Sequential subspace methods on Stiefel manifold optimization problems *

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Abstract

We study the minimization of a quadratic over Stiefel manifolds (the set of all orthogonal r-frames in \(\mathbb{R}^n\)), which has applications in high-dimensional semi-supervised classification tasks. To reduce the computational complexity, sequential subspace methods (SSM) are employed to convert the high-dimensional minimization problems to low-dimensional ones. In this paper, we are interested in attaining an optimal solution of good quality, i.e., a “qualified” critical point. Qualified critical points are those critical points, at which the associated multiplier matrix meets some upper bound condition. These critical points enjoy the global optimality in special quadratic problems. For a general quadratic, SSM computes a sequence of “qualified critical points” in its low-dimensional “surrogate regularized models”. The convergence to a qualified critical point is ensured, whenever each SSM subspace is constructed by the following vectors: (i) a set of orthogonal unit vectors associated with the current iterate, (ii) a set of vectors corresponding to the gradient of the objective, and (iii) a set of eigenvectors associated with the smallest r eigenvalues of the system matrix. In addition, when Newton direction vectors are included in subspaces, the convergence of SSM can be accelerated significantly.

Keywords: Procrustes problem, Stiefel manifold, Sequential subspace methods, Trust region methods.

1 Introduction

Optimization problems on smooth manifolds arise in science and engineering as a result of natural geometry and have various applications in machine learning, computer vision, robotics, scientific computing, and signal processing [EAS01, AM01, AMS08, MMSY07]. Let \(\text{St}(n,r)\) denote Stiefel manifold defined as

\[
\text{St}(n,r) := \{X \in \mathbb{R}^{n \times r} : X^\top X = I_r\}. \tag{1}
\]

In short, \(\text{St}(n,r)\) is the set of matrices in \(\mathbb{R}^{n \times r}\) whose columns are orthonormal in \(\mathbb{R}^n\) with respect to the inner product \(\langle x, y \rangle = \text{tr}(x^\top y)\). In this paper, we propose one efficient algorithm to solve the problem

\[
\min_{X \in \text{St}(n,r)} \{f(X) = \frac{1}{2} \text{tr}(X^\top AXC) - \text{tr}(B^\top X)\}, \tag{2}
\]

where \(A\) is symmetric, \(C\) is symmetric positive definite, and \(B \in \mathbb{R}^{n \times r}\). When \(C = I_r\), the problem in (2) is equivalent to the (unbalanced) Procrustes problem [Sch66, EP99, ZQD07].

The large-scale quadratic optimization problems \(n \gg r\) with orthogonality constraints are a fundamental class of matrix optimization problems that are widely applied across machine learning, statistics,
and signal processing. For instance, the problem \( \text{(2)} \) with \( C = I_r \) and \( B = 0 \) is the major task in Principal Component Analysis (PCA), which is one visualization tool in unsupervised data preprocessing \([JC16,Sha15]\). Specific instances of \( \text{(2)} \) also appear in one popular technique for multiple signal processing, independent component analysis \([Com94,Nis,ACG17,AVGA23]\), where the search for a demixing (uncorrelated) matrix is reduced to the separation of orthogonal signals under proper statistical principles. More recently, in deep learning the weights of a layer are parametrized by an orthogonal matrix to overcome the difficulty in training deep networks \([ASB16,BCW15]\).

The matrix \( A \) in \( \text{(2)} \) is constructed from the graph Laplacian, computed from some data graph. Laplacian Eigenmap \([BN03]\) is a graph embedding framework that relies on computing the spectrum of a matrix derived from an underlying data graph to identify certain characterizations of the data—e.g. its cluster structure or geometry. A large body of subsequent work including \([CLL05]\) use global eigenvectors of the graph Laplacian to perform dimensionality reduction and data representation, in unsupervised and semi-supervised settings \([TSL00,ZBL03,BN03,BN04,BNS06]\). In this work, we shall study one prominent application of \( \text{(2)} \) in the context of graph machine learning, namely, semi-supervised graph embedding, where collecting labeled data is generally costly and time-consuming, but there is a wealth of unlabeled data. In semi-supervised graph embedding, we are interested in acquiring useful insights into the clustering structure from the additional label information, in particular, only a small amount of pre-specified labeled data. The minimization problem in \( \text{(2)} \) provides one model for the \( r \)-way classification with partial labeling. (See section 4.1 for the details.) In contrast to global eigenvectors in \( \text{(2)} \), the minimizer \( X \) here is viewed as one local-biased set of the graph Laplacian eigenvectors under the perturbation \( tr(B^TX) \) in \( \text{(4)} \).

The constrained optimization problem in \( \text{(2)} \) can be handled by various optimization algorithms. For instance, the gradient projection method is one effective method when projections on constrained sets can be easily implemented \([God64,LP66,Ber76,Ber16]\). From the perspective of manifold optimization, the Stiefel manifold in \( \text{(2)} \) is a smooth manifold with special quadratic constraints, and one can implement conjugate gradient methods and Newton methods over geodesic paths on the manifold \([EAS01]\). The computational complexity of geodesics can be reduced, if we adopt line-search procedures on tangent spaces with proper retractions \([Man02,AMS08]\) or use the Cayley transform to directly construct a feasible curve on the manifold \([WY13]\). In this paper, we propose one algorithm for the large-scale problems in \( \text{(2)} \) with \( n \gg r \). For \( r = 1 \), the minimization task is the minimization of a quadratic over a unit sphere, arising in trust region methods \([Sor82,CGT00]\). In \([HP05]\), authors propose Sequential Subspace Methods (SSM) to compute a global minimizer of large-scale problems. In this paper, we generalize the application of SSM to the optimization over the Stiefel manifold with \( r > 1 \).

When the problem dimension \( n \) is large, many local solutions can exist in \( \text{(2)} \), and most of them are saddles, which are far away from global minimizers of \( \text{(2)} \). To ensure the solution quality, observing the eigendecomposition
\[
A = [v_1, v_2, \ldots, v_n] \text{diag}(d_1, \ldots, d_n)[v_1, v_2, \ldots, v_n]^{\top},
\]
we use the ground eigenvectors \( \{v_1, \ldots, v_r\} \) to construct a “regularized” system \( \tilde{A} \) via modifying the ground eigenvalues of \( A \),
\[
\tilde{A} := A + \sum_{k=1}^{r-1} (d_r - d_k) v_k v_k^{\top} = A + V_g(d_r I_r - \text{diag}(d_1, \ldots, d_r))V_g^{\top}, \quad V_g := [v_1, \ldots, v_r] \in \mathbb{R}^{n \times r}.
\]
Here, assume the spectral gap \( d_{r+1} > d_r \) in \( A \). When the ground eigenvectors of \( A \) are precomputed, SSM introduce a sequence of small dimensional subspaces \( \{S_k : k = 1, \ldots\} \) to compute the global minimizers \( X_k \) of the induced regularized problems,
\[
\min_X \left\{ f(X; \tilde{A}, B_k, C) := \frac{1}{2} \langle X, \tilde{A}XC \rangle - \langle B_k, X \rangle \right\} \quad \text{subject to} \quad X \in \text{St}(n, r) \cap S_k.
\]
Here, each \( B_k \in \mathbb{R}^{n \times r} \) is properly constructed to ensure that each regularized problem is a tight surrogate model for \( \text{(2)} \). The details are described in section 4.3.

In this work, we aim to provide one theoretical and algorithmic framework to solve \( \text{(2)} \). Even though the objective discussed is restricted to quadratic functions, the results in this paper can shed some light on the minimization of general objectives over Stiefel manifolds. The following outlines the contribution
In this work, we examine the optimality condition of minimizers in \([2]\). Some optimal conditions with \(C = I\) were reported in \([EP99,ZQD07]\). Since we are concerned with local solutions of good quality with \(C \geq 0\), we introduce the computation of “qualified” critical points, at which the first order condition holds and the associated multiplier matrix \(\Lambda\) meets the condition \(\Lambda \preceq d\cdot C\). For the system matrix \(A\) with identical ground eigenvalues, i.e., a regularized system \(A = \tilde{A}\), any qualified critical point is a global minimizer. In general, when all singular values of \(V\top B\) exceed the gap \(d_r - d_1\), any qualified critical point is also a global minimizer. See Prop. 2.10.

For large-scale problems, we minimize a sequence of surrogate regularized functions in \([5]\) to reach one qualified critical point of \([2]\). SSM construct isometric matrices \(\tilde{V} \in \mathbb{R}^n \times 4r\) (the column space is associated with \(S_k\)) to convert \([5]\) to a sequence of low dimensional sub-problems, called “SSM core problems”,

\[
\min_{\tilde{X}} f(\tilde{X}; \tilde{V}\top \tilde{A}\tilde{V}, \tilde{V}\top B_k, C), \quad \text{subject to} \quad \tilde{X} \in S_t(4r, r),
\]

(6)

When these subspaces \(S_k\) are spanned by columns of \(X\), \(AXC - B\) and \(V_g\), SSM is globally convergent, i.e., a limit of subproblem solutions is a qualified critical point. It is worth mentioning that retractions are implemented on these small dimensional problems, which greatly reduces the computation efforts.

Problem dimension is typically enormous in practical applications. Fast convergence can be obtained if a Newton direction \(Z_k\) is included in \(S_k\), where \(Z_k\) is constructed to reach the maximal reduction of some model functions. Empirically, the computation of \(Z_k\) is the most time-consuming part during the update of \(X\). We impose the orthogonality between \(Z_k\) and \(V_g\) in the Newton direction computation, which improves the condition of the Hessian operator and reduces the total number of CG iterations used.

In many applications, one may wish to solve a “locally-biased” problem, for example, find a partitioning or clustering that is informed by a prespecified “ground-truth” partitioning of a seed set of vertices. Locally-biased problems of this sort are particularly challenging for popular eigenvector-based machine learning and data analysis tools. We demonstrate the effectiveness of SSM on various artificial test cases. The classification accuracy relies on the solution quality of these local solutions. Numerical studies indicate that the proposed SSM obtains high-quality clusters both in terms of balanced graph cut metrics and in terms of the accuracy of the labeling assignment on several real-world datasets, thanks to the solution of good quality.

The paper is organized as follows. In section 2 we start with some known results in the spherical case, i.e., \(S_t(n, 1)\). Next, we derive the necessary and sufficient conditions of the local minimizers in \([2]\). One of our major results is stated in Theorem 2, where each local minimizer of the regularized problem in \([5]\) is a global minimizer. In section 3 we describe sequential subspace methods and show the convergence property. Finally, we demonstrate numerical results, which validate the effectiveness of the proposed algorithms in solving one \(r\)-way classification problem, described in section 4.

Throughout this paper, \(r\) is a positive integer, (much) less than \(n\). We use \(\mathbb{R}^n\) as the \(n\) dimensional real vector space. The inner product \((A, B)\) is the trace of the matrix \(AB\top\) for \(A, B\) of the same size. Let \(\|X\|\) denote the Frobenius norm for a matrix \(X\). Let \(I\) denote the identity matrix, and \(I_n\) denote the identity matrix with size \(n \times n\). Consider the Riemannian metric, inner product on \(S_t(n, r)\),

\[
(u, v) = \text{tr}(u\top v), \quad \text{for any} \quad u, v \in S_t(n, r).
\]

(7)

Let \(\Lambda_{\text{sym}}\) denote the symmetric matrix \((\Lambda + \Lambda\top)/2\) for a square matrix \(\Lambda\). Let \(\text{diag}(x_1, \ldots, x_n)\) denote the diagonal matrix with \(x_1, \ldots, x_n\) lying on the main diagonal. Let \(O\) be the orthogonal group, i.e., \(Q \in O\), if and only if \(Q \in \mathbb{R}^{r \times r}\) and \(Q\top Q = I_r\). Let \(e_i\) denote the canonical basis vector \([0, \ldots, 1, 0, \ldots]\), whose entries are all 0, except for the \(i\)-th entry being 1. Let \(1_n\) denote the \(n\)-dimensional column vector with entries all ones.
2 Local optimality conditions

Define Stiefel manifolds $St(n, r)$ as

$$ St(n, r) := \{ X \in \mathbb{R}^{n \times r} : X^T X = I_r \}. \quad (8) $$

In this paper, we are interested in the minimization of some smooth function $f$ over one Steifel manifold, which has applications in providing initializations of good quality for nonconvex optimization.

2.1 Preliminaries: Quadratic minimization over a sphere

Consider the application of the trust region method on the minimization

$$ \min_{z} f(z), \; z \in \mathbb{R}^n. \quad (9) $$

Let $\Delta > 0$ be the trust-region radius. The trust region method updates the current iterate $z = z_k$ to $z_{k+1} = z_k + x$, where the update vector $x \in \mathbb{R}^n$ solves a quadratic minimization subproblem \[CGT00\] \[HP05\] \[NW06\],

$$ \min_{x} \{ x^T Ax - 2\langle x, b \rangle : \|x\| \leq \Delta, x \in \mathbb{R}^n \}, \quad (10) $$

the vector $b \in \mathbb{R}^n$ is the differential $\partial f$ at the current iterate $z = z_k \in \mathbb{R}^n$, and the symmetric matrix $A$ is the Hessian matrix $\partial^2 f$. Note that the problem in (10) is exactly the special case of (2) with $r = 1$.

The following propositions indicate that the global solution of the quadratic minimization in (10) is the critical point associated with a multiplier $\lambda$ bounded above by the smallest eigenvalue $d_1$ of $A$.

**Proposition 2.1.** \[Sor82\] A vector $x \in \mathbb{R}^n$ is a global solution of (10), if and only if

$$ \|x\| = 1, \; (A - \lambda I)x = b $$

holds for some $\lambda \in \mathbb{R}$.

**Proposition 2.2.** \[Hag01\] Consider the eigenvector decomposition $A = V_A \text{diag}(d_1, d_2, \ldots, d_n)V_A^T$. Let $V_g$ be the matrix whose columns are the “ground eigenvectors” of $A$, i.e., corresponding to eigenvalue $d_1$.

Then a solution $x$ can be determined in the following way.

- **Degenerate case:** Suppose $V_g^T b = 0$ and $c_\perp := \|(A - d_1 I)^{1/2} v_g\| \leq 1$.

  Then $\lambda = d_1$ and

  $$ x = (1 - c_\perp^2)^{1/2} v_g + (A - d_1 I)^{1/2} b $$

  for any unit eigenvector $v_g$ of $A$ associated with eigenvalue $d_1$.

- **Nondegenerate case:** If the condition in (12) does not hold, then a solution is $x = (A - \lambda I)^{-1} b$ for some $\lambda < d_1$ with $\|x\| = 1$.

**Remark 2.3.** Note that for $\lambda \leq d_1$, $\|(A - \lambda I)^{-1} b\|$ decreases monotonically with respect to $\lambda$. Since $\lambda$ in (17) is determined to meet that condition $\|x\| = 1$, we can obtain a tighter bound on $\lambda$ from

$$ (d_1 - \lambda)^{-2} \|V_g b\|^2 \leq 1 = \|(A - \lambda I)^{-1} b\|^2 \leq (d_1 - \lambda)^{-2} \|b\|^2. \quad (14) $$

That is, $\lambda$ lies in the interval $[d_1 - \|b\|, d_1 - \|V_g b\|]$.

2.2 Optimality conditions

Return to the problem

$$ \min_X \left\{ f(X; A, B, C) := \frac{1}{2}(X, AXC) - \langle B, X \rangle \right\}, \text{ subject to } X \in St(n, r) \quad (15) $$
where $C \in \mathbb{R}^{r \times r}$ is a positive definite matrix and $B \in \mathbb{R}^{n \times r}$. To proceed, we adopt standard approaches used in manifold optimization [Man02, AMS08, Bou04]. Introduce two projections $P_M$ and $Proj$ to handle manifold optimization over $\mathcal{M} := St(n, r)$. For each $Y \in \mathbb{R}^{n \times r}$, the polar projection $P_M$ on the manifold $St(n, r)$ is $P_M Y = U_Y V_Y^\top$, where $Y = U_Y D_Y V_Y^\top$ is the reduced SVD of $Y$. Equivalently, the projection can be expressed as

$$P_M Y = (Y^\top Y)^{-1/2} Y.$$

(16)

For each $X \in St(n, r)$, let $X_\perp \in \mathbb{R}^{n \times (n-r)}$ completes the orthonormal basis in $\mathbb{R}^n$ (formed by columns of $X$ and $X_\perp$). The tangent space and the normal space to $St(n, r)$ at $X$ are

$$T_X St(n, r) = \left\{ X\Delta_0 + X_\perp \Delta_1 : \Delta_0 \in \text{Skew}(r), \Delta_1 \in \mathbb{R}^{(n-r) \times r} \right\}, \quad N_X St(n, r) = \left\{ X\Delta_2 : \Delta_2 \in \text{Sym}(r) \right\}.$$

(17)

**Definition 1.** For each $U \in \mathbb{R}^{n \times r}$, define the projection $Proj_X$ on the tangent space $T_X St(n, r)$,

$$Proj_X U = U - X (X^\top U)_{\text{sym}},$$

(18)

where $\Lambda_{\text{sym}} = (\Lambda + \Lambda^\top)/2$ for each $\Lambda \in \mathbb{R}^{r \times r}$.

We analyze the optimal solutions of (15). Regarding $\mathcal{M} = St(n, r)$ as a Riemannian submanifold of $\mathbb{R}^{n \times r}$, for a point $X \in \mathcal{M}$ and a vector $v \in T_X \mathcal{M}$, we introduce the metric projection retraction

$$R_X (v) = \arg\min_{y \in \mathcal{M}} \|X + v - y\|^2 = P_M (X + v),$$

(19)

and construct a retraction curve $c(t) = R_X (tv)$. In the following, if no confusion, we shall write $f(X)$ for $f(X; A, B, C)$. For each tangent vector $v$ at $T_X \mathcal{M}$, $R_X (v)$ is a second-order retraction. Then we have

$$f(R_X (tv)) = f(X) + t \langle \text{grad} f(X), v \rangle + \frac{t^2}{2} \langle \text{Hess} f(X)[v], v \rangle + O(t^3),$$

(20)

where the Riemannian gradient $\text{grad} f$ and the Riemannian Hessian $\text{Hess} f$ are the Euclidean gradient and Hessian followed by the orthogonal projection to tangent spaces.\(^1\)

- For a local optimal solution $X$ in (15), the Riemannian gradient $\text{grad} f$ must vanish, i.e., the Euclidean gradient $\nabla f(X) = AXC - B$ must lie in the normal space to $St(n, r)$ at $X$. This condition is known as the first-order optimal condition.

- Since the Riemannian Hessian is the covariant derivative of the gradient vector,

$$\text{Hess} f(X)[v] = \nabla_v \text{grad} f(X) = \text{Proj}_X \{X\nabla^2 f(X)[v] - v(X^\top \nabla f(X))_{\text{sym}}\}$$

(21)

and

$$\text{Proj}_X \{AvC - v\Lambda_{\text{sym}}\}. \quad \text{(22)}$$

(23)

The second-order condition implies that for all $v \in T_X \mathcal{M}$,

$$\langle v, AvC \rangle - \langle v, v\Lambda_{\text{sym}} \rangle \geq 0.$$  

(24)

**Remark 2.4.** Mathematical models of optimization are generally represented by a constraint set and an objective function. The constraint set consists of the available decisions, which are commonly regarded as vectors. For (1), we may introduce long vectors $\tilde{X} = [x_1^\top, \ldots, x_r^\top]^\top$, $\tilde{B} = [b_1^\top, \ldots, b_r^\top]^\top$ for each $X = [x_1, \ldots, x_r] \in St(n, r)$ and $B = [b_1, \ldots, b_r] \in \mathbb{R}^{n \times r}$. Introduce a multiplier matrix $\Lambda = (\lambda_{i,j}) \in \mathbb{R}^{r \times r}$ for the orthonormal constraints in $St(n, r)$. To solve (1), we form the Lagrangian function $L$,

$$L(\tilde{X}, \lambda_1, \ldots, \lambda_r) := f(X; A, B, C) - \sum_{i=1}^r \sum_{j=1}^r \frac{\lambda_{i,j}}{2} (\langle x_i, x_j \rangle - \delta_{i,j}).$$

(25)

\(^1\)See Prop. 5.44 in [Bou04] for the derivation details.
The Hessian matrix $H_L$ of the Lagrangian function $L$ is

$$H_L := C \otimes A - \Lambda \otimes I_n, \tag{26}$$

where $\otimes$ is the Kronecker product. For each point $X$ in $\text{St}(n,r)$, the gradients of the $r(r+1)/2$ constraints $\{\langle x_i, x_j \rangle = \delta_{ij} : 1 \leq i \leq j \leq r\}$ are independent, thus each point on $\text{St}(n,r)$ is a regular point. For a critical point $\hat{X}$, the first-order necessary condition (chapter 11, [LY16] or chapter 12 [NW06]) can be expressed as

$$H_L \hat{X} = \hat{B}. \quad \text{Equivalently, } AXC = X\Lambda + B \tag{27}$$

holds for some symmetric matrix $\Lambda$. In addition, the condition in (24) is also known as the projected Hessian test (see section 11.6 [LY16]): the Riemannian Hessian $\text{Hess}_f(X)$, which is the projected Hessian matrix to the tangent space is positive semidefinite.

In general, there could exist a lot of critical points $X$ fulfilling the condition in (27). These points are called stationary points (maximizers, minimizers, or saddle points). The quality of these critical points $X$ is directly related to the eigenvalues of the associated matrix $\Lambda C^{-1}$. For completeness, we verify the optimality condition in Prop. 2.5 via a geodesic on $\text{St}(n,r)$. Observe that $\text{St}(n,r)$ is one sub-manifold of $O(n)$. According to (17), we can introduce a differentiable curve $\rho(t)$ passing $X$ on $\text{St}(n,r)$, where $\Delta_1 \in \mathbb{R}^{r \times (n-r)}$ is a nonzero matrix and $\Delta_0 \in \mathbb{R}^{r \times r}$ is a skew-symmetric matrix. Indeed, $\rho(t)^\top \rho(t) = I_r$ holds, i.e., $\rho(t) \in \text{St}(n,r)$ and $\rho(0) = X$, $\rho'(0) = X\Delta_0 + X_\bot \Delta_1$. The following geometric viewpoint indicates that eigenvalues of $\Lambda C^{-1}$ should meet some upper bound conditions at a local minimizer $X$.

**Proposition 2.5.** Let $X \in \text{St}(n,r)$ be a stationary point of (15). Then

$$X \Lambda = AXC - B \tag{29}$$

holds for some symmetric matrix $\Lambda$. In addition, suppose $X$ is a local minimizer in $\text{St}(n,r)$. Let $Y := X\Delta_0 + X_\bot \Delta_1 \in T_X \text{St}(n,r)$, where $[X, X_\bot] \in O(n)$ holds for some matrix $X_\bot \in \mathbb{R}^{n \times (n-r)}$. Then

$$-\langle Y^\top Y, \Lambda \rangle + \langle Y, AYC \rangle \geq 0 \tag{30}$$

holds. Let $d_{\min}^\bot$ be the smallest eigenvalue of $X_\bot^\top AX_\bot$ and let $\gamma_1, \gamma_2, \ldots, \gamma_r$ be eigenvalues of $\Lambda C^{-1}$. Then

$$d_{\min}^\bot \geq \max(\gamma_1, \ldots, \gamma_r). \tag{31}$$

**Proof.** From (28), computation shows

$$\frac{d}{dt} f(X(t)) = \langle \rho'(t), A\rho(t)C \rangle - \langle \rho'(t), B \rangle \tag{32}$$

and

$$\frac{d^2}{dt^2} f(X(t)) = \langle \rho'(t), A\rho'(t)C \rangle + \langle \rho''(t), A\rho(t)C - B \rangle, \tag{33}$$

and

$$\rho'(0) = [X, X_\bot] \Omega_{n,r}, X\Delta_0 + X_\bot \Delta_1, \tag{34}$$

$$\rho''(0) = [X, X_\bot] \Omega^2 I_{n,r} = X(\Delta_0^2 - \Delta_\bot^\top \Delta_1) + X_\bot \Delta_1 \Delta_0. \tag{35}$$

Then $f(\rho(t))$ is a strictly local minimizer at $t = 0$, if and only if the following two optimal conditions hold. First, (32) indicates (29), since

$$\frac{d}{dt} f(\rho(t))|_{t=0} = \langle AXC - B, X\Delta_0 + X_\bot \Delta_1 \rangle = 0 \tag{36}$$

\footnote{Let vec($X$) be the vectorization operator applied on $X$. Kronecker product is one convenient way to express vec($AXC$), i.e., vec($AXC$) = ($A \otimes C$)vec($X$).}
holds for any matrix $\Delta_1$ and any skew-symmetric matrix $\Delta_0$. Second, let $Y := X\Delta_0 + X_\perp \Delta_1$. We should have
\[
\frac{d^2}{dt^2} \langle \rho(t) \rangle |_{t=0} = \langle \rho''(0), A\rho(0)C - B \rangle + \langle \rho'(0), A\rho(0)C \rangle
\]
and
\[
= -\langle Y^\top Y, \Lambda \rangle + (Y, AYC) \geq 0,
\]
where we use the first order condition in (29). Now set $\Delta_0 = 0$ and $\Delta_1 = u_1 u_0^\top C^{-1/2}$, where $u_1$ is a unit eigenvector of $X_\perp^\top AX_\perp$ associated with eigenvalue $d_{\text{min}}^2$ and $u_0$ is a unit eigenvector of $C^{-1/2}AC^{-1/2}$. Then (38) implies (31).

\[\square\]

2.3 Qualified critical points

For our application in (2), we would like to sharpen further the upper bound condition in (31) to identify a global minimizer $X$. The following Prop. 2.6 and Prop. 2.7 together indicate that the multiplier $\Lambda$ associated with a global minimizer $X$ satisfies $\Lambda \preceq d_r C$. Motivated by the observation, we introduce the set: **qualified critical points** defined below. The existence of the qualified critical points is ensured by the existence of the global minimizer.

**Definition 2.** We say that $X$ is a **qualified** critical point of (3), if
\[
AXC = B + X\Lambda, \quad \Lambda \preceq d_r C
\]
hold for some symmetric multiplier matrix $\Lambda$. Equivalently, introduce the eigenvector decomposition,
\[
\Gamma := C^{-1/2}\Lambda C^{-1/2} = U\text{diag}([\gamma_1, \ldots, \gamma_r])U^{-1}
\]
via some orthogonal $U$. The associated eigenvalues $\gamma_i$ of $\Gamma$ in (40) are bounded above by $d_r$.

Before stating Prop. 2.7, we introduce auxiliary variables
\[
Y := X C^{1/2} U = [y_1, \ldots, y_r] \text{ and } B' := B C^{-1/2} U = [b_1, \ldots, b_r].
\]
From (40), we can determine $X$ in (29) from the decoupled system,
\[
AY = B' + Y \text{diag}(\gamma_1, \ldots, \gamma_r), \text{ i.e., } A y_i = b_i + \gamma_i y_i, \quad i = 1, \ldots, r.
\]
First, we shall point out the optimality of each $y_i$ from the perspective of Prop. 2.1. Thanks to the symmetric role of $i$, it suffices to consider the case $i = 1$.

**Proposition 2.6.** Suppose $C > 0$. Suppose $X$ is a global minimizer of (15). Introduce $Y, B'$ and $y_1, b_1$, as in (47). Write $Y = [y_1, y_2, \ldots, y_r] = [y_1, Y_\perp]$. Let $V \in \mathbb{R}^{n \times (n-(r-1))}$ be an isometric matrix, orthogonal to $[y_2, \ldots, y_r]$. Let
\[
C' := Y^\top Y = U^\top C U = \begin{pmatrix} C_{1,1} & C_{1,2} \\ C_{2,1} & C_{2,2} \end{pmatrix}, \quad C_{1,1} \in \mathbb{R}^{1,1}, \quad C_{2,2} \in \mathbb{R}^{(r-1) \times (r-1)}.
\]
Then $y_1$ in (42) is the global minimizer of
\[
\min_{y_1} \left\{ \frac{1}{2} y_1^\top A y_1 - \langle b_1, y_1 \rangle \right\} \quad \text{subject to } \|V^\top y_1\|^2 = C_{1,1} - C_{1,2} C_{2,2}^{-1} C_{2,1}.
\]

**Proof.** Choose $U$ as in (40), so that $\gamma_1$ is the largest eigenvalue of $\Gamma$. First, we shall show the optimality of $Y$. By assumption, $X$ is a global minimizer in (2). Thanks to $\langle Y, B' \rangle = \langle X, B \rangle$, $Y$ is a global minimizer of
\[
\min_Y \left\{ f(Y; A, B', I) = \frac{1}{2} (Y, AY) - \langle Y, B' \rangle \right\} \quad \text{subject to } Y^\top Y = C' := U^\top C U.
\]

7
Indeed, for any $\tilde{Y} \in \mathbb{R}^{n \times r}$ with $\tilde{Y}^\top \tilde{Y} = C'$, construct $\tilde{X} := \tilde{Y} C'^{-1/2} U \in St(n, r)$ from (41). Then
\[ f(\tilde{Y}; A, B', I) = f(\tilde{X}; A, B, C) \geq f(X; A, B, C) = f(Y; A, B', I) \tag{46} \]
verifies the global optimality of $Y$.

Keep $Y_\bot$ fixed and examine the optimality of $y_1$. Write
\[ y_1 = V z + Y_\bot c \tag{47} \]
for some vectors $z \in \mathbb{R}^{n-r+1}$ and $c \in \mathbb{R}^{r-1}$. Note that $Y = [y_1, y_2, \ldots, y_r] = [y_1, Y_\bot]$ satisfies the constraint
\[ [y_1, Y_\bot]^\top [y_1, Y_\bot] = Y^\top Y := C' = \left( \begin{array}{cc} C_{1,1} & C_{1,2} \\ C_{2,1} & C_{2,2} \end{array} \right). \tag{48} \]
Thus, $c$ is actually determined by (48), i.e.,
\[ C_{2,1} = Y_\bot^\top y_1 = Y_\bot^\top Y_\bot c \text{ gives } c = C_{2,2}^{-1} C_{2,1}. \tag{49} \]
Hence, the global optimality of $y_1$ is determined by the global optimality of $z$, which is subject to the norm constraint
\[ \|z\|^2 = \|V^\top y_1\|^2 = \|y_1\|^2 - \|Y_\bot c\|^2 = C_{1,1} - C_{1,2} C_{2,2}^{-1} C_{2,1} > 0. \tag{50} \]

**Proposition 2.7** (Existence of qualified critical points). *Let $X$ be a global minimizer of (3) with multiplier matrix $\Lambda$. Introduce one isometric matrix $V$ as in Prop. 2.6 Then
\[ \gamma_1 \text{ in (40) is a lower bound for the eigenvalues of } V^\top AV. \tag{51} \]

*Proof.* Continue the proof in Prop. 2.6. The $y_1$-minimization problem
\[ \min_{y_1} \left\{ \frac{1}{2} y_1^\top A y_1 - \langle b_1, y_1 \rangle \right\} \text{ subject to } Y^\top Y = C' \tag{52} \]
can be formulated as the $z$-minimization
\[ \min_z \left\{ \frac{1}{2} z^\top V^\top AV z + \frac{1}{2} c^\top Y_\bot^\top AY_\bot c - \langle b_1 - AY_\bot c, Vz \rangle - \langle b_1, Y_\bot c \rangle \right\} \tag{53} \]
subject to the constraint in (50). Introduce a multiplier $\mu$ for the constraint in (50). The optimality condition of $y_1$ is
\[ V^\top AV z + V^\top (AY_\bot c - b_1) - \mu z = 0. \tag{54} \]
According to Prop. 2.1, the optimal $z$ is
\[ z = (V^\top AV - \mu I)^{-1} \{ V^\top (-AY_\bot c + b_1) \} \tag{55} \]
where $\mu$, not greater than the eigenvalues of $V^\top AV$, is chosen to meet the norm condition in (50). Obviously the proof is complete, if we show $\mu = \gamma_1$. Indeed, observe (42) and (54). When $y_1$ satisfies (42), then $\gamma_1$ satisfies
\[ AV z + AY_\bot c = b_1 + \gamma_1(V z + Y_\bot c). \tag{56} \]
Applying $V^\top$ on (56) yields
\[ V^\top AV z = (V^\top b_1 - V^\top AY_\bot c) + \gamma_1 z. \tag{57} \]
Comparing (54) and (57), we have $\mu = \gamma_1$ from $\|z\| > 0$. \qed

By Courant-Fischer min-max theorem (Theorem 4.2.11 [HJ85]), since $V$ has $r$ columns, then $d_r$ is a lower bound for the maximal eigenvalue of $V^\top AV$ in (51). Thus Prop. 2.7 actually implies $\gamma_1 \leq d_r$. In summary, we have the following theorem.
**Theorem 1.** Let $X$ be a global optimal solution of $f(X; A, B, C)$ and let $\Lambda$ be its associated multiplier, 
\[ \Lambda = X^\top (AXC - B). \] 
Then $(X, \Lambda)$ is qualified, i.e., it satisfies the first-order condition, 
\[ AXC = B + X\Lambda, \] 
and the second-order condition, 
\[ \Lambda \succeq d_r C. \]

2.4 Global optimal minimizers

2.4.1 Optimality in regularized problems

On the other hand, a qualified critical point is not necessarily a global minimizer. The following illustrates that a qualified critical point $X$ in (2) fulfilling a tighter condition in (62) is a global minimizer.

**Proposition 2.8 (Global solutions).** Let $d_1$ be the smallest eigenvalue of $A$. Let $X'$ be a stationary point of 
\[ \min_X f(X; A, B, C) \text{ subject to } X \in St(n, r). \] 
Let $\Lambda'$ be the associated multiplier matrix in (27). Suppose 
\[ d_1 C \succeq \Lambda'. \] 
Then $X'$ is a global minimizer. In addition, suppose 
\[ d_1 C \succ \Lambda'. \] 
Then $X'$ is the unique global minimizer.

**Proof.** For $\Lambda' \in \mathbb{R}^{r \times r}$ and $X \in St(n, r)$, let 
\[ \mathcal{L}(X, \Lambda') := \frac{1}{2} \langle X, AXC \rangle - \langle B, X \rangle - \frac{1}{2} \langle \Lambda', X^\top X - I \rangle. \] 
Reformulate (63) in terms of Taylor series of $X - X'$ around $X'$:

\[ f(X) = \mathcal{L}(X, \Lambda') \]
\[ = \mathcal{L}(X', \Lambda') + \frac{1}{2} \{ \langle (X - X'), A(X - X')C \rangle - \langle (X - X'), (X - X')\Lambda' \rangle \}, \]
\[ \geq \mathcal{L}(X', \Lambda') + \frac{1}{2} \langle (X - X')^\top (X - X'), d_1 C - \Lambda' \rangle \geq f(X'), \]
where the linear term is dropped due to (29). Since $\Lambda'$ satisfies $d_1 C \succeq \Lambda'$, then (64) implies that 
\[ f(X) = \mathcal{L}(X, \Lambda') \geq \mathcal{L}(X', \Lambda') = f(X') \]
for each $X \in St(n, r)$, i.e., $X'$ is a global minimizer. On the other hand, suppose $f(X) = f(X')$ holds for some $X \in St(n, r)$. The condition $d_1 C \succ \Lambda'$ implies the uniqueness from $(X - X')^\top (X - X') = 0$. \qed

When $C = I$, the sufficient condition for a global minimizer was reported in Theorem 4.1 [ZQD07], where authors studied the unbalanced Procrustes problem. Generally, when $d_1 \neq d_\gamma$, the condition in (62) could be too strict to be fulfilled for any critical points. To proceed, we consider approximate “regularized” models, where the eigenvalues of the system matrix are adjusted (lifted), $A \rightarrow \tilde{A}$. Under the circumstance, since the conditions in (62,60) coincide, Prop. 2.8 implies that a qualified critical point is automatically a global minimizer.

**Theorem 2.** Consider the regularized problem in (5). A qualified critical point is one global solution.
2.4.2 When does a qualified critical point become a global minimizer in (2)?

In addition to Theorem 2, we further list a few more cases, where we can identify which qualified critical point is a global minimizer. The first case is $A = d_1 I_n$. Then (2) reduces to

$$\min_X \left\{ f(X) = \frac{d_1}{2} r(C) - \langle X, B \rangle \right\}.$$ 

The minimizer $X$ is the polar projection of $B$ on $\text{St}(n, r)$, i.e., (16). The second case is that $B = V_g V_g^T B$ and $C = I$. The global minimizer is also $X = P_M B$.

**Proposition 2.9.** Suppose $C = I$. Assume the reduced SVD: $B = U_B D_B V_g^T$ with rank $r$. Suppose left singular vectors of $B$ lie in the column space of $V_g$, i.e., $U_B = \text{span}\{ V_g \}$. Then a global minimizer $X$ in (2) is

$$X = U_B V_g^T = P_M B.$$ 

In this situation, $X^T B$ is symmetric and positive semidefinite, and $\gamma_j \leq d_j$ for $j = 1, \ldots, r$.

**Proof.** The objective $f$ has a lower bound: for any $X \in \text{St}(n, r)$,

$$f(X; A, B, I) \geq \frac{1}{2} (d_1 + \ldots + d_r) - \|B\|_*,$$ 

where $\|B\|_*$ is the nuclear norm, i.e., the sum of singular values of $B$. Note that the lower bound in (77) is reached at $X = V_g V_g^T$, which verifies the optimality of $X$. In addition, $\Lambda$ satisfies

$$\Lambda = X^T AX - X^T B = V_B (Q_B \text{diag}([d_1, \ldots, d_r]) Q_B - D_B) V_g^T.$$ 

Since the diagonal of $D_B$ is nonnegative, then $\gamma_j \leq d_j$ for all $j = 1, \ldots, r$.

**Definition 3.** Let $\sigma$ be the smallest singular value of $V_g^T B C^{-1}$. Suppose $\sigma > 0$. The problem in (2) is said to be non-degenerate.

Motivated by the second case, we propose one non-degenerate condition on $V_g^T B$ to fill the gap between (62) and (60). The following safeguard estimate shows that when the projection of $B$ on $V_g$ is sufficiently large, compared with the spectral gap $d_r - d_1$, then any qualified critical point $X$ will be a global minimizer in (15).

**Proposition 2.10 (Safeguard estimate).** Let $V_g = [v_1, v_2, \ldots, v_r] \in \mathbb{R}^{n \times r}$ be the ground eigenvector matrix. Let $(X, \Lambda)$ be a qualified critical point. Let $\sigma$ be the smallest singular value of $V_g^T B C^{-1}$. Then

$$d_r - \gamma_j \geq \sigma$$ 

for $j = 1, \ldots, r$. (70)

In addition, suppose

$$\sigma > d_r - d_1.$$ 

(71)

Then all eigenvalues $\gamma_1, \ldots, \gamma_r$ of multiplier matrix $\Lambda C^{-1}$ are less than $d_1$. Thus, $X$ is one global minimizer.

**Proof.** Start with the first-order condition $AX = X \Lambda C^{-1} + BC^{-1}$. Let $u_j$ be a unit eigenvector of $\Lambda C^{-1}$ corresponding to eigenvalue $\gamma_j$. Taking the product of the first order condition with $u_j$ and $v_i$ from the right and left-hand sides yields

$$d_i v_i^T X u_j = v_i^T A X u_j = (v_i^T X) \Lambda C^{-1} u_j + v_i^T B C^{-1} u_j,$$ 

which implies

$$(d_i - \gamma_j) v_i^T X u_j = v_i^T B C^{-1} u_j.$$ 

(73)

From Prop. 2.7, the second-order condition of $X$ indicates

$$\gamma_j \leq d_r$$ 

for $j = 1, 2, \ldots, r$. (74)
Note that \( \|V_g\|_2 = 1 = \|X\|_2 \), then \( \|V_g^T X u_j\| \leq \|X u_j\| \leq 1 \). Since \( |v_i^T B C^{-1} u_j| \) is bounded below by the smallest singular value of \( V_g^T B C^{-1} \), then with \( i = r \),

\[
d_r - \gamma_j \geq (d_r - \gamma_j)|v_i^T X u_j| = |v_i^T B C^{-1} u_j| \geq \sigma. \tag{75}
\]

From \( \frac{71}{74} \), we have \( \gamma_j < d_1 \) for each \( j = 1, \ldots, r \).

### 2.4.3 Initialization in SSM

The following proposition will be used in the initialization of \( X \) and \( \Lambda \) in SSM. Let \( V \) be an isometric matrix, \( V \in \text{St}(l, r) \), \( n > l \geq r \). Let \( S \) be the induced subspace, \( S = \{V \overline{X} : \overline{X} \in \text{St}(l, r)\} \). Consider the subspace-restricted regularized problem,

\[
\min_{\overline{X}} \{f(X; \tilde{A}, B, C) : X = V \overline{X} \in S, X \in \text{St}(n, r)\} = \min_{\overline{X}} \{f(X; V^T A \overline{V}, V^T B, C) : \overline{X} \in \text{St}(l, r)\}. \tag{76}
\]

Here, the objective in \( \frac{76}{76} \) is one surrogate model for \( f(X; A, B, C) \) thanks to \( \tilde{A} \succeq A \). On the other hand, the objective has one lower bound: for any \( X \in \text{St}(n, r) \),

\[
f(X; \tilde{A}, B, C) \geq \frac{1}{2} (\text{tr}(C) d_r) - \|B\|. \tag{77}
\]

The lower bound is attained, if columns of \( B \) lie in \( V_g \) and \( X = P_M B \).

**Proposition 2.11** (Initialization). Consider \( V = V_g \) in \( \frac{76}{76} \), i.e., the approximate regularized problem

\[
\min_{X} \{f(X; \tilde{A}, V_g V_g^T B, C) : X \in \text{St}(n, r)\}. \tag{78}
\]

Then \( X = P_M B \) is a global minimizer and the associated multiplier \( \Lambda = X^T (\tilde{A} X C - V_g V_g^T B) \) satisfies \( \Lambda \preceq d_r C \).

**Proof.** Let \( X = V_g Q \), where \( Q \) is one orthogonal matrix, which maximizes \( \langle Q, V_g^T B \rangle \). Since the lower bound in \( \frac{77}{77} \) is reached, we have the optimality of \( X \). Note that

\[
\Lambda = X^T (\tilde{A} X C - B) = d_r C - Q^T V_g^T B \tag{79}
\]

is symmetric. Hence, \( \Lambda \) can be expressed as the difference between two Hermitian matrices, and by Weyl's inequality, the proof is complete.

### 2.4.4 Degeneracy of regularized problems

The optimality condition in the degenerate case can be complicated. When \( V_g^T B \) becomes singular, multiple qualified minimizers \( X \) can exist. Here we briefly mention one case, where singular values of \( V_g^T B C^{-1} \) are all zero.

**Proposition 2.12.** Consider the regularized problem in \( \frac{3}{3} \). Suppose \( V_g^T B C^{-1} = 0 \) and the spectral norm bound holds:

\[
\|(\tilde{A} - d_1 I)^\dagger (BC^{-1})\|_2 \leq 1. \tag{80}
\]

Then there exists some \( U \in \mathbb{R}^{r \times r} \), such that a global solution \( X \) exists in the form of

\[
X = V_g U + (\tilde{A} - d_1 I)^\dagger BC^{-1}. \tag{81}
\]

In this case, the multiplier is \( \Lambda = d_1 C \).

**Proof.** We shall construct a global solution \( X \) with \( \Lambda C^{-1} = d_1 I_r \), i.e., \( \gamma_1 = \gamma_2 = \ldots = \gamma_r = d_1 \). The first-order condition in \( \frac{27}{27} \) indicates

\[
(\tilde{A} - d_1 I)X = BC^{-1}. \tag{82}
\]
Under some matrix $U \in \mathbb{R}^{r \times r}$, \[82\] has a solution (due to eigenvalue $d_1$)

$$X = V_g U + (\bar{A} - d_1 I)^\dagger BC^{-1}. \quad (83)$$

From \[83\], to meet the condition $X \in St(n, r)$, we need

$$I = X^\top X = U^\top U + C^{-1} B^\top ((\bar{A} - d_1 I)^\dagger )^\top (\bar{A} - d_1 I)^\dagger BC^{-1}. \quad (84)$$

Here, the existence of $U$ is ensured (e.g., by Cholesky decomposition), thanks to \[80\]. Indeed, we can solve $U$ from \[84\]. The optimal $X$ is given by \[83\]. \hfill \Box

Conversely, the following indicates that the full rank of $V_g^\top B$ ensures $\gamma_k < d_1$ for $k = 1, \ldots, r$.

**Proposition 2.13.** Consider a qualified critical point $X$ to the regularized problem

$$\min_X f(X; \bar{A}, B, C). \quad (85)$$

Suppose $V_g^\top B \in \mathbb{R}^{r \times r}$ has rank $k$ with $0 \leq k < r$. Then at least $k$ eigenvalues $\gamma_1, \ldots, \gamma_k$ of $\Gamma$ are less than $d_1$.

**Proof.** We prove it by contradiction. Suppose $\gamma_k = d_1$ for the eigenvalues $\gamma_1 \leq \ldots \leq \gamma_r$. Since $X$ is a qualified critical point, then $\gamma_k = \gamma_{k+1} = \ldots = \gamma_r = d_1$. The first-order condition implies that for $j = k, \ldots, r$,

$$(\bar{A} - d_1 I)x_j = b_j, \text{ i.e., } V_g^\top (\bar{A} - d_1 I)x_j = V_g^\top b_j = 0. \quad (86)$$

Thus, $V_g^\top BC^{-1}$, which has at least $r - k + 1$ zero columns, has rank at most $k - 1$. The contradiction completes the proof. \hfill \Box

Readers should be aware of the non-uniqueness of the global minimizers from the non-uniqueness of $U$ in \[82\]. Finally, we provide one toy example, which demonstrates the existence of multiple qualified minimizers under the small $B$ compared with the spectral gap. Roughly, computing a global minimizer becomes challenging under a small norm of $B$.

**Example 2.14.** Consider the problem in \[15\],

$$A = \begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix}, \quad B = \begin{bmatrix} \delta_1 & 0 \\ 0 & \delta_2 \\ 0 & 0 \end{bmatrix}, \quad C = I_2, \quad (87)$$

with $\delta_1 > 0$, $\delta_2 > 0$ and $d_1 < d_2 < d_3$. Examine the following two critical points on $St(n, r)$:

$$X = X_1 = [e_1, e_2], \text{ and } X = X_2 = [-e_1, e_2]. \quad (88)$$

We have $f(X_1) < f(X_2)$, since

$$f(X_1) = (d_1 + d_2)/2 - (\delta_1 + \delta_2), \quad f(X_2) = (d_1 + d_2)/2 - (-\delta_1 + \delta_2). \quad (89)$$

The associated multiplier matrices are $\Lambda = X^\top AX - X^\top B$,

$$\Lambda = \Lambda_1 = \text{diag}(d_1 - \delta_1, d_2 - \delta_2), \quad \Lambda = \Lambda_2 = \text{diag}(d_1 + \delta_1, d_2 - \delta_2). \quad (90)$$

From \[17\], the tangent space $T_X St(n, r)$ for $X = X_1$ or $X = X_2$ has a set of basis vectors,

$$v_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad v_2 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad v_3 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix}. \quad (91)$$
From (24), the corresponding Riemannian Hessians $H_1, H_2$ can be expressed in terms of basis $\{v_1, v_2, v_3\}$,

$$
H_1 = \begin{bmatrix}
\frac{\delta_1 + \delta_2}{2} & 0 & 0 \\
0 & d_3 - d_1 + \delta_1 & 0 \\
0 & 0 & d_3 - d_2 + \delta_2
\end{bmatrix}, \quad H_2 = \begin{bmatrix}
\frac{\delta_1 - \delta_2}{2} & 0 & 0 \\
0 & d_3 - d_1 - \delta_1 & 0 \\
0 & 0 & d_3 - d_2 + \delta_2
\end{bmatrix}.
$$

(92)

Since $X_1 = \mathcal{P}_M B$, from Prop. 2.9, $X_1$ is the global minimizer, and also a qualified critical point. On the other hand, the optimality of $X_2$ can vary, depending on the choices of $\delta_1, \delta_2$.

- When $\delta_1 \in (0, d_2 - d_1)$, then $X_2$ is a qualified critical point. When $\delta_1 > d_2 - d_1$, $X_2$ is no longer a qualified critical point.
- $X_2$ is a local minimizer, when $\delta_1 \in (0, d_3 - d_1)$ and $\delta_2 \in (0, \delta_1)$, i.e., $H_2$ is positive definite.

### 3 Algorithms

#### 3.1 Gradient projection methods

Projected gradient methods or gradient methods with retractions can be used to reach a local solution of (2).

- Note that when $Y \in T_X M$ and $X \in St(n, r)$, $X + Y$ has singular values all not less than 1, i.e., eigenvalues of $(X + Y)^\top (X + Y) = I + Y^\top Y$ are not less than 1. Hence, the metric retraction $\mathcal{R}_X(Y)$ is actually the projection of $X + Y$ on the convex hull of $St(n, r)$. Since the Euclidean gradient of $f$ is given by $\nabla f = \nabla f(X) = AXC - B$, we can use the standard gradient projection method, i.e., the iterations

$$
X^{(k+1)} = \mathcal{P}_M(X_k - \alpha(AX_k C - B)), \quad k = 1, 2, \ldots,
$$

with proper step size $\alpha > 0$. The convergence analysis under the Armijo rule can be found in Prop. 2.3.3 [Ber16].

- The Riemannian gradient descent method is one standard method to solve (2) numerically. Gradient projected on $St(n, r)$, the gradient vector at $X$ is given by

$$
\text{grad } f(X) = \text{Proj}_X [AXC - B] = (AXC - B) - X\Lambda_{sym},
$$

(94)

(95)

where $\Lambda = X^\top (AXC - B)$. The Riemannian gradient descent is

$$
X_{k+1} = \mathcal{R}_{X_k}(-\alpha_k \text{grad } f(X_k));
$$

(96)

For the gradient method with the Armijo rule, the convergence to a stationary point is verified in Theorem 4.3.1 [AMS08] or Cor. 4.13 [Bou04].

- When $X_k$ is near a critical point, we can use the Newton method to speed up the convergence,

$$
X_{k+1} = \mathcal{R}_{X_k}(\alpha_k Z);
$$

(97)

where the Newton direction $Z \in \mathbb{R}^{n \times r}$ is computed from

$$
\text{Hess } f(X)[Z] = -\text{grad } f(X),
$$

(98)

The right-hand side is

$$
\text{grad } f(X) = \text{Proj}_X (\nabla f(X)) = AXC - B - X\Lambda_{sym}, \quad \Lambda = X^\top (AXC - B)
$$

(99)

(100)
and the left-hand side (the calculation is based on (7.29), (7.39) in [Bou04]) is

\[
\text{Hess } f(X)[Z] = \text{Proj } X \{\nabla^2 f(X)[Z] - Z( X^\top \nabla f(X))_{\text{sym}} \} \quad (101)
\]

\[
= \text{Proj } X \{AZC - ZA_{\text{sym}}\}. \quad (102)
\]

From the perspective of optimization, the scheme can be viewed as one local SQP (Sequential quadratic programming. See section 18.1 [NW06]). Hence, when \( X_k \) is quite far from a critical point, the system in (103) is not positive definite and the computation of \( Z \) can be ineffective. In particular, \( Z \) can not be a descent direction. In the next section, we shall propose the determination of \( \Lambda \) in regularized problems to overcome this issue.

### 3.2 Sequential subspace methods (SSM)

Manifold optimization requires many retractions in each step length determination, which can be time-consuming if \( n \gg r \). Sequential subspace methods have been proposed to solve the sphere minimization in (10) [HP05], where the retractions are conducted in a small dimensional problem. The reduction of the computational complexity is one apparent advantage of SSM, when handling large-scale problems. In this section, we generalize the framework to solve the \( St(n, r) \)-minimization, stated in (2).

For a general smooth function \( f \) on \( St(n, r) \), the idea of SSM is to introduce/find proper isometric matrices \( V \in St(n, l) \) with \( r < l < n \) to express \( X = V \tilde{X} \) with \( \tilde{X} \in St(l, r) \), and convert the original problem as a low dimensional problem (i.e., on \( St(l, r) \)),

\[
\min_{\tilde{X}} \{ \tilde{f}(\tilde{X}) := f(V \tilde{X}) \}. \quad (103)
\]

For (2), we have

\[
\min_{X \in St(n, r)} f(X; A, B, C) = \min_V \min_{X \in St(n, r)} \{ f(V^\top X; V^\top AV, V^\top B, C) : V^\top V = I, \, V \in \mathbb{R}^{n \times 4r} \}. \quad (104)
\]

The matrix \( V \) can be regarded as one descriptor of one subspace \( S_k \) of the \( n \times r \) matrices, whose columns are spanned by

- column vectors of \( V_0^r \): the ground eigenvectors \( \{v_1, v_2, \ldots , v_r\} \) of \( A \) corresponding to the smallest eigenvalues \( d_1, \ldots , d_r \),

- column vectors of \( X_k \),

- column vectors of \( \text{SQP direction} \, Z_k \) (the computation is deferred in section 3.4.2),

- column vectors of \( \text{gradient } \nabla f(X_k) = AX_k C - B \) of the cost function at \( X_k \).

In other words, we compute an approximate solution \( X_{k+1} \) from the low dimensional space

\[
S_k = \{ [V_g, X_k, AX_k C - B, Z_k] S : S \in \mathbb{R}^{4r \times r} \} \subset \mathbb{R}^{n \times r}. \quad (105)
\]

Expressing \( S \) as \( S = [S_1^T, S_2^T, S_3^T, S_4^T]^T \), we have \( S_k = \{ V_g S_1 + X_k S_2 + (AX_k C - B) S_3 + Z_k S_4 : S_1, S_2, S_3, S_4 \in \mathbb{R}^{r \times r} \} \). If no confusion, we shall write \( S_k = \text{span} \{ V_g, X_k, AX_k C - B, Z_k \} \).

As a “basis” of the subspace \( S_k \), we use one isometric matrix \( V = V_k \), from the qr-factroization of \([V_g, X_k, AX_k C - B, Z_k]\) to express each \( X \in St(n, r) \) \( \cap S_k \) as \( X = V_k \tilde{X} \) for some \( \tilde{X} \in St(4r, r) \). From (104), we can determine \( X_{k+1} \) from the SSM core problem,

\[
\min_{X \in St(n,r) \cap S_k} f(X) = \min_{\tilde{X} \in St(4r,r)} f(\tilde{X}; V_k AV_k^\top, V_k^\top B, C). \quad (106)
\]

That is, for each \( V_k \), we introduce

\[
A_k := V_k^\top AV_k, \quad B_k := V_k^\top B. \quad (107)
\]
Figure 1: Illustration of surrogate models \( f_k(X) \) of \( f(X; A, B, C) \), where \( f_k(X) \) in (113) is constructed from the tangent point \( X_k \). The minimizer \( X_{k+1} \) of \( \min_X \{ f_k(X) : X \in S_k \} \) provides one estimate for the minimizer of \( \min_X f(X; A, B, C) \).

Then \( X_{k+1} = V_k \tilde{X}_k \in \mathbb{R}^{d_k \times r} \), where \( \tilde{X} = \tilde{X}_k \) is one local solution,

\[
\tilde{X}_k := \arg\min_{X \in \mathbb{R}^{d_k \times r}} f(\tilde{X}; A_k, B_k, C).
\] (108)

The sequence \( \{ f(X_k) \} \) monotonically decreases with respect to \( k \). Indeed, the monotonic property is the result of the computation:

\[
f(X_{k+1}) = \frac{1}{2} \langle X_{k+1}, AX_{k+1}C - 2B \rangle \]
\[
\leq \min_X \left\{ \frac{1}{2} \langle V_k \tilde{X}, AV_k \tilde{X}C - 2B \rangle = \frac{1}{2} \langle \tilde{X}, A_k \tilde{X}C - 2B_k \rangle \right\} \]
\[
\leq \frac{1}{2} \langle X_k, AX_kC - 2B \rangle = f(X_k). \] (111)

### 3.3 Regularized surrogate models

To accelerate the convergence of SSM, we include some Newton direction in the subspace selection of \( S_k \). However, when the Hessian matrix in (102) is not positive semidefinite, the Newton step is not a descent direction. To bypass the difficulty, we replace the objective \( f \) in (104) by a surrogate regularized model as shown in (113). The advantages are twofold. First, according to Cor. 2 its qualified critical point is automatically a global minimizer. Second, the computed qualified multiplier ensures that we can use conjugate gradient methods to compute a Newton step, which is automatically a descent direction.

Prop. 3.1 describes the design of a surrogate regularized model. As shown in Fig. 1.3 for each \( k \), we construct a surrogate model \( \{ f_k(X) : X \in S_k \} \), which is tangent to \( f \) at \( X_k \), i.e.,

\[
f_k(X) := f(X; A, B_k, C) + \text{constant} \geq f(X; A, B, C),
\] (112)

where \( B_k \) is given by (113). Then compute its minimizer \( X_{k+1} \).

**Proposition 3.1** (Convergence of SSM). Let \( D := \tilde{A} - A \succeq 0 \) and \( C \succ 0 \). At each base point \( X_k \in St(n, r) \), introduce one surrogate model \( f_k(X) \) of \( f(X; A, B, C) \),

\[
f_k(X) := \frac{1}{2} \langle X, \tilde{A}XC \rangle - \langle X, B_k \rangle + \frac{1}{2} \langle X, DX_kC \rangle, \quad \text{with} \ B_k = B + DX_kC.
\] (113)
Let $X_{k+1}$ be one global minimizer of the regularized problem

$$
\min_X \{ f_k(X) : X \in St(n, r) \cap S \}, \quad \text{where} \quad S = \text{span}\{ X_k, AX_k C - B \}.
$$

(114)

If $X_k$ is not a stationary point, then

$$
f_k(X_{k+1}) \leq f_k(X_{k+1}) = \min_{X \in St(n, r) \cap S} f_k(X) < f_k(X_k) = f(X_k).
$$

(115)

**Proof.** Claim: For each $k$, we have

$$
f_k(X) \geq f(X; A, B, C), \quad f_k(X_k) = f(X_k; A, B, C).
$$

(116)

Indeed, for each $X = X_k$ in $St(n, r)$ with $C > 0$, we have the monotonicity,

$$
2f_k(X) := \langle X, AX(C) \rangle - 2\langle X, B + DX_k C \rangle + \langle X, DX_k C \rangle \geq 2f(X; A, B, C).
$$

Hence,

$$
f_k(X_k; A, B, C) = f_k(X_k) \geq f_k(X_{k+1}) \geq f(X_{k+1}; A, B, C).
$$

Suppose $X_k$ is not a stationary point. Since $\nabla f(X_k) = \nabla f_k(X_k)$, then

$$
g := \text{grad } f_k(X_k) = \text{grad } f(X_k) = AX_k C - B - X_k \Lambda_k
$$

(122)

does not vanish, where $\Lambda_k = (X_k^T (AX_k C - B))_{\text{sym}}$. Note that $g \in S$. Define $c(\alpha) := R_{X_k}(-\alpha g)$. Then

$$
\frac{d}{d\alpha} f(c(\alpha)) = \langle AX_k C - B, \frac{dc(\alpha)}{d\alpha} \rangle = -\langle AX_k C - B, g \rangle = -\|g\|^2 \neq 0.
$$

(123)

Hence, for positive $\alpha$ near 0, we have $f_k(c(\alpha)) < f_k(c(0)) = f_k(X_k)$, which implies (115).

\[ \Box \]

Prop. 3.2 shows that the solutions to these regularized problems converge to one qualified critical point of the original problem in $\textbf{2}$. Due to the difference $A - \tilde{A}$, the adjustment $B \rightarrow B_k$ is introduced to ensure the gradient condition:

$$
AX_k C - B = \tilde{A}X_k C - B_k, \quad \text{i.e.,} \quad B_k = B + (\tilde{A} - A)X_k C.
$$

(124)

This difference also induces the difference of two multipliers. At the updated base point $X_{k+1}$, the multiplier $\Lambda_{k+1}$ associated with $f_k$ is different from the multiplier $\tilde{\Lambda}_{k+1}$ associated with $f$. That is, from [124] and

$$
\tilde{\Lambda}_{k+1} = X_{k+1}^T (AX_{k+1} C + B), \quad \Lambda_{k+1} = X_{k+1}^T (\tilde{A}X_{k+1} C + B_k),
$$

(125)

we have

$$
\tilde{\Lambda}_{k+1} - \Lambda_{k+1} = X_{k+1}^T (DX_{k+1} C - (B_k - B)) = X_{k+1}^T D(AX_{k+1} - X_k) C.
$$

(126)

**Proposition 3.2.** For each $k$, let $X_{k+1}$ be a solution to the regularized problem in (114) with the associated multiplier $\Lambda_{k+1}$,

$$
\Lambda_{k+1} = X_{k+1}^T (\tilde{A}X_{k+1} C + B_k).
$$

(127)

Let $g_k = \text{grad } f_k(X_k; A, B, C)$. Then $\lim_{k \rightarrow \infty} g_k = 0$. Suppose in addition $V_k^T B C^{-1}$ is nonsingular. Let $(X_*, \Lambda_*)$ be a limit point of $\{(X_k, \Lambda_k) : k\}$. Then $X_*$ is a qualified critical point of $\min_X f(X; A, B, C)$.

**Proof.** Introduce a curve $c(\alpha) = R_{X_k}(\alpha s)$ on $St(n, r) \cap S$ with $s = -\|g_k\|^{-1}g_k$. The Taylor expansion around $X_k$ yields

$$
f_k(R_{X_k}(\alpha s)) = f_k(X_k) + \langle \text{grad } f_k(X_k), \alpha s \rangle + \frac{1}{2} \langle \text{Hess } f_k(X_k)[\alpha s], \alpha s \rangle + o(\alpha^2).
$$

(128)
Thanks to [113, 127], \( \|B_k\| \) and \( \|\Lambda_k\| \) are bounded above on \( St(n, r) \). Then \( \|\text{Hess} f_k(X)\| \) is bounded above on \( St(n, r) \). Hence, we can find some constant \( M > 0 \), such that

\[
f(X_{k+1}) \leq f_k(X_{k+1}) \leq f_k(X_k) - \|g_k\|\alpha + \frac{1}{2}M\alpha^2 = f(X_k) - \|g_k\|\alpha + \frac{1}{2}M\alpha^2 
\]  

(129)

whenever \( \alpha \in [0, 0.5] \). Since \( \|g_k\| \) is bounded over all choices of \( X \in St(n, r) \), we can choose \( M \) sufficiently large to ensure that \( \|g_k\|/M \leq 0.5 \). Take \( \alpha = \|g_k\|/M \) in (129), and we have \( f(X_{k+1}) \leq f(X_k) - \|g_k\|^2/(2M) \). Thus, \( \lim_{k \to \infty} \|g_k\| = 0 \) holds according to

\[
f(X_{k+1}) \leq f(X_1) - \sum_{j=1}^k \|g_j\|^2/(2M). 
\]  

(130)

By assumption, \( V_g^TBC^{-1} \) is nonsingular. From Prop. 2.10, \( d_r - \gamma_j \geq \sigma \) holds for some \( \sigma > 0 \). Expanding \( f_k \) around \( X_k \), we have for each \( X \in St(n, r) \cap \mathcal{S} \),

\[
f_k(X) = f_k(X_k) + \langle X - X_k, g_k \rangle + \frac{1}{2}\langle X - X_k, \text{Hess} f_k(X) [X - X_k] \rangle. 
\]  

(131)

Hence,

\[
\frac{\sigma}{2} \|X_{k+1} - X_k\|^2 \leq f_k(X_{k+1}) - f_k(X_k) - \langle X_{k+1} - X_k, g_k \rangle \leq \|g_k\| \|X_{k+1} - X_k\|. 
\]  

(132)

Together with \( \lim_{k \to \infty} g_k = 0 \), we have \( \lim_{k \to \infty} \|X_{k+1} - X_k\| = 0 \). Finally, observe that as \( k \to \infty \),

\[
\hat{\Lambda}_{k+1} - \Lambda_{k+1} = X_{k+1}^T(DX_{k+1} - (B_k - B)) = X_{k+1}^T(D(X_{k+1} - X_k)C) \to 0. 
\]  

(133)

For each \( k \), the global optimality of \( X_{k+1} \) ensures \( \hat{\Lambda}_{k+1} \leq d_r C \). Together with (133), the limit \( \hat{\Lambda}_* \) of \( \{\hat{\Lambda}_{k+1}\} \) satisfies \( \hat{\Lambda}_* = \Lambda_* \leq d_r C \).

3.4 Subspace selection in \( \mathcal{S} \)

We shall examine the solution quality of each regularized problem

\[
\min_{X \in \mathcal{S} \cap St(n, r)} \left\{ f_k(X) = f_k(X; \tilde{\Lambda}_k B_k, C) + \frac{1}{2}\langle X, (\tilde{\Lambda}_k - \Lambda)X_kC \rangle \right\} 
\]  

(134)

under the subspace selection \( \mathcal{S} \). Similar to (106), let

\[
\tilde{\Lambda}_k = V_k^T \tilde{\Lambda} V_k, \tilde{B}_k = V_k^T B_k. 
\]  

(135)

The update of the base point is given by \( X_{k+1} = V_k \tilde{X} \) in (134), where \( \tilde{X} \) is the solution to

\[
\min_{\tilde{X}} \left\{ f(\tilde{X}; \tilde{\Lambda}_k, \tilde{B}_k, C) : \tilde{X} \in St(4r, r) \right\}. 
\]  

(136)

The problem in (136) is called the SSM core problem.

3.4.1 \( V_g \) in \( \mathcal{S} \)

**Proposition 3.3.** Suppose \( \tilde{X} \) is a stationary point of (134) and \( \tilde{X} \) is not a global minimizer. For \( \mathcal{S} = \text{span}\{V_g, \tilde{X}\} \), i.e., \( \mathcal{S} = \{V_gU_1 + \tilde{X}U_2 : U_1 \in \mathbb{R}^{r \times r}, U_2 \in \mathbb{R}^{r \times r}\} \), we have

\[
\min_{X \in \mathcal{S} \cap St(n, r)} f_k(X) \leq f_k(\tilde{X}). 
\]  

(137)

**Proof.** Let \( \hat{\Lambda} \) be the multiplier associated with the stationary point \( \tilde{X} \). Then

\[
f_k(X) = f_k(\tilde{X}) + \frac{1}{2}\langle (X - \tilde{X}), \hat{\Lambda}(X - \tilde{X})C \rangle - \frac{1}{2}\langle (X - \tilde{X})\hat{\Lambda}_*, (X - \tilde{X}) \rangle. 
\]  

(138)
Claim: Suppose $\bar{A}C^{-1}$ has at least one eigenvalue $\gamma_1$ larger than $d_r$. Then $\bar{X}$ is not a global minimizer. Indeed, there exists one orthogonal eigenvector matrix $U$, so that
\begin{equation}
\Gamma := U^T C^{-1/2} \bar{A}C^{-1/2} U = \text{diag}(\gamma_1, \ldots, \gamma_r)
\end{equation}
holds. Let
\begin{equation}
\bar{Y} = \bar{X} C^{1/2} U = [\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_r].
\end{equation}
Since $V_g$ has rank $r$, we may choose one unit vector $v_1$ in the column space of $V_g$, which is orthogonal to $\bar{y}_2, \ldots, \bar{y}_r$. Starting with $v_1$, we construct a set of unit orthogonal bases $\{v_1, v_2, \ldots, v_n\}$ of the column space of $V_g$. Together with the eigenvectors $\{v_{r+1}, \ldots, v_n\}$ of $A$, we have a set of unit orthogonal basis $\{v_1, \ldots, v_n\}$ in $\mathbb{R}^n$. We can express $\bar{y}_1 = \sum_{j=1}^n \xi_j v_j$ for some scalars $\xi_j$.

Suppose $\xi_1 \neq 0$. Take $Y = X C^{1/2} U = [\bar{y}_1, \bar{y}_2, \ldots, \bar{y}_r]$ with
\begin{equation}
y_1 = \bar{y}_1 - 2\xi_1 v_1 = -\xi_1 v_1 + \sum_{j=2}^n \xi_j v_j.
\end{equation}
The transformation $\bar{Y} \rightarrow Y$ can be regarded as one Householder reflection about the hyperplane orthogonal to $v_1 e^T_1$, where $e_1 = [1, 0, \ldots, 0]^T \in \mathbb{R}^r$. Clearly, $X \in \text{St}(n, r)$, since
\begin{equation}
X^T X = (Y^T C^{-1/2})^T (Y U^T C^{-1/2}) = (Y U^T C^{-1/2})^T (Y U^T C^{-1/2}) = X^T \bar{X} = I,
\end{equation}
where we used
\begin{equation}
Y^T Y = (Y - 2\xi_1 v_1 e^T_1)^T (Y - 2\xi_1 v_1 e^T_1) = Y^T \bar{Y}.
\end{equation}
Observe that $X - \bar{X} = (Y - \bar{Y}) U C^{-1/2} = -2\xi_1 v_1 e^T_1 U^T C^{-1/2}$ implies (137), since
\begin{equation}
f_k(X) - f_k(\bar{X}) = \frac{1}{2} \langle (X - \bar{X}), \tilde{A}(X - \bar{X}) C \rangle - \frac{1}{2} \langle (X - \bar{X})\Lambda, (X - \bar{X}) \rangle
\end{equation}
\begin{equation}
= \frac{1}{2} \langle -2\xi_1 v_1 e^T_1, \Lambda(-2\xi_1 v_1 e^T_1) \rangle - \frac{1}{2} \langle (-2\xi_1 v_1 e^T_1) \Gamma, (-2\xi_1 v_1 e^T_1) \rangle
\end{equation}
\begin{equation}
\leq 2\xi_1^2 (d_r - \gamma_1) < 0.
\end{equation}

On the other hand, suppose $\xi_1 = 0$, i.e., $v_1$ is orthogonal to all the vectors $\bar{y}_1, \ldots, \bar{y}_r$. Then
\begin{equation}
V' = v_1 e^T_1 U^T C^{-1/2} \in T_X \text{St}(n, r).
\end{equation}
Indeed, $\text{Proj}_X(V') = V' - \bar{X}(\bar{X} V')_{\text{sym}} = V'$, where $V' = V' - \bar{X} V' \bar{X} = V' \bar{X} U^T C^{-1/2} = 0$. Consider a smooth curve $c(\alpha) \in \text{St}(n, r)$ passing through $c(0) = \bar{X}$ and $c'(0) = V'$. Then we have (137), since for sufficiently small $\alpha > 0$, from (20),
\begin{equation}
f_k(c(\alpha)) = f_k(\bar{X}) + \alpha^3 (V', \text{Hess } f_k(\bar{X}) V') + O(\alpha^3)
\end{equation}
\begin{equation}
= f_k(\bar{X}) + \alpha^2 (d_r - \gamma_1) + O(\alpha^3) < f_k(\bar{X}).
\end{equation}

\subsection{SQP direction $Z_k$ in $S_k$}

To accelerate the convergence speed of SSM in solving (134), we shall include the Newton step (SQP direction) $Z_k$ in the subspace $S_k$ to yield a maximum decrease of the regularized model $f_k(X) := f_k(X; \bar{A}, B_k, C)$ in the tangent space at $X_k \in \text{St}(n, r)$.

\textbf{Proposition 3.4 (SQP direction).} Consider the minimization of the unconstrained objective function
\begin{equation}
\min_{X \in \mathbb{R}^{n \times r}} \left\{ m(X) := f_k(X) - \frac{1}{2} \langle \Lambda_k, XX^T - I \rangle \right\}.
\end{equation}
Introduce some $Z_k \in \mathbb{R}^{n \times r}$ to express the minimizer $X$ as

$$X = X_k w_k + Z_k + V_g u_k$$

(152)

for some $u_k, w_k$ in $\mathbb{R}^{r \times r}$, i.e., $X \in \text{span}\{X_k, Z_k, V_g\}$. Assume the orthogonality between $Z_k$ and $\text{span}\{X_k, V_g\}$. Let $V_{X,g}$ be an isometric matrix from the qr-factorization of $[V_g, X_k]$ and let $P_k$ denote the projection

$$P_k = I - V_{X,g} V_{X,g}^T.$$  

(153)

Then $Z_k$ satisfies $P_k Z_k = Z_k$ and

$$P_k \tilde{A} P_k Z_k - Z_k \Lambda_k = P_k E_k, \quad \text{where } E_k := -\tilde{A} X_k C + B_k + X_k \Lambda_k.$$  

(154)

Proof. Express the minimizer $X$ as $X = X_k + z$ for some $z \in \mathbb{R}^{n \times r}$. Expanding the function $m$ around $X_k$, introduce $m_k(z) = m(X)$ and write

$$\min_{z \in \mathbb{R}^{n \times r}} m_k(z) = \min_{X \in \mathbb{R}^{n \times r}} m(X).$$  

(155)

The optimal $z$ satisfies $\tilde{A} z C - z \Lambda_k = E_k$, according to the computation

$$m_k(z) = \frac{1}{2} \langle \tilde{A} (X_k + z), (X_k + z) C \rangle - \langle X_k + z, B_k \rangle - \frac{1}{2} \langle \Lambda_k, (X_k + z) (X_k + z)^T - I \rangle$$  

(156)

$$= m_k(0) + \langle z, \tilde{A} X_k C - B_k - X_k \Lambda_k \rangle + \frac{1}{2} \langle (\tilde{A} z C, z) - \langle \Lambda_k, z^T z \rangle \rangle$$  

(157)

$$= m_k(0) - \langle z, E_k \rangle + \frac{1}{2} \langle (\tilde{A} z C, z) - \langle \Lambda_k, z^T z \rangle \rangle.$$  

(158)

Applying $P_k$ on both sides of the equation, we have $m_k(z) = m_k(0) + \langle z, E_k \rangle$.

Note that the matrices $V_g$ and $X_k$ are included in each subspace $S_k$. Suppose the spectral gap $d_{r+1} > d_r$ holds in $A$. With $\Lambda_k \preceq d_r C$, (154) is one positive definite system and we can employ conjugate gradient methods to determine one Newton direction $Z_k$ orthogonal to $V_{X,g}$.

### 3.4.3 Outline of Algorithm

In summary, we have the following algorithm to compute a qualified critical point.

**Algorithm 1:** Sequential subspace methods to solve (15)

<table>
<thead>
<tr>
<th>Data: Symmetric matrix $A \in \mathbb{R}^{n \times n}$ with spectral gap $d_r &lt; d_{r+1}$. Let $B \in \mathbb{R}^{n \times r}$ and $C \in \mathbb{R}^{r \times r}$ with $C \succeq 0$. Stopping criterion parameters: $\epsilon &gt; 0$ and $k_{\max} \in \mathbb{Z}$. Construct $V_g = [v_1, \ldots, v_r]$. Use $V_g$ to construct $\tilde{A}$ from (4).</th>
</tr>
</thead>
<tbody>
<tr>
<td>Result: A qualified critical point $X_k \in \mathcal{M} := \text{St}(n, r)$.</td>
</tr>
</tbody>
</table>

1. **Initialization:** $k = 1$, $X_1 = P_{\mathcal{M}}(V_g V_g^T B)$. $\Lambda_1 = X_1^T \tilde{A} X_1 C - X_1^T B \preceq d_r C$.  
2. **while** $\|\text{grad} f(X_k; A, B, C)\| > \epsilon$ or $k \leq k_{\max}$ do  
3. \hspace{1em} In (154), use conjugate gradient methods to compute $Z_k$ in the subspace orthogonal to $\text{span}\{X_k, V_g\}$.  
4. \hspace{1em} Let $S_k = \text{span}\{V_g, X_k, \tilde{A} X_k C - B, Z_k\}$ and let $V_k \in \mathbb{R}^{n \times 4r}$ be the isometric matrix associated with $S_k$. Compute $B_k$ from (124) and $\tilde{A}_k, \tilde{B}_k$ from (135).  
5. \hspace{1em} Let $X_{k+1} = V_k \tilde{X}$, where $\tilde{X} \in \mathbb{R}^{4r \times r}$ is the solution to (136) via Alg. 2.  
6. \hspace{1em} $k \rightarrow k + 1$.  
7. **end**

**Remark 3.5.** First, $\Lambda_1 = X_1^T \tilde{A} X_1 C - X_1^T B \preceq d_r C$ from Prop. 2.11. Second, according to Prop. 3.1, a limit of the sequence $\{X_k\}$ is a qualified critical point $X_\ast$. Third, various algorithms can be used to solve the small dimensional problem in (136). See the dual projection method and Riemannian Newton methods in section 3.5.
### 3.5 SSM core problems

In this section, we shall describe the computation of one qualified critical point \(X = X_{k+1}\) of the regularization problem in (134),

\[
\min_{X} f_k(X).
\] (159)

#### 3.5.1 Dual projected methods

We start with one dual projected method. For each \(\Lambda\) with \(\Lambda \preceq d_rC\), we relax the feasible set from \(St(n, r)\) to \(\mathbb{R}^{n \times r}\), introduce the Lagrangian and the dual objective,

\[
L(X, \Lambda) := f_k(X) - \frac{1}{2} \langle \Lambda, X^\top X - I \rangle, \quad h(\Lambda) := \min_X \{L(X, \Lambda) : X \in \mathbb{R}^{n \times r}\}. \tag{160}
\]

In the computation of \(h\), since \(L\) is convex in \(X\) for each feasible \(\Lambda\), then we can determine the corresponding minimizer \(X \in \mathbb{R}^{n \times r}\) by solving the linear system,

\[
\tilde{A}XC = B_k + X\Lambda. \tag{161}
\]

According to Remark 3.7, we can express \(X\) as a function \(g\) of \(\Lambda\), i.e., \(X = g(\Lambda)\). Here is the duality relation.

**Proposition 3.6.** The optimal solution \(X_{k+1}\) in (159) satisfies \(X_{k+1} = g(\Lambda') \in St(n, r)\), where \(\Lambda = \Lambda'\) is the maximizer of \(\max h(\Lambda)\) and \(g\) is given in Remark 3.7.

**Proof.** First, observe the weak duality: for each \(\bar{X} \in St(n, r)\) and each feasible \(\bar{\Lambda}\),

\[
h(\bar{\Lambda}) = \min_X L(X, \bar{\Lambda}) \leq f_k(\bar{X}). \tag{162}
\]

Second, let \(\bar{X} = \min_X L(X, \bar{\Lambda}) = f_k(\bar{X})\). Comparing (162) and (164), \(\Lambda'\) is one maximizer of the problem

\[
\max_{\bar{\Lambda}} \{h(\bar{\Lambda}) : \bar{\Lambda} \preceq d_rC\} \tag{165}
\]

and the corresponding minimizer \(g(\Lambda')\) lies in \(St(n, r)\).

Since the gradient \(dh/d\Lambda = X^\top X - I\) (Danskin’s min-max theorem\[Ber16\]), we iterate

\[
\Lambda \to \Lambda + \alpha (X^\top X - I_r) \tag{166}
\]

with proper step size \(\alpha > 0\) to maximize \(h(\Lambda)\). To impose the qualified condition \(\Lambda \preceq d_rC\) in (165) during the iterations, it is convenient to introduce the following safeguard mapping \(s(\Lambda)\), according to Prop. 2.10.

**Definition 4.** Let \(\sigma\) be the smallest singular value of \(V^\top B_k C^{-1}\). Suppose \(\sigma > 0\). Introduce the following safeguard mapping \(\Lambda \to s(\Lambda)\), so that \(s(\Lambda) \preceq d_rC\). Diagonalize \(\Lambda\) as

\[
C^{-1/2} \Lambda C^{-1/2} = UTU^{-1}, \quad \Gamma = \text{diag}(\gamma_1, \ldots, \gamma_r). \tag{167}
\]

Update

\[
\Lambda \to s(\Lambda) := C^{1/2} U \text{diag}(\bar{\gamma}_1, \ldots, \bar{\gamma}_r) U^{-1} C^{1/2}, \tag{168}
\]
where
\[ \tilde{\gamma}_i = \min(\gamma_i, d_r - \sigma), \quad i = 1, \ldots, r. \]  

(169)

**Remark 3.7** (Minimizer $X$). For each qualified multiplier $\Lambda$, we can express the minimizer $X$ in (160) as $X = \mathbf{g}(\Lambda)$. Indeed, let $U$ be the orthogonal matrix diagonalizing $C^{-1/2} \Lambda C^{-1/2}$, i.e.,
\[ UTU^{-1} = C^{-1/2} \Lambda C^{-1/2} \]

(170)

for a matrix $\Gamma = \text{diag}(\gamma_1, \ldots, \gamma_r)$. From (161), with $B' = B_k C^{-1/2}$, introduce $Y := XC^{1/2}U$, which satisfies
\[ \tilde{A}Y = B'U + Y \Gamma \]

(171)

Write $Y := [y_1, \ldots, y_r]$,
\[ y_i = (\tilde{A} - \gamma_i I)^{-1} (B'U)_i, \quad \text{for} \quad i = 1, \ldots, r. \]

(172)

Then we have $X = YU^{-1}C^{-1/2}$. Note that the minimizer matrix $X$ does not lie in $\text{St}(n, r)$, unless $\Lambda$ is the maximizer of (163).

### 3.5.2 Riemannian Newton methods

Suppose $X_{k+1}$ is in the proximity of $X_k$. Empirically, the Riemannian Newton method in Alg. 2 is a fast algorithm to solve the SSM core problems in (136),
\[ X_{k+1} = \arg \min_X f_k(X; \hat{A}, B_k, C), \]

(173)

where $f_k$ is the regularized model based at $X_k \in \text{St}(4r, r)$. The associated multiplier $\Lambda_{k+1}$ meets the condition $d_r C \succeq \Lambda_{k+1}$.

To avoid the subscript/notion confusion, we drop the subscript $k$ in (173), and replace $(X, A)$ with $(Y, \Xi)$. Write (173) as
\[ Y^* = \arg \min_Y f(Y; \hat{A}, B, C) \in \text{St}(4r, r). \]

(174)

That is,
\[ \tilde{A}Y^* C - Y \Xi^* = B \]

(175)

holds for some symmetric multiplier $\Xi^*$ with $\Xi^* \preceq d_r C$. The optimal solution $Y^*$ is expected to be in the proximity of the current base point $X_k$. The Riemannian Newton method uses a Newton direction $Z = Z_j$ to iterate $Y = Y_j$,
\[ Y_j \rightarrow Y_{j+1} = \mathbf{R}_{Y_j}(\alpha Z_j). \]

(176)

**Remark 3.8.** The equation in (177) is the linearization of (175) with $Y^* = Y_j + Z_j$. Thanks to the safeguard $s$ on $\Xi_j$, the system in (177) is positive semi-definite in $Z$. Thus, $Z_j$ can be determined by conjugate gradient methods.
Equivalently, for each vertex \( v \) in the context of \( r \)-way classification, we are interested in finding an optimal partitioning \( \chi_S \) of \( S \) for the indicator vector of \( S \). The optimal partitioning (labeling) in (182) can be

4 Numerical Simulations

We present one experiment on the \( r \)-way classification with partial labeling to illustrate the effectiveness of SSM.

4.1 Spectral graph embedding with partial labeling

Introduce the graph \( G = (V, E, W) \), where \( V = \{v_1, v_2, \ldots, v_{m'}\} \) is the vertex set, \( E \) is the edge set and \( W \) is the weight matrix whose entries \( w_{ij} \geq 0 \) are the edge weights between \( v_i \) and \( v_j \). Assume that the graph is symmetric, i.e., \( w_{ij} = w_{ji} \). Define the degree \( d_i = \sum_{j=1}^{m'} w_{ij} \) for each \( v_i \in V \). For each subset \( S \) in \( V \), define the volume \( \text{vol}(S) \) of \( S \) and the cut \( \text{cut}(S) \),

\[
\text{vol}(S) = \sum_{i \in S} d_i, \quad \text{cut}(S) = \sum_{(i,j) \in E(S)} w_{ij},\quad E(S) := \{i,j) : v_i \in S, v_j \in S^c\},
\]

where \( S^c \) is the complement set of \( S \). The conductance \( \phi(S) \) is defined as

\[
\phi(S) := \frac{\text{cut}(S)}{\min\{\text{vol}(S), \text{vol}(S^c)\}}.
\]

In the context of \( r \)-class classification, we are interested in finding an optimal partitioning \( S_1 \cup S_2 \cup \ldots \cup S_r = V \) for the minimization problem,

\[
\min_{S_i} \sum_{i=1}^{r} \phi(S_i).
\]

Equivalently, for each vertex \( v_i \), we assign a label \( y_i \) from the \( r \) standard basis vectors \( \{e_1, e_2, \ldots, e_r\} \) of the form \( e_i = [0, \ldots, 0, 1, 0, \ldots, 0] \), i.e., a one-hot row vector. Then the set \( S_i \) consists of the vertices with labels \( y_i \).

For simplicity, consider the cardinality-fixed minimization problem (replacing \( \text{vol}(S_i) \) in (180) with the cardinality \( |S_i| \) in \( S \)),

\[
\min_{S_i} \sum_{i=1}^{r} \text{cut}(S_i), |S_i| = c_i \in \mathbb{Z}, \quad i = 1, \ldots, r.
\]

Write \( \chi_{S_i} \in \mathbb{Z}^{m'} \) for the indicator vector of \( S_i \). The optimal partitioning (labeling) in (182) can be
described by the binary matrix

\[
Y := \begin{bmatrix}
y_1 \\
\vdots \\
y_m'
\end{bmatrix} = [\chi_{S_1}, \chi_{S_2}, \ldots, \chi_{S_r}] \in \mathbb{Z}^{m' \times r},
\]  

(183)

where \([c_1, \ldots, c_r]\) is the column sum of \(Y\). The spectral approximation of \([182]\) can be computed via relaxing the min-cut problem \([182]\) over binary matrices to real matrices. Let \(L\) denote the combinatorial graph Laplacian, \(L = \text{diag}([d_1, \ldots, d_m]) - W\). An embedding of the labeling of vertices is given by the eigen functions \(X\) corresponding to the smallest nontrivial eigenvalues,

\[
\min_{X \in \mathbb{R}^{m' \times r}} \langle X, LX \rangle, \quad X^\top X = I_r.
\]  

(184)

Consider the semi-supervised learning task, where a set of pre-specified labeled data is available: The first \(m\) vertices \(V_1 := \{v_1, v_2, \ldots, v_m\}\) are assigned labels \(\{y_1, y_2, \ldots, y_m\}\), where \(0 < m \ll m'\). Let \(n\) denote the number of unlabeled vertices, \(n = m' - m\). The task of the semi-supervised learning is to smoothly propagate the labels over the unlabeled vertices \(V_u := \{v_{m+1}, v_{m+2}, \ldots, v_{m'}\}\). Write

\[
L = \begin{bmatrix} L_{i,i} & L_{i,u} \\ L_{u,i} & L_{u,u} \end{bmatrix}, \quad Y = \begin{bmatrix} Y_1 \\ Y_u \end{bmatrix}, \quad Y_l = [y_1, \ldots, y_m]^\top, \quad X = \begin{bmatrix} X_l \\ X_u \end{bmatrix}.
\]  

(185)

where subscripts \(l\) and \(u\) correspond to labeled and unlabeled indices, respectively. Let \(X_l\) represent the labeled vertices with cardinality \(m\), i.e., \(X_l = Y_l\). Introduce the associated constraint set

\[
\mathcal{X} := \{X \in \mathbb{R}^{n \times r} : 1_n^\top X = c^\top, X^\top X = X_l^\top X_l + X_u^\top X_u = \text{diag}(c)\}.
\]  

(186)

The following proposition indicates that the unknown matrix \(X_u\) can be computed from one quadratic minimization problem over a Stiefel manifold, i.e., \([190]\).

**Proposition 4.1.** Introduce \(X, L\) in \([185]\). Given some binary matrix \(X_l \in \mathbb{R}^{m \times r}\) and \(c \in \mathbb{R}^r\), consider the minimization

\[
\min_{X_u \in \mathbb{R}^{n \times r}} \{\langle X, LX \rangle : X \in \mathcal{X}\}.
\]  

(187)

Let \(c_l\) be the column sum of \(X_l\), i.e., \(c_l = X_l^\top 1_m\). Let \(c_u = c - c_l\). Introduce \(P = I_n - n^{-1}1_n 1_n^\top\) and

\[
A = PL_{u,u}P, \quad B = P(n^{-1}L_{u,u}1_n c_u^\top + L_{u,l}X_l), \quad C = \text{diag}(c) - X_l^\top X_l - n^{-1}c_u c_u^\top.
\]  

(188)

Let \(X_u''\) be the minimizer of

\[
\min_{X_u''} \{\langle X_u'', AX_u'' C \rangle + 2\langle X_u'', BC^{1/2} \rangle : X_u'' \in \text{St}(n, r)\}
\]  

(189)

Then \(X_u\) is given by

\[
X_u = X_u'' C^{1/2} + n^{-1}1_n c_u^\top.
\]  

(190)

**Proof.** Introduce

\[
X'_u := X_u - n^{-1}1_n c_u^\top.
\]  

(191)

Then \(X'_u\) has zero column sum, \(1_n^\top X'_u = 0\). Reformulate the problem in \([187]\) in terms of \(X'_u\): The constraint part is

\[
\text{diag}(c) = X^\top X = X_l^\top X_l + X_u^\top X_u = X_l^\top X_l + X'_u^\top X'_u + n^{-1}c_u c_u^\top;
\]  

(192)

The objective is

\[
\langle X_u, L_{u,u} X_u \rangle + 2\langle X_u, L_{u,l} X_l \rangle + \text{constant}.
\]  

(193)

Thanks to \([188]\) and \([191]\), \(X'_u\) is the minimizer of the problem

\[
\min_{X'_u} \{\langle X'_u, AX'_u \rangle + 2\langle X'_u, B \rangle\},
\]  

(194)
subject to
\[ X_u^T X_u = \text{diag}(c) - X_l^T X_l - n^{-1} c_u c_u^T = C \in \mathbb{R}^{r \times r}. \]  
(195)

The proof is completed by writing \( X_u' = X_u' C^{1/2} \).

However, the matrix \( C \) in (188) has rank at most \( r - 1 \), since \( C \) has a null vector \( 1_r \), i.e.,
\[ C1_r = c - X_l^T 1_m - n^{-1} c_u n = c - c_l - c_u = 0, \quad \text{where we used } X_l 1_r = 1_m, \quad c_u 1_r = n. \]  
(196)
Likewise, \( BC^{1/2} \) has rank at most \( r - 1 \). Thanks to \( X_u' 1_r = 1_n \), \( X_u' \) in (195) has rank at most \( r - 1 \). Thus we cannot employ SSM on (198) directly. To alleviate this difficulty, assume that the rank of \( C \) is \( r - 1 \). Take the eigen decomposition:
\[ C = \tilde{Q} \tilde{C} \tilde{Q}^T \] with isometric \( \tilde{Q} \in \mathbb{R}^{r \times (r-1)} \) and positive definite \( \tilde{C} \in \mathbb{R}^{(r-1) \times (r-1)} \).

Introduce
\[ Y := X_u' \tilde{Q}, \quad \tilde{B} = B \tilde{Q} \in \mathbb{R}^{n \times (r-1)} \]  
(197)
to eliminate \( X_u' \) in (189). Then \( Y \) is a minimizer to
\[ \min \left\{ \langle Y, AY \tilde{C} \rangle + 2 \langle Y, \tilde{B} \tilde{C}^{1/2} \rangle : \ Y \in \text{St}(n, r-1) \right\}. \]  
(198)
According to Prop. 4.1, once \( Y \) is obtained via SSM, we can compute \( X_u \),
\[ X_u = Y \tilde{Q}^T \tilde{C}^{1/2} + n^{-1} 1_n c_u^T. \]  
(199)

4.2 Experimental setup

We evaluate SSM on synthetic and three image datasets: MNIST [Den12], Fashion-MNIST [XRV17] and Cifar-10 [Kri09]. On CIFAR-10 we preprocess images using a pre-trained autoencoder as a feature extractor. The autoencoder architecture, loss, and training, were derived from the AutoEncodingTransformations architecture from [ZQWL19], with all the default parameters from their paper, and we normalized the features to unit vectors. We also evaluate SSM on a variety of real-world networks including the Cora citation network, which demonstrates that our method generalizes beyond \( k \)-NN graphs. In this benchmark, the vertices of the graph represent documents and their links refer to citations between documents, while the label corresponds to the topic of the document.

4.2.1 Synthetic datasets

To illustrate the concept of semi-supervised learning, we apply SSM to a small synthetic benchmark. We consider three concentric circles centered at the origin with radii 1, 2, and 3 for each circle, we randomly sample 2000 points, normally distributed with standard deviation 0.2. We construct a graph over the data. The graph was constructed as a \( k \)-nearest neighbor graph with Gaussian edge weights given by \( w_{ij} = \exp\left(-4||x_i - x_j||^2/d_k(x_j)^2\right) \) where \( d_k(x_j) \) is the distance between \( x_i \) and its \( k \)th nearest neighbor. We used \( k = 10 \) in all experiments and symmetrize \( W \) by replacing \( W \) with \( \frac{1}{2}(W + W^T) \). From each circle, we uniformly randomly select 5 points to use as supervision and then construct matrices \( A, B, \) and \( C \) as stated in Prop. 4.1 and run SSM to get predictions. Figure 2 illustrates this procedure.
4.2.2 Image datasets

We construct a graph over the pixel space. We used all available data to construct the graph for MNIST and Fashion-MNIST, and for Cifar-10. The graph was constructed as a $k$-nearest neighbor graph with Gaussian edge weights as did in section 4.2.1. To construct $Y_l$, we uniformly sample 1 vertex for each of the 5 classes, i.e. $m = 5$.

4.2.3 Citation networks

We also evaluate the Cora citation network, demonstrating that our method generalizes beyond $k$-NN graphs. In this benchmark, the graph is given. The vertices represent documents and their links refer to citations between documents, while the label corresponds to the topic of the document.

Table 1 demonstrates the comparison of SSM with other methods, including R-TRUST REGION, R-CONJUGATE GRADIENT, and R-GRADIENT to solve $X_u$ from (199). \(^3\) For a fair comparison, all four methods start with the same initialization $P_M(V_g V_g^T B)$.

- SSM is Algorithm 1 in section 3.
- R-TRUST REGION is the trust region method described in section 6.4 [Bou04].
- R-CONJUGATE GRADIENT is the Riemannian conjugate gradient method proposed in [Sat22].
- R-GRADIENT is the iterative method given in [96].

The computation of $V_g$ is necessary to compute both the initialization of SSM and is used to compute the sequence of subspaces. We employ locally optimal block preconditioned conjugate gradient methods (LOBPCG) [Kny01], a matrix-free algorithm with Jacobi preconditioning to compute the principal eigenvectors of $A$, $V_g$ in nearly linear time. For instance, we compute the smallest four eigenvalues and corresponding eigenvectors of $A$ to generate $V_g$ with rank 4 for the MNIST dataset. Here, the first 6 positive eigenvalues of $A$ for the MNIST dataset are

\[
\begin{align*}
   d_1 &= 4.9439 \times 10^{-4}, & d_2 &= 9.7915 \times 10^{-4}, & d_3 &= 1.1816 \times 10^{-3}, \\
   d_4 &= 1.2345 \times 10^{-3}, & d_5 &= 2.1650 \times 10^{-3}, & d_6 &= 2.4785 \times 10^{-3}.
\end{align*}
\]

Table 1 indicates that a better classification accuracy is obtained, if a lower objective is reached. Compared to the methods R-CONJUGATE GRADIENT and R-GRADIENT, both SSM and R-TRUST REGION can reach a lower objective value, see the column of $f(X)$. On the other hand, even though these methods are guaranteed to monotonically reduce the objective via line search, SSM rapidly converges to one qualified critical point, while the projected gradient method fails to converge, even after hundreds of iterations. See the column $\|AXC - B - XA\|$ for the norm of the first-order condition.

\(^3\)The code and experiments can be found at https://github.com/choltz95/SSM-on-stiefel-manifolds.

\(^4\)Random initialization produces poor objective values in the methods: R-TRUST REGION, R-CONJUGATE GRADIENT, and R-GRADIENT. We omit these results.
<table>
<thead>
<tr>
<th>MNIST</th>
<th>f(X)</th>
<th>|AXC − B − XA|</th>
<th># EVALUATIONS L^1 x</th>
<th>RUNTIME (s)</th>
<th>ACCURACY</th>
</tr>
</thead>
<tbody>
<tr>
<td>SSM</td>
<td>15.57</td>
<td>0.0</td>
<td>19</td>
<td>33.1</td>
<td>97.61%</td>
</tr>
<tr>
<td>R-Trust Region</td>
<td>15.57</td>
<td>0.0</td>
<td>43</td>
<td>97.3</td>
<td>97.61%</td>
</tr>
<tr>
<td>R-Conjugate Gradient</td>
<td>25.08</td>
<td>0.07</td>
<td>0</td>
<td>72.3</td>
<td>75.31%</td>
</tr>
<tr>
<td>R-Gradient</td>
<td>25.08</td>
<td>0.09</td>
<td>0</td>
<td>117.9</td>
<td>75.22%</td>
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<table>
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<tbody>
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<td>0.0</td>
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<td>53.57%</td>
</tr>
<tr>
<td>R-Trust Region</td>
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<td>231.4</td>
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<tr>
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<tr>
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<td>162.1</td>
<td>33.96%</td>
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<table>
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<tr>
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<td>0</td>
<td>79.10</td>
<td>37.03%</td>
</tr>
</tbody>
</table>

One may also ask how our method compares to traditional second-order methods (i.e., Riemannian Trust-region). Column RUNTIME shows that SSM converges faster than R-TRUST REGION. The L^1 column reports the number of calls to the conjugate gradient solver for each method (to compute the Newton direction). In theory, SSM employs a special set of vectors to estimate the Hessian information to update the search direction via subspace minimization. As a result, the Hessian information estimated from SSM is usually better than the Hessian estimated from CG or BFGS methods typically used for trust-region type approaches. Take MNIST as one example. The smallest eigenvalue of Hessian in SSM is about $1.3 \times 10^{-3}$ near the critical point, while the smallest eigenvalue of Hessian in R-TRUST REGION is less than $2.05 \times 10^{-5}$.

### 4.3 Complexity of SSM

Last, we briefly analyze the computational cost of SSM, which is dominated by the SQP routine to compute the SQP directions Z (Newton directions). The SQP direction Z is the solution to the system characterized by the linearization of the first-order optimality conditions. Namely, within each iteration of our procedure, we compute the Lagrangian multipliers as well as the SQP update for X. As in Newton’s method for unconstrained problems, SQP-based methods necessitate the computation of inverse-vector products involving symmetric PSD linear systems. Assume that by exploiting the sparsity of the graph Laplacian L, vector-vector and matrix-matrix multiplication can be done in linear time. The primary overhead of our method lies in the computation Z, which necessitates the computation of the solution to a certain linear system in the subspace orthogonal to span\{X_k, V_g\}. We empirically show that this linear system is well-conditioned. In summary, SSM is an efficient tool to compute a qualified critical point of large-dimensional problems in 4.
References


