 \leq i \leq \ell$ only. Optimization problem (5.1) with $T = T_{2a}$ for $t = 0$ and $\phi(x) = \sum_{i=1}^{\ell} x_i$ gives the key optimization problem in the uniform multidimensional scaling (UMDS) method [80].

Comparing the conclusion here and that of Example 5.2 (for all $P_i = P$), we don't require $\phi_{\ell+j} \geq 0$ for $1 \leq j \leq t$ here, everything else being equal. In particular, both require $A_i \geq 0$ for all i . Next, we explain how to make the NEPv approach work on $f = \phi \circ T_{2a}$ even if some $A_i \not\geq 0$, yielding yet another example for which the NEPv approach works but the NPDo approach may not. Let $\delta_i \in \mathbb{R}$ such that $\hat{A}_i = A_i - \delta_i I \geq 0$ for $1 \leq i \leq \ell$. This is always possible by letting δ_i be some lower bound of the eigenvalues of A_i , and numerically, δ_i can be estimated cheaply [82].

Notice that

$$\text{tr}((P^T A_i P)^2) = \text{tr}((P^T \hat{A}_i P)^2) + 2\delta_i \text{tr}(P^T \hat{A}_i P) + k\delta_i^2.$$

Define

$$\hat{T}_{2a} : P \in \text{St}(k, n) \rightarrow \hat{T}_{2a}(P) := \begin{bmatrix} \text{tr}((P^T \hat{A}_1 P)^2) \\ \vdots \\ \text{tr}((P^T \hat{A}_\ell P)^2) \\ \text{tr}(P^T \hat{A}_1 P) \\ \vdots \\ \text{tr}(P^T \hat{A}_\ell P) \\ \|P^T D_1\|_F^2 \\ \vdots \\ \|P^T D_t\|_F^2 \end{bmatrix} \in \mathbb{R}^{2\ell+t}, \quad (8.10)$$

and an affine transformation: $\mathcal{A} : \hat{\mathbf{x}} \in \mathbb{R}^{2\ell+t} \rightarrow \mathbf{x} \in \mathbb{R}^{\ell+t}$ by

$$\mathbf{x} = \mathcal{A}(\hat{\mathbf{x}}) = \begin{bmatrix} \hat{\mathbf{x}}_{(1:\ell)} + 2\Delta \hat{\mathbf{x}}_{(\ell+1:2\ell)} + k\mathbf{d} \\ \hat{\mathbf{x}}_{(2\ell+1:2\ell+t)} \end{bmatrix},$$

where $\hat{\mathbf{x}}_{(i:j)}$ is the sub-vector of $\hat{\mathbf{x}}$ from its i th entry to j th entry, $\Delta = \text{diag}(\delta_1, \dots, \delta_\ell) \in \mathbb{R}^{\ell \times \ell}$, and $\mathbf{d}^T = [\delta_1^2, \dots, \delta_\ell^2]$. Finally, $f(P) = \hat{\phi} \circ \hat{T}_{2a}(P)$ where $\hat{\phi}(\hat{\mathbf{x}}) = \phi(\mathbf{x}) \equiv \phi(\mathcal{A}(\hat{\mathbf{x}}))$ is convex in $\hat{\mathbf{x}}$ [13, p.79]. It can be verified that

$$\hat{\phi}_i(\hat{\mathbf{x}}) := \frac{\partial \hat{\phi}(\hat{\mathbf{x}})}{\partial \hat{x}_i} = \begin{cases} \phi_i(\mathbf{x}), & \text{for } 1 \leq i \leq \ell, \\ 2\delta_{i-\ell} \phi_{i-\ell}(\mathbf{x}), & \text{for } \ell+1 \leq i \leq 2\ell, \\ \phi_{i-\ell}(\mathbf{x}), & \text{for } 2\ell+1 \leq i \leq 2\ell+t. \end{cases}$$

Theorem 8.1 is now applicable to $f(P) = \hat{\phi} \circ \hat{T}_{2a}(P)$, but requiring only $\phi_i \geq 0$ for $1 \leq i \leq \ell$ and without requiring any of $A_i \geq 0$.

Example 8.3 Consider T_{3a} , a special case of T_3 in (5.11),

$$T_{3a} : P \in \text{St}(k, n) \rightarrow T_{3a}(P) := \begin{bmatrix} \text{tr}((P^T A_1 P)^{m_1}) \\ \vdots \\ \text{tr}((P^T A_\ell P)^{m_\ell}) \\ \text{tr}((P^T D)^{m_{\ell+1}}) \end{bmatrix} \in \mathbb{R}^{\ell+1}, \quad (8.11)$$

where integer $m_i \geq 1$ for all $1 \leq i \leq \ell+1$ and $D \in \mathbb{R}^{n \times k}$. It reduces to an even more special case of Example 8.1 if all $m_i = 1$ for $1 \leq i \leq \ell+1$. Either $\ell = 0$ or without

the last component $\text{tr}((P^T D)^{m_{\ell+1}})$ is allowed. For optimization problem (5.1) with $f = \phi \circ T_{3a}$, we will use

$$\begin{aligned}
 H(P) = & \sum_{i=1}^{\ell} \phi_i(T_{3a}(P)) \underbrace{2m_i A_i (P P^T A_i)^{m_i-1}}_{=: H_i(P)} \\
 & + \phi_{\ell+1}(T_{3a}(P)) \underbrace{m_{\ell+1} [D(P^T D)^{m_{\ell+1}-1} P^T + P(D^T P)^{m_{\ell+1}-1} D^T]}_{=: H_{\ell+1}(P)},
 \end{aligned} \tag{8.12}$$

for which $H(P)P - \mathcal{H}(P) = P[\phi_{\ell+1}(T_{3a}(P)) m_{\ell+1} (D^T P)^{m_{\ell+1}}]$ for $P \in \text{St}(k, n)$. Any solution P to NEPv (6.3) with $H(P)$ in (8.12) such that $(D^T P)^{m_{\ell+1}}$ is symmetric is a solution to the KKT condition (2.3). Suppose all $A_i \succeq 0$ and let $\mathbb{P} = \text{St}(k, n)_{D+}$. Then the consistency conditions in (8.5) are satisfied with $\underline{\alpha} = 2$, $\underline{\beta}_i = 2(m_i - 1)$ for $1 \leq i \leq \ell + 1$, by Theorems 7.4 and 7.5. In applying Theorem 8.1 with $T_0 = T_{3a}$ we need $\phi_i \geq 0$ for $1 \leq i \leq \ell + 1$ because now we are not sure if any of the inequalities in (8.5b) is an equality. Lastly, the best Q_i at Line 4 of Algorithm 6.1 when applied to $\phi \circ T_{3a}$ is an orthogonal polar factor of $[\widehat{P}^{(i)}]^T D$ and vice versa.

Remark 8.1 We conclude this section by commenting on the applicability of the results of this section to the objective functions in Table 1 via convex compositions of atomic functions for NEPv. Essentially our results are applicable to all but OLDA and SumTR, for which the corresponding composing functions ϕ are x_2/x_1 and $x_2/x_1 + x_3$, respectively. Both are non-convex, and yet the **NEPv Ansatz** still holds for OLDA but does not for SumTR. With the generic $H(P)$ as in (6.5), SumCT can be handled too through the convex composition of atomic functions but the resulting NEPv approach may not be competitive to the NPDo approach (see [42, sect. 8.2]). The composing function for OCCA is $x_2/\sqrt{x_1}$, which is not convex but whose square x_2^2/x_1 is convex for $x_2 \geq 0$ and $x_1 > 0$. For Θ TR, the theory in this section can only handle $0 \leq \theta \leq 1/2$ and also on the objective function squared, however:

$$[f(P)]^2 = \phi \circ T(P) \quad \text{with } T(P) = \begin{bmatrix} \text{tr}(P^T B P) \\ \text{tr}(P^T A P) \\ \text{tr}(P^T D) \end{bmatrix}, \quad \phi(\mathbf{x}) = \frac{(x_2 + x_3)^2}{x_1^{2\theta}}, \tag{8.13}$$

where $\mathbf{x} \equiv [x_1, x_2, x_3]^T$. This T has the form of T_{1a} of Example 8.1 and it can be verified that the associated symmetric matrix-valued function $H(P)$ by (8.6) differs from the one in (6.4) [68] by a scalar factor only. We claim that ϕ is convex for $x_1 > 0$ and $x_2 + x_3 \geq 0$, provided $0 \leq \theta \leq 1/2$, and, since also $\phi_3(\mathbf{x}) := \partial\phi(\mathbf{x})/\partial x_3 \geq 0$ for $x_1 > 0$ and $x_2 + x_3 \geq 0$, Theorem 8.2 applies. We note that $\phi_0(x, y) = y^2/x^{2\theta}$ for $x > 0$ and $y \geq 0$ is convex if $0 \leq \theta \leq 1/2$ but is not convex if $\theta > 1/2$. In fact, the

Hessian matrix of ϕ_0 is

$$\begin{bmatrix} 2\theta(2\theta+1)y^2/x^{2\theta+2} & -4\theta y/x^{2\theta+1} \\ -4\theta y/x^{2\theta+1} & 2/x^{2\theta} \end{bmatrix} = \frac{2}{x^{2\theta}} \begin{bmatrix} y/x & \\ & 1 \end{bmatrix} \begin{bmatrix} \theta(2\theta+1) & -2\theta \\ -2\theta & 1 \end{bmatrix} \begin{bmatrix} y/x & \\ & 1 \end{bmatrix}$$

which is positive semidefinite for $x > 0$ and $y \geq 0$ if and only if $0 \leq \theta \leq 1/2$. This implies $\phi(\mathbf{x}) \equiv \phi_0(x_1, x_2 + x_3)$ is convex for $x_1 > 0$ and $x_2 + x_3 \geq 0$, provided $0 \leq \theta \leq 1/2$. However, the results in [68] says that the NEPv approach works on f for Θ TR for $0 \leq \theta \leq 1$, much bigger range for θ than what Theorem 8.2 for f^2 implies. Theorem 8.2 also yields an inequality on how much the objective function squared, f^2 , increases, in contrast to the previous (6.11) which is for the original objective function, f , for $0 \leq \theta \leq 1$ and OCCA. In any case, the best Q_i at Line 4 of Algorithm 6.1 when applied to Θ TR is an orthogonal polar factor of $[\hat{P}^{(i)}]^T D$ and $\mathbb{P} = \text{St}(k, n)_{D+}$.

9 A Brief Comparison of the NPDo and NEPv Approaches

The developments of the frameworks for both NPDo and NEPv follow the same pattern: an ansatz that implies the global convergence of their respective SCF iterations, the definition of atomic functions for an approach, and the fulfillment of the ansatz by the atomic functions for the approach and their convex compositions. Subtly, between the two approaches, there are differences in applicabilities and numerical implementations, making them somewhat complementary to each other. We outline some notable differences below.

The NEPv approach requires weaker conditions. We have demonstrated that **the NPDo Ansatz** demands more on an objective function than **the NEPv Ansatz**, and hence the NEPv approach provably works on a wider collection of maximization problems (1.1) on the Stiefel manifold than the NPDo approach.

- i. The NPDo approach requires that the KKT condition $\mathcal{H}(P) \equiv \partial f(P)/\partial P = P\Lambda$ is a polar decomposition at optimality, in order for the approach to be even considered, whereas the NEPv approach does not impose that the KKT condition must be an NPDo at optimality;
- ii. **The NPDo Ansatz** implies **the NEPv Ansatz** with the generic symmetric matrix-valued function $H(P)$ in (6.5) (see Theorem 6.2);
- iii. Atomic functions for NPDo are also atomic functions for NEPv with the generic symmetric matrix-valued function $H(P)$ in (6.5) (see Theorem 7.1);
- iv. Among those in Table 1, the NEPv approach is guaranteed to work for three more than the NPDo approach does (Table 2 vs. Table 4);
- v. When it comes to the concrete atomic functions $[\text{tr}((P^T A P)^m)]^s$ where integer $m \geq 1$ and scalar $s \geq 1$, it is required that $A \geq 0$ always for the NPDo approach, whereas for the NEPv approach A being symmetric suffices for $m \in \{1, 2\}$ and $s = 1$ (see Examples 8.1 and 8.2);
- vi. As a further demonstration, in Table 6, we summarize what are required by both approaches on three convex compositions of matrix-trace functions, and it clearly

Table 6 NPDo vs. NEPv on three convex compositions of matrix traces

<i>f</i>	NPDo		NEPv	
	conditions	by	conditions	by
$\phi \circ T_{1a}$	$A_i \geq 0, 1 \leq i \leq \ell$ $\phi_j \geq 0, 1 \leq j \leq \ell$	Theorem 5.2	none	Theorem 8.2
$\phi \circ T_{2a}$	$A_i \geq 0, 1 \leq i \leq \ell$ $\phi_j \geq 0, 1 \leq j \leq \ell + t$	Example 5.2	$\phi_j \geq 0, 1 \leq j \leq \ell$	Example 8.2
$\phi \circ T_{3a}$	$A_i \geq 0, 1 \leq i \leq \ell$ $\phi_j \geq 0, 1 \leq j \leq \ell + 1$	Example 5.3	$A_i \geq 0, 1 \leq i \leq \ell$ $\phi_j \geq 0, 1 \leq j \leq \ell + 1$	Example 8.3

$\phi_j(\mathbf{x}) := \partial \phi(\mathbf{x}) / \partial x_j$ for $\mathbf{x} = [x_j]$

indicates that NEPv requires weaker conditions than NPDo does for both $\phi \circ T_{1a}$ and $\phi \circ T_{2a}$.

The NPDo approach is easier to use. The NPDo approach, if it provably works, is easier to implement and more flexible to use.

- The NPDo approach relies on SVDs of tall and skinny matrices [17, 24] during its SCF iterations, whereas the NEPv approach needs solutions to potentially large scale eigenvalue problems [3, 36, 41, 52, 57], not to mention that the NEPv approach requires constructing a symmetric matrix-valued function $H(P)$.
- In general for the NPDo approach, the atomic functions in a convex composition are allowed to be of submatrices of P consisting of a few, not necessarily all, columns of P , such as P_i in $\text{tr}(P_i^T A_i P_i)$ of SumCT in Table 1, but, more generally, different P_i can share common columns of P , whereas no P_i in SumCT share common columns of P ; For the NEPv approach, allowing such flexibility in the involved atomic functions in the convex composition forces us to use the generic symmetric matrix-valued function $H(P)$ in (6.5) and ask for the same conditions as the NPDo approach requires, and hence we may as well go for the NPDo approach in the first place (see [42, sect. 8.2]).

10 Concluding Remarks

The first order optimality condition, also known as the KKT condition, for optimizing a function f over the Stiefel manifold takes the form

$$\mathcal{H}(P) := \frac{\partial f(P)}{\partial P} = P \Lambda \quad \text{with} \quad \Lambda^T = \Lambda \in \mathbb{R}^{k \times k}, \quad P^T P = I_k. \quad (10.1)$$

This is an $n \times k$ matrix equation in P on the Stiefel manifold, upon noticing $\Lambda = [P^T \mathcal{H}(P) + \mathcal{H}(P)^T P]/2$. Any maximizer is a solution. Except for very special objective functions such as $\text{tr}(P^T A P)$ or $\text{tr}(P^T D)$, solving this equation rightly and efficiently for a maximizer is a challenging task. For example, it often has infinitely many solutions and maximizers hide among them. Hence we need to not only solve the nonlinear equation of the KKT condition but also find the right ones. Inspired by recent works [67, 68, 75–78], in this paper, we establish two unifying frameworks, one for the NEPv approach and the other for the NPDo approach, for optimization on the Stiefel manifold. Our frameworks are built upon two fundamental ansatzes, **the NPDo Ansatz** and **the NEPv Ansatz**. When a respective ansatz is satisfied, the corresponding approach, the NPDo or NEPv approach, is guaranteed to work in the sense of global convergence from any given initial point. To expand the applicability of the approaches, we propose the theories of atomic functions for each approach and show that any convex composition $\phi \circ T$ of atomic functions for any of the two approaches satisfies the corresponding ansatz under some mild conditions. It is demonstrated that the commonly used matrix-trace functions

$$[\text{tr}((P^T A P)^m)]^s, \quad [\text{tr}((P^T D)^m)]^s \quad \text{for integer } m \geq 1 \text{ and real scalar } s \geq 1$$

are concrete atomic functions for both approaches (A may be required to be positive semidefinite depending on circumstances), and that nearly all optimization problems on the Stiefel manifold recently investigated in the literature for various machine learning applications are about some compositions of these concrete matrix-trace functions. Although not all of them are convex compositions, some may still satisfy **the NEPv Ansatz**. These concrete atomic functions in combination with convex compositions lead to a large collection of objective functions on which one of or both approaches work.

However when an ansatz fails to hold for a given objective function, the conclusions from our global convergence analysis will likely fail. In the case for the NEPv approach, a remedy via the level-shifting SCF exists to ensure locally linear convergence when $f(P)$ is right-unitarily invariant [4] or when $f(P)$ contains and increases with $\text{tr}(P^T D)$ [47], where sharp estimations of linear convergence rate are obtained. But there are more works to do, especially for the NPDo approach for which a remedy remains to be found. In [63], it is investigated how $\text{tr}(P^T D)$ may help determine a particular P among all orthonormal basis matrices of a subspace.

Not all objective functions (or their simple transformations like f^2 for ΘTR as explained in Remark 8.1) that satisfy the ansatz(es) take the form of some convex compositions of atomic functions, even for some of those in Table 1. For example, in the case of OLDA, $f(P) = \phi \circ T(P)$ where $\phi(x) = x_1/x_2$ and $T(P) = \begin{bmatrix} \text{tr}(P^T A P) \\ \text{tr}(P^T B P) \end{bmatrix}$. Although this $f(P)$ is not a convex composition of $\text{tr}(P^T A P)$ and $\text{tr}(P^T B P)$, it still satisfies **the NEPv Ansatz**. In fact, OLDA is a special case of ΘTR : $\theta = 1$ and $D = 0$, and inequality (6.11) applies and yields, for OLDA, that if $\text{tr}(\widehat{P}^T H(P) \widehat{P}) - \text{tr}(P^T H(P) P) \geq 0$, then

$$f(\widetilde{P}) \geq f(P) + \frac{1}{2} \cdot \frac{s_k(B)}{S_k(B)} \left[\text{tr}(\widehat{P}^T H(P) \widehat{P}) - \text{tr}(P^T H(P) P) \right],$$

assuming $B \succeq 0$ and $\text{rank}(B) > n - k$, where $\widetilde{P} = \widehat{P}$ and $H(P)$ is given by (6.4) upon setting $\theta = 1$ and $D = 0$.

Numerical demonstrations on the performances of the NEPv approach and the NPDo approach on various machine learning applications have been well documented by the author and his collaborators in their recent works [67, 68, 75, 78]. We expect more to come as the unifying frameworks in this paper have significantly expanded the domains on which the approaches provably work.

Throughout the article, we limit ourselves to the Stiefel manifold in the standard inner product $\langle x, y \rangle = y^T x$ for $x, y \in \mathbb{R}^n$ and to the field of real numbers, because that is where most optimization on the Stiefel manifold from machine learning dominantly falls into. But our developments can be extended to the field of complex numbers and other inner-products, separately and combined. For the case of the field of complex numbers, minor modifications suffice: replacing transpose $(\cdot)^T$ with conjugate transpose $(\cdot)^H$ and $\text{tr}((P^T D)^m)$ with $\Re(\text{tr}((P^H D)^m))$ (where $\Re(\cdot)$ takes the real part of a complex number). However, extending to the case of the M -inner product requires additional algebraic manipulations and analysis. An outline on how to proceed is explained in [42, appendix E].

A Canonical Angles

We introduce a metric on Grassmann manifold $\mathcal{G}_k(\mathbb{R}^n)$, the collection of all k -dimensional subspaces in $\mathbb{R}^n$. Let $\mathcal{X} = \mathcal{R}(X)$ and $\mathcal{Y} = \mathcal{R}(Y)$ be two points in $\mathcal{G}_k(\mathbb{R}^n)$, where $X, Y \in \text{St}(k, n)$. The canonical angles $\theta_1(\mathcal{X}, \mathcal{Y}) \geq \dots \geq \theta_k(\mathcal{X}, \mathcal{Y})$ between $\mathcal{X}$ and $\mathcal{Y}$ are defined by [59]

$$0 \leq \theta_i(\mathcal{X}, \mathcal{Y}) := \arccos \sigma_i(X^T Y) \leq \frac{\pi}{2} \quad \text{for } 1 \leq i \leq k,$$

and accordingly, the diagonal matrix of the canonical angles between $\mathcal{X}$ and $\mathcal{Y}$ is

$$\Theta(\mathcal{X}, \mathcal{Y}) = \text{diag}(\theta_1(\mathcal{X}, \mathcal{Y}), \dots, \theta_k(\mathcal{X}, \mathcal{Y})) \in \mathbb{R}^{k \times k}.$$

It is known that

$$\text{dist}_2(\mathcal{X}, \mathcal{Y}) := \|\sin \Theta(\mathcal{X}, \mathcal{Y})\|_2 = \sin \theta_1(\mathcal{X}, \mathcal{Y}), \quad (\text{A.1})$$

$$\text{dist}_F(\mathcal{X}, \mathcal{Y}) := \|\sin \Theta(\mathcal{X}, \mathcal{Y})\|_F = \left[\sum_{i=1}^k \sin^2 \theta_i(\mathcal{X}, \mathcal{Y}) \right]^{1/2} \quad (\text{A.2})$$

are two unitarily invariant metrics on the Grassmann manifold $\mathcal{G}_k(\mathbb{R}^n)$ [60, p.99].

B Preliminary Lemmas

In this section, we collect a few results, some known and some likely new, that we need in our proofs. We will point out an earliest reference, if known, to each one. Some likely appear before but we are not aware of any reference to. For completeness, we will provide proofs for those we cannot find references.

Lemma B.1 (Young's Inequality) *Given $a, b \geq 0$, and $p, q \geq 1$ such that $\frac{1}{p} + \frac{1}{q} = 1$, we have*

$$a^{1/p} b^{1/q} \leq \frac{1}{p} a + \frac{1}{q} b.$$

In particular for $p = q = 2$, it becomes $2\sqrt{ab} \leq a + b$.

Lemma B.2 *For $a, b \geq 0$, and $\mu, v \geq 0$ such that $\mu + v \geq 1$, we have*

$$a^\mu b^v \leq \frac{\mu}{\mu + v} a^{\mu+v} + \frac{v}{\mu + v} b^{\mu+v}.$$

Proof Let $\tau := \mu + v \geq 1$. Then $\mu/\tau + v/\tau = 1$. Using Young's Inequality, we get

$$a^\mu b^v = (a^{\mu/\tau} b^{v/\tau})^\tau \leq \left(\frac{\mu}{\tau} a + \frac{v}{\tau} b \right)^\tau \leq \frac{\mu}{\tau} a^\tau + \frac{v}{\tau} b^\tau,$$

as was to be shown, where the last inequality follows from that fact that x^τ with $\tau \geq 1$ is convex on $[0, \infty)$. $\square$

Lemma B.3 Let $\phi : \mathcal{D} \subseteq \mathbb{R}^N \rightarrow \mathbb{R}$ be convex and differentiable and let $\mathbf{x}, \tilde{\mathbf{x}} \in \mathcal{D}$, where $\mathcal{D}$ is a convex domain in $\mathbb{R}^N$. If

$$\nabla \phi(\mathbf{x})^T \tilde{\mathbf{x}} \geq \nabla \phi(\mathbf{x})^T \mathbf{x} + \eta,$$

then $\phi(\tilde{\mathbf{x}}) \geq \phi(\mathbf{x}) + \eta$.

Proof Likely, the result of this lemma is known, and it has a short proof. Since ϕ is convex, we have

$$\begin{aligned} \phi(\tilde{\mathbf{x}}) &\geq \phi(\mathbf{x}) + [\nabla \phi(\mathbf{x})]^T (\tilde{\mathbf{x}} - \mathbf{x}) \\ &= [\nabla \phi(\mathbf{x})]^T \tilde{\mathbf{x}} + \phi(\mathbf{x}) - [\nabla \phi(\mathbf{x})]^T \mathbf{x} \\ &\geq [\nabla \phi(\mathbf{x})]^T \mathbf{x} + \eta + \phi(\mathbf{x}) - [\nabla \phi(\mathbf{x})]^T \mathbf{x} \\ &= \phi(\mathbf{x}) + \eta, \end{aligned}$$

as was to be shown. $\square$

Lemma B.4 (von Neumann's trace inequality [65], [28, p.183]) For $B, C \in \mathbb{R}^{n \times k}$, we have

$$|\operatorname{tr}(B^T C)| \leq \sum_{i=1}^k \sigma_i(B) \sigma_i(C).$$

In the next four lemmas, any arbitrary nonnegative power of a positive semidefinite matrix B is understood as $B^\mu = U \Lambda^\mu U^T$ for any $\mu \geq 0$, where $B = U \Lambda U^T$ is the eigendecomposition of B , and Λ^μ is obtained by taking the μ th power of every diagonal entry of Λ .

Lemma B.5 For $B, C \in \mathbb{R}^{k \times k}$ that are positive semidefinite, and $\mu, \nu \geq 0$ such that $\mu + \nu \geq 1$, we have

$$\operatorname{tr}(B^\mu C^\nu) \leq \|B^\mu C^\nu\|_{\operatorname{tr}} \leq \frac{\mu}{\mu + \nu} \operatorname{tr}(B^{\mu+\nu}) + \frac{\nu}{\mu + \nu} \operatorname{tr}(C^{\mu+\nu}).$$

Proof That $\operatorname{tr}(B^\mu C^\nu) \leq \|B^\mu C^\nu\|_{\operatorname{tr}}$ is a corollary of Weyl's majorant theorem [8, p.42]. Let $Q \in \operatorname{St}(k, k)$ such that $Q^T B^\mu C^\nu \succeq 0$, which yields $\|B^\mu C^\nu\|_{\operatorname{tr}} = \operatorname{tr}(Q^T B^\mu C^\nu)$. Note that $B \succeq 0$ and thus $(Q^T B^\mu)^T (Q^T B^\mu) = B^{2\mu}$, implying the singular values of $Q^T B^\mu$ are given by $\{[\sigma_i(B)]^\mu\}_{i=1}^k$. Since $C \succeq 0$, the singular values of C^ν are $\{[\sigma_i(C)]^\nu\}_{i=1}^k$. Hence by Lemma B.4 and then by Lemma B.2, we get

$$\begin{aligned} \|B^\mu C^\nu\|_{\operatorname{tr}} &= \operatorname{tr}([Q^T B^\mu] C^\nu) \\ &\leq \sum_{i=1}^k [\sigma_i(B)]^\mu [\sigma_i(C)]^\nu \end{aligned} \tag{B.1}$$

$$\begin{aligned}
 &\leq \sum_{i=1}^k \left(\frac{\mu}{\mu + \nu} [\sigma_i(B)]^{\mu+\nu} + \frac{\nu}{\mu + \nu} [\sigma_i(C)]^{\mu+\nu} \right) \\
 &= \frac{\mu}{\mu + \nu} \operatorname{tr}(B^{\mu+\nu}) + \frac{\nu}{\mu + \nu} \operatorname{tr}(C^{\mu+\nu}), \quad (\text{B.2})
 \end{aligned}$$

as expected. $\square$

Lemma B.6 For $B, C \in \mathbb{R}^{k \times k}$ where C is positive semidefinite, and $\nu \geq 0$, we have

$$\operatorname{tr}(BC^\nu) \leq \|BC^\nu\|_{\operatorname{tr}} \leq \frac{1}{1+\nu} \operatorname{tr}((Q^T B)^{1+\nu}) + \frac{\nu}{1+\nu} \operatorname{tr}(C^{1+\nu}),$$

where $Q \in \operatorname{St}(k, k)$ such that $Q^T B \succeq 0$.

Proof Again $\operatorname{tr}(BC^\nu) \leq \|BC^\nu\|_{\operatorname{tr}}$ is a corollary of Weyl's majorant theorem. Despite that B may not be positive semidefinite (possibly not even symmetric), we still have (B.1) with $\mu = 1$ so long as $Q^T B C^\nu \succeq 0$. Also note $(Q^T B)^T (Q^T B) = B^T B$ and hence the singular values of $Q^T B$ are given by $\{\sigma_i(B)\}_{i=1}^k$. So we still get (B.2) with $\mu = 1$. The proof is completed upon noticing the eigenvalues of $Q^T B$ are the same as the singular values of B . $\square$

Lemma B.7 For $X, Y \in \mathbb{R}^{n \times k}$ and $\mu, \nu \geq 0$, we have

$$\begin{aligned}
 &\operatorname{tr}((X^T X)^\mu X^T Y (Y^T Y)^\nu) \\
 &\leq \frac{1+2\mu}{2(\mu+\nu+1)} \operatorname{tr}((X^T X)^{\mu+\nu+1}) + \frac{1+2\nu}{2(\mu+\nu+1)} \operatorname{tr}((Y^T Y)^{\mu+\nu+1}).
 \end{aligned}$$

Proof The singular values of $(X^T X)^\mu X^T$ and $Y(Y^T Y)^\nu$ are $\{[\sigma_i(X)]^{1+2\mu}\}_{i=1}^k$ and $\{[\sigma_i(Y)]^{1+2\nu}\}_{i=1}^k$, respectively. Hence by Lemma B.4 and then by Lemma B.2, we get

$$\begin{aligned}
 &\operatorname{tr}((X^T X)^\mu X^T Y (Y^T Y)^\nu) \\
 &\leq \sum_{i=1}^k [\sigma_i(X)]^{1+2\mu} [\sigma_i(Y)]^{1+2\nu} \\
 &\leq \sum_{i=1}^k \left(\frac{1+2\mu}{2(\mu+\nu+1)} [\sigma_i(X)]^{2(\mu+\nu+1)} + \frac{1+2\nu}{2(\mu+\nu+1)} [\sigma_i(Y)]^{2(\mu+\nu+1)} \right) \\
 &= \frac{1+2\mu}{2(\mu+\nu+1)} \operatorname{tr}((X^T X)^{\mu+\nu+1}) + \frac{1+2\nu}{2(\mu+\nu+1)} \operatorname{tr}((Y^T Y)^{\mu+\nu+1}),
 \end{aligned}$$

as was to be shown. $\square$

Lemma B.8 ([78, Lemma 3]) For $H \in \mathbb{R}^{k \times k}$, we have $|\operatorname{tr}(H)| \leq \|H\|_{\operatorname{tr}}$. If $|\operatorname{tr}(H)| = \|H\|_{\operatorname{tr}}$, then H is symmetric and is either positive semi-definite when $\operatorname{tr}(H) \geq 0$, or negative semi-definite when $\operatorname{tr}(H) \leq 0$.

Remark B.1 ([67]) As a corollary of Lemma B.8, for any $H \in \mathbb{R}^{k \times k}$, if $H \not\geq 0$ (which means either H is not symmetric or H is symmetric but indefinite or even negative semidefinite), then $\text{tr}(H) < \|H\|_{\text{tr}}$. Now let $H = U \Sigma V^T$ be the SVD of H [24] where $\Sigma \in \mathbb{R}^{k \times k}$ and set $Q = UV^T$, an orthogonal polar factor of H . Then $Q^T H = V \Sigma V^T \geq 0$ and $\text{tr}(Q^T H) = \|H\|_{\text{tr}} > \text{tr}(H)$.

The next lemma are likely well-known. For example, they are implied in the discussion in [67] before [67, Lemma 3.2] there.

Lemma B.9 Let $B \in \mathbb{R}^{n \times k}$.

- $\text{tr}(P^T B) \leq \|B\|_{\text{tr}}$ for any $P \in \text{St}(k, n)$;
- $\text{tr}(P^T B) = \|B\|_{\text{tr}}$ where $P \in \text{St}(k, n)$ if and only if $B = P \Lambda$ with $\Lambda \geq 0$;
- We have

$$\max_{P \in \text{St}(k, n)} \text{tr}(P^T B) = \|B\|_{\text{tr}}$$

and the optimal value $\|B\|_{\text{tr}}$ is achieved by any orthogonal polar factor P_* of B .

Lemma B.9 says that $\text{tr}(P^T B)$ is bounded above by $\|B\|_{\text{tr}}$ always and the upper bound $\|B\|_{\text{tr}}$ is achieved by any orthogonal polar factor P_* of B and also any maximizer of $\text{tr}(P^T B)$ over $P \in \text{St}(k, n)$ is an orthogonal polar factor of B . For numerical computation, an orthogonal polar factor of B can be constructed from the thin SVD $B = U \Sigma V^T$ as $P_* = UV^T$ of B .

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