Abstract

Recent literature has advocated the use of randomized methods for accelerating the solution of various matrix problems arising throughout data science and computational science. One popular strategy for leveraging randomization is to use it as a way to reduce problem size. However, methods based on this strategy lack sufficient accuracy for some applications. Randomized preconditioning is another approach for leveraging randomization, which provides higher accuracy. The main challenge in using randomized preconditioning is the need for an underlying iterative method, thus randomized preconditioning so far have been applied almost exclusively to solving regression problems and linear systems. In this article, we show how to expand the application of randomized preconditioning to another important set of problems prevalent across data science: optimization problems with (generalized) orthogonality constraints. We demonstrate our approach, which is based on the framework of Riemannian optimization and Riemannian preconditioning, on the problem of computing the dominant canonical correlations and on the Fisher linear discriminant analysis problem. For both problems, we evaluate the effect of preconditioning on the computational costs and asymptotic convergence, and demonstrate empirically the utility of our approach.

1 Introduction

Matrix sketching has recently emerged as a powerful tool for accelerating the solution of many important matrix computations, with widespread use throughout data science and computational science. Important examples of matrix computations that have been accelerated using matrix sketching include linear regression, low rank approximation, and principal component analysis (see recent surveys [57, 58]). Matrix sketching is one of the main techniques used in so-called Randomized Numerical Linear Algebra.

Roughly speaking, matrix sketching provides a transformation that embeds a high dimensional space in a lower dimensional space, while preserving some desired properties of the high dimensional space [57]. There are several ways in which such an embedding can be used. The most popular approach is sketch-and-solve, in which matrix sketching is used to form a smaller problem. That is, sketch-and-solve based algorithms attempt to find a “good” approximate solution by sketching the input problem so that with high probability the exact solution of the sketched problem is a good approximate solution to the original problem. For example, the sketch-and-solve approach for solving unconstrained overdetermined linear regression problem, i.e., \( \min_w \|Xw - y\|_2 \), where \( X \in \mathbb{R}^{n \times d} \) (\( n \geq d \)) is assumed to be full rank matrix, is to randomly generate a matrix \( S \in \mathbb{R}^{s \times n} \) and solve the reduced size problem \( \min_w \|SXw - Sy\|_2 \) [19]. If \( S \) is chosen appropriately, then with high probability the solution of the sketched problem, \( \hat{w} \), is close to the exact solution, \( w^* \), in the sense that the inequality \( \|X\hat{w} - y\|_2 \leq (1 + \varepsilon)\|Xw^* - y\|_2 \) holds, and that \( SX \) and \( Sy \) can be computed quickly.

Sketch-and-solve algorithms have been proposed for a wide spectrum of linear algebra problems: linear regression [19], principal component analysis [30], canonical correlation analysis (CCA) [2], kernelized
methods [5], low-rank approximations [10], structured decompositions [19], etc. However, there are two main drawbacks to the sketch-and-solve approach. First, it is unable to deliver highly accurate results (typically, for sketch-and-solve algorithms, the running time dependence on the accuracy parameter $\epsilon$ is $\Theta(\epsilon^{-2})$). The second drawback is that sketch-and-solve algorithms typically have only Monte-Carlo type guarantees, i.e., they return a solution within the prescribed accuracy threshold only with high probability (on the positive side, the running time is deterministic).

These drawbacks have prompted researchers to develop a second approach, typically termed sketch preconditioning or randomized preconditioning. The main idea in randomized preconditioning is to use an iterative method which, in turn, uses a preconditioner that is formed using a sketched matrix. For example, consider again the unconstrained overdetermined linear regression problem problem. It is possible to accelerate the solution of $\min_w \|Xw - y\|_2$ by first sketching the matrix $X$ to form $SX$, and then using a factorization of $SX = QR$ to form a preconditioner, $R$, for an iterative Krylov method (e.g., LSQR). By choosing $S$ properly, with high probability the preconditioner $R$ is such that the condition number governing the convergence of the Krylov method, $\kappa(XR^{-1})$, is bounded by a small constant [44, 4, 37, 16]. Thus, when using a Krylov method to solve $\min_w \|XR^{-1}w - y\|_2$ only a small number of iterations are necessary for convergence.

More generally, by using an iterative method, it is typically possible to reduce the running time dependence on the accuracy parameter to be logarithmic instead of polynomial. Furthermore, since we can control the stopping criteria of the iterative methods, sketch preconditioning algorithms typically entertain Las-Vegas type guarantees, i.e., they return a solution within the accuracy threshold, albeit at the cost of probabilistic running time.

The sketch-and-solve approach is more prevalent in the literature than sketch preconditioning. Indeed, in one way or the other, almost all sketch preconditioning method have essentially been designed for linear regression or solving linear systems. The main reason is that sketch preconditioning requires an iterative method that can be preconditioned, and such a method is not always known for the various problems addressed by sketching. Indeed, linear regression and solving linear systems are cases for which the use of preconditioning is straightforward.

The goal of this paper is to go beyond linear regression, and design sketch preconditioning algorithms for another important class of problems: optimization problems under generalized orthogonality constraints. In general, we are interested in solving problems of the form

$$\min f(X_1, \ldots, X_k) \ \text{s.t.} \ \ X_i^T B_i X_i = I_p \quad (i = 1, \ldots, k) \quad (1.1)$$

where $f(X_1, \ldots, X_k) : \mathbb{R}^{d_1 \times p} \times \cdots \times \mathbb{R}^{d_k \times p} \to \mathbb{R}$ is a smooth function, and $B_i \in \mathbb{R}^{d_i \times d_i}$ are fixed symmetric positive definite (SPD) matrices. An important example of such problems is the problem of finding the dominant subspace: given a SPD matrix $A \in \mathbb{R}^{n \times n}$, if $f(X_1) = -\text{Tr}(X_1^T A X_1)$ and $B_1 = I_n$, then Problem (1.1) corresponds to finding a basis for the dominant eigenspace.

Problems of the form of Eq. (1.1) frequently appear in data science applications. Typically, in data science applications, the constraint matrices $B_i$ can be written as the Gram matrix of a tall-and-skinny data matrix $Z_i$, i.e., $B_i = Z_i^T Z_i$ for $Z_i \in \mathbb{R}^{n_i \times d_i}$, or more generally $B_i = Z_i^T Z_i + \lambda_i I_d$ where $\lambda_i \geq 0$ is some regularization parameter. We assume that $Z_1, \ldots, Z_k$ are given as input and not $B_i$. Our aim is to design algorithms that use $O(nd^2)$ operations to find the preconditioner, and use $O(nd)$ per iteration, where $n = \max_i n_i$ and $d = \max_i d_i$.

Two important unsupervised machine learning methods that reduce to Problem (1.1) are canonical correlation analysis (CCA) and Fisher linear discriminant analysis (FDA). We illustrate our approach, demonstrating its effectiveness both theoretically and empirically, on both of these problems. In particular, we improve on the $\Theta(nd^2)$ running time possible for both problems using direct methods.

The underlying iterative methods we precondition are based on the framework of Riemannian optimization [11, 7]. Riemannian optimization is well suited for problems with manifold constraints, e.g., under generalized orthogonality constraints [21]. It makes use of the Riemannian geometry components associated with the constraining manifolds, which in the case of Eq. (1.1) are products of generalized Stiefel manifolds. Riemannian
Preconditioning [41], which is a technique for preconditioning Riemannian optimization algorithms based on carefully choosing the Riemannian metric is another component of our proposed method. By combining randomized preconditioning with Riemannian preconditioning we obtain faster methods for solving Eq. (1.1).

1.1 Related Work

Matrix Sketching The literature on sketching has so far mostly focused on the sketch-and-solve approach. In particular, in the context of solving problems with generalized orthogonality constraints, a sketch-and-solve based approach for CCA was developed in [2]. Sketch preconditioning was predominantly applied to linear least-squares regression problems (e.g., [4, 37]), and also to non least-squares variants (e.g., \( \ell_1 \) - regression [36]). For a regularized version of FDA, a randomized iterative method was developed in [15]. Even though the method in [15] does not use sketch preconditioning per se, it can be viewed as a preconditioned Richardson iteration. A randomized iterative method for solving LP problems was proposed in [14], where sketch preconditioning is used to find the Newton search direction as part of an interior point method. To the best of our knowledge, sketch preconditioning has neither been applied to CCA before, nor has it been used in the context of Riemannian optimization.

Riemannian Optimization and Reimannian Precondioning Recent works introducing Riemannian optimization are [1, 7]. Earlier works are [34, 24, 47], and specifically, using Riemannian optimization to solve problems under orthogonality constraints is presented in the seminal work of Edelman et al. [21].

Preconditioning of Riemannian optimization methods based on the cost function alone is presented in several works, see e.g., [42, 40, 45, 60]. Most of the aforementioned work attempt to perform preconditioning by approximating the Euclidean Hessian of the cost function. However, the Riemannian Hessian and the Euclidean Hessian are quite different even for simple examples (see [46, Section 3.5]). The Riemannian Hessian is related to the Hessian of the Lagrangian, and indeed in [41] it is shown that selecting the Riemannian metric inspired by the Hessian of the Lagrangian affects convergence of Riemannian steepest-descent, coining the term Riemannian preconditioning for judiciously choosing the Riemannian metric in order to accelerate convergence. Unlike [41], we present a randomized preconditioning strategy, and analyze the condition number of the Riemannian Hessian at the optimum for specific examples (CCA and FDA), which allows us to quantify the quality of the proposed preconditioner.

Additional works regarding preconditioning of Riemannian methods are a work by Kressner et al. where they proposed a Riemannian analogue to the preconditioned Richardson method [33], and a work by Vandereycken and Vandewalle where they proposed a Riemannian version of preconditioning the trust-region subproblem (which to some extent can be also viewed as Riemannian metric selection) [53]. We remark that no previous work proposed to use randomized preconditioners in the context of Riemannian preconditioning.

Iterative Methods for CCA and FDA Several iterative methods for solving CCA have been proposed in the literature. Golub et al. presented an iterative method for CCA based on alternating least squares [26]. Each iteration requires the solution of two least squares problems. The authors suggest using LSQR for that task. Wang et al. proposed to replace LSQR with either accelerated gradient descent, stochastic variance reduce gradient (SVRG) or accelerated SVRG [56]. They also proposed a different approach based on shift-and-invert preconditioning. Ma et al. developed an algorithm for CCA based on augmented approximate gradients [35]. Ge et al. provided an iterative algorithm for the generalized eigenvalue problem, and used a standard reduction of CCA to generalized eigenvalue problems to derive an algorithm for CCA [25]. They assume a fast black box access to an approximate linear system solver.

Convergence bounds of all the aforementioned algorithms depend on the condition number of the input matrices, which might be large. In contrast, the condition number bounds for our proposed sketching based algorithms are independent of the conditioning of the input matrices. As aside, Yger et al. proposed a Riemannian method for adaptive CCA [59].
In the context of FDA, a recent work by Chowdhury et al. proposed an iterative, sketching-based algorithm for regularized FDA [15]

2 Preliminaries

2.1 Notation and Basic Definitions

In this paper we use standard notation. Scalars are denoted by lower case letters $\alpha, \beta, ..., x, y, ...$, while vectors are denoted by bold letters $\alpha, \beta, ..., x, y, ...$, and matrices are denoted by bold uppercase English letters $A, B, ...$ or upper case Greek letters. We use the convention that vectors are column-vectors. We denote the element of a diagonal matrix $A$ by $A_i$ and a block diagonal matrix by $\text{blkdiag} (\cdot)$.

We denote by $(\cdot, \cdot)_M$ the inner-product with respect to a matrix $M$: for $U$ and $V$, $(U, V)_M := \text{Tr} (U^T M V)$ where $\text{Tr} (\cdot)$ denotes the trace operator. The $s \times s$ identity matrix is denoted $I_s$. The $s \times s$ zero matrix is denoted $0_s$. We denote by $\mathcal{S}_{\text{sym}}(p)$ and $\mathcal{S}_{\text{skew}}(p)$ the set of all symmetric and skew-symmetric matrices (respectively) in $\mathbb{R}^{p \times p}$. The symmetric and skew-symmetric components of $A$ are denoted by $\text{sym}(A) := (A + A^T)/2$ and $\text{skew}(A) := (A - A^T)/2$ respectively.

For a SPD matrix $B \in \mathbb{R}^{d \times d}$, we denote by $B^{1/2}$ the unique SPD matrix such that $B = B^{1/2} B^{1/2}$, obtained by keeping the same eigenvectors and taking the square root of the eigenvalues. We denote the inverse of $B^{1/2}$ by $B^{-1/2}$.

The eigenvalues of a symmetric $d \times d$ matrix $A$ are denoted by $\lambda_1(A) \geq \lambda_2(A) \geq \cdots \geq \lambda_d(A)$. The condition number of $A$, i.e., the ratio between the largest and smallest eigenvalues in absolute value, is denoted by $\kappa(A)$. The generalized condition number of a matrix pencil $(A, B)$, which is the ratio between largest and smallest generalized eigenvalues, is denoted by $\kappa(A, B)$, and it holds that if $B$ is a SPD matrix, then $\kappa(A, B) = \kappa(B^{-1/2} A B^{-1/2})$.

For differential geometry objects we use the following notations: tangent vectors (of a manifold) are denoted using lower case Greek letters with a subscript indicating the point of the manifold for which they correspond (e.g., $\eta_x$), while normal vectors (of a manifold) are denoted using bold lower and upper case letters with a subscript (e.g., $u_x$). We denote by $\mathbf{St}_B(p,d)$ the generalized Steifel manifold, which is a submanifold of $\mathbb{R}^{d \times p}$ defined by

$$\mathbf{St}_B(p,d) := \{ X \in \mathbb{R}^{d \times p} : X^T B X = I_p \}.$$  

Given a function defined on $\mathbf{St}_B(p,d)$, a smooth extension of that function to the entire $\mathbb{R}^{d \times p}$ is denoted by a bar decorator. For example, given a smooth function $f : \mathbf{St}_B(p,d) \rightarrow \mathbb{R}$, we use $\bar{f} : \mathbb{R}^{d \times p} \rightarrow \mathbb{R}$ to denote a smooth function on $\mathbb{R}^{d \times p}$ such that on $\mathbf{St}_B(p,d)$ that function agrees with $f$.

2.2 Riemannian Optimization and Preconditioning for the Generalized Stiefel Manifold

In this subsection we detail several necessary components in order to develop our preconditioning strategy: Riemannian optimization, Riemannian preconditioning, and the geometric optimization components of the generalized Steifel manifold with a non-standard metric. In following sections we make use of these components to present our randomized Riemannian preconditioning strategy.

Riemannian optimization [1, 7] is a framework of designing algorithms for solving constrained optimization problems, where the constraints form a smooth manifold $\mathcal{M}$. The general idea of these algorithms is to make use of the differential geometry components of $\mathcal{M}$ in order to generalize iterative methods for unconstrained optimization. Iterative algorithms for smooth problems such as gradient methods, trust-region, and conjugate gradient (CG), are adopted to the Riemannian setting using the following components: a Riemannian metric which is a smoothly varying inner product $x \mapsto g_x$ on the tangent bundle $T\mathcal{M}$ such that $(\mathcal{M}, g)$ becomes a Riemannian manifold, a retraction mapping $R_x : T_x \mathcal{M} \rightarrow \mathcal{M}$ which allows to take a step at point $x \in \mathcal{M}$ in
a direction $\xi_x \in T_xM$, a vector transport $T_{\eta_x} : T_xM \to T_{R_\eta \xi}M$ which allows operations between tangent vectors from two different tangent spaces, a Riemannian gradient $\text{grad} f(x) \in T_xM$, and a Riemannian Hessian $\text{Hess} f(x) : T_xM \to T_xM$. Another important notion in the context of this paper is the notion of Riemannian submanifold, which allows to easily compute the aforementioned geometric components if they are known for the ambient manifold. Usually, a Riemannian optimization algorithm is built from iterations on the tangent space $T_xM$ which are then retracted to the manifold. For example, Riemannian gradient methods are given by the formula $x_{k+1} = R_{x_k}(\tau_k \text{grad} f(x_k))$ where $\tau_k$ is the step size. Many of the Riemannian algorithms and common manifolds are implemented in MANOPT, which is a MATLAB library [6]. There is also a PYTHON parallel for MANOPT called PYMANOPT [50]. The experiments reported in Section 6 use the MANOPT library.

Preconditioning of iterative methods is often challenging since it is not initially clear how the actually precondition the problem for an iterative method. Riemannian preconditioning [41] generalizes preconditioning for Riemannian optimization methods. In Riemannian preconditioning, preconditioning is performed via a Riemannian metric selection, i.e., the preconditioner is incorporated via the Riemannian metric.

A motivation for metric selection is the observation that the condition number of the Riemannian Hessian at the optimum affects the asymptotic convergence rate of Riemannian optimization (e.g., [1] Theorem 4.5.6, Theorem 7.4.11 and Equation 7.5), [7] Definition 4.5 and Section 4.6], and in the case of convex objective function (in the Riemannian sense [32 Chapter 3.2]) there are also global convergence results, e.g., [32 Chapter 7, Theorem 4.2]. Thus, selecting a metric such that this condition number is lowered should improve convergence.

In this paper, we propose to utilize randomized preconditioning to accelerate the solution of orthogonality constrained problems by using Riemannian preconditioning. Optimization problems under generalized orthogonality constraints can be written as Riemannian optimization problems on the generalized Stiefel manifold. The standard Riemannian metric for the generalized Stiefel manifold (e.g., [21] [6]) is

$$g_x(\xi_x, \eta_x) := (\xi_x, \eta_x)_B = \text{Tr} \left( \xi_x^T B \eta_x \right).$$

The use of this metric has two possible shortcomings. First, it might might not be the optimal metric with respect to convergence of Riemannian optimization methods. Second, and more relevant for this paper, the computation of most Riemannian components requires taking products of $B^{-1}$ with a vector. Computing $B$ and/or factorizing is in many cases as costly as solving the problem directly, e.g., for CCA (see Section 7).

In order to overcome these shortcoming, we leverage our recently developed geometric components for the generalized Stiefel manifold with a Riemannian metric which is based on a preconditioning scheme $X \to M_X$ instead of $B$ [40]. In this paper, we apply a preconditioning scheme independent of $X$, i.e., $M_X := M$ for all $X \in \text{St}_B(p, d)$ (see Section 3). As a reference we summarize (without proofs) in Table 1 the various geometric components developed in [40].

In addition, we also address optimization problems that are constrained on a product of generalized Stiefel manifolds such as CCA. In this case, the Riemannian components of the generalized Stiefel manifold can be generalized to be the Riemannian components of a product of generalized Stiefel manifolds in a straightforward way (see Section 4).

### 3 Randomized Riemannian Preconditioning

In this section we present our main contribution: randomized Riemannian preconditioners for optimization problems which feature generalized orthogonality constraints defined by Gram matrices. That is, our goal is to address constraints of the form $X_i^T B_i X_i = I_p$ ($i = 1, \ldots, k$), where $B_i$ can be written as a regularized Gram matrix of a tall-and-skinny matrix $Z_i \in \mathbb{R}^{n_i \times d}$ with a regularization parameter $\lambda \geq 0$, i.e., $B_i = Z_i^T Z_i + \lambda I_d$. As alluded earlier, our proposed solution incorporates a preconditioner by selecting a non-standard metric for $\text{St}_{B_1} \times \cdots \times \text{St}_{B_k}$.
Table 1: Summary of various Riemannian components of the generalized Stiefel manifold \[46\].

| Component                                                                 | Formula                                                                                                                                 |
|---------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------|
| Tangent space \(T_X\text{St}_\mathcal{B}(p, d)\)                         | \(\{ \mathbf{Z} \in \mathbb{R}^{d \times p} : \mathbf{Z}^T \mathbf{B} \mathbf{X} + \mathbf{X}^T \mathbf{B} \mathbf{Z} = \theta_p \}\) |
| Tangent space \(T_X\text{St}_\mathcal{B}(p, d)\) alternative form     | \(\{ \mathbf{Z} = \mathbf{X} \mathbf{\Theta} + \mathbf{X}_\perp \mathbf{K} \in \mathbb{R}^{d \times p} : \mathbf{\Theta} = -\mathbf{T}^T, \ \mathbf{K} \in \mathbb{R}^{(d-p) \times p} \} \) such that \(X_{\parallel}^T B X_{\parallel} = I_{d-p}, X_{\perp}^T B X_{\perp} = 0_{(d-p) \times p}\) |
| The Riemannian metric                                                    | \(g_\mathcal{X}(\mathbf{\xi}, \mathbf{\eta}) = \langle \mathbf{\xi}, \mathbf{\eta} \rangle_M = \text{Tr}(\mathbf{\xi}^T \mathbf{M} \mathbf{\eta})\) |
| Normal space with respect to the Riemannian metric                       | \((T_X\text{St}_\mathcal{B}(p, d))^\perp = \{ \mathbf{M}^{-1} \mathbf{B} \mathbf{X} S : \mathbf{S} = \mathbf{S}^T \}\) |
| Polar-based retraction                                                   | \(R_X^{\text{pol}}(\mathbf{\xi}) = (\mathbf{X} + \mathbf{\xi})(\mathbf{I}_p + \mathbf{\xi}_2 \mathbf{B} \mathbf{\xi}_2)^{-1/2}\) |
| QR-based retraction                                                      | \(R_X^{\text{QR}}(\mathbf{\xi}) = \mathbf{B}^{-1/2} \text{qr} \left( \mathbf{B}^{1/2} (\mathbf{X} + \mathbf{\xi}) \right)\) |
| Orthogonal projection on the normal space                               | \(\Pi_\mathcal{X}(\mathbf{\xi}) = \mathbf{M}^{-1} B \mathbf{X} s_{\mathcal{X}}\) |
| Orthogonal projection on the tangent space                               | \(\Pi_\mathcal{X}(\mathbf{\xi}) = (\text{id}_{T_X\text{St}_\mathcal{B}(p, d)} - \Pi_\mathcal{X}^T) \mathbf{\xi} = \mathbf{\xi} - \mathbf{M}^{-1} B \mathbf{X} \mathbf{s}_{\mathcal{X}}\) |
| Sylvester equation for \(s_{\mathcal{X}}\) (orthogonal projection)     | \((\mathbf{X}^T \mathbf{B}^{-1} \mathbf{B} \mathbf{X}) \mathbf{s}_{\mathcal{X}} + \mathbf{s}_{\mathcal{X}} (\mathbf{X}^T \mathbf{B}^{-1} \mathbf{B} \mathbf{X}) = \mathbf{X}^T \mathbf{B} \mathbf{\xi} + (\mathbf{X}^T \mathbf{B} \mathbf{\xi})^T\) |
| Vector transport                                                        | \(\tau_\mathcal{X}(\mathbf{\xi}) = \Pi_\mathcal{X}(\mathbf{\eta}_\mathcal{X}(\mathbf{\xi})) \} \mathbf{\xi})\) |
| Riemannian gradient                                                      | \(\text{grad}/(\mathbf{X}) = \Pi_\mathcal{X} \left( \mathbf{M}^{-1} \nabla \mathcal{f}(\mathbf{X}) \right)\) |
| Riemannian Hessian applied on a tangent vector                          | \(\text{Hess}(\mathbf{[X][\mathcal{X}]}) = \Pi_{\mathcal{X}}(\mathbf{M}^{-1} (\nabla^2 \mathcal{f}(\mathbf{X}) \mid_{\mathcal{X}} - B_{\mathcal{X}}(\mathbf{X}^T \nabla \mathcal{f}(\mathbf{X}) - \mathbf{X}^T \text{grad}/(\mathbf{X}))))\) |

For simplicity, let us focus our exposition on the case of \(k = 1\) and drop the subscript from \(B_i, Z_i\) etc. Generalization to an arbitrary \(k\) is straightforward. We define the metric on \(\text{St}_\mathcal{B}\) using a matrix \(\mathbf{M}\) formed from sketching \(\mathbf{Z}\) prior to computing the Gram matrix. Our proposed construction of \(\mathbf{M}\) requires \(O(nd^2)\) operations, which is cheaper than computing \(\mathbf{B}\) as required with the use of the standard metric.

Our randomized construction of \(\mathbf{M}\) is based on the following observation: in many cases, if \(\mathbf{M}\) approximates \(\mathbf{B}\) in the sense that the condition number \(\kappa(\mathbf{B}, \mathbf{M})\) is small, then convergence will be fast. Conceptually, the last observation is synonymous with the observation that usually the standard metric is a good choice iteration complexity-wise, albeit a computationally expensive choice, and thus we should aim at cheaply approximating it. Mathematically, the underlying reason is that in many cases the condition number of the Riemannian Hessian at the optimum is bounded by the product of \(\kappa(\mathbf{B}, \mathbf{M})\) and a problem/input dependent quantity which is typically small. It is known in the Riemannian optimization literature that the convergence rate can be analyzed by inspecting the condition number of the Riemannian Hessian at the optimum (e.g., [1] Section 4.1 and Theorem 4.5.6), [7] Definition 4.5 and Section 4.6).

We demonstrate the observation that when \(\mathbf{M}\) approximates \(\mathbf{B}\) well then the Riemannian Hessian at the optimum is well conditioned on two important use-cases: CCA and FDA (see Theorems 5 and 10). Indeed, we show that under certain assumptions, both for CCA and FDA we can bound the condition number at the optimum by the product of some baseline condition number that depends on eigengaps, and the condition number of \(\kappa(\mathbf{B}, \mathbf{M})\).

We propose to construct \(\mathbf{M}\) using the technique of sketching [57]. Let \(\mathbf{S} \in \mathbb{R}^{s \times n}\) is some sketching matrix (a certain distribution on matrices; we discuss a concrete choice in the next paragraph). We then use \(\mathbf{M} = \mathbf{Z}^T \mathbf{S}^T \mathbf{S} \mathbf{Z} + \lambda I_d\). However, we do not propose to actually compute \(\mathbf{M}\). Using the metric defined by \(\mathbf{M}\) requires only taking products with \(\mathbf{M}\) and \(\mathbf{M}^{-1}\) (see Table (1)). Suppose we have already computed \(\mathbf{SZ}\). The product of \(\mathbf{M}\) with a vector can be computed in \(O(\text{nnz}(\mathbf{S}^T \mathbf{Z}))\) operations. As for \(\mathbf{M}^{-1}\), by computing a QR factorization of \(\mathbf{SZ} \sqrt{\lambda I_d} \) \((O(sd^2)\) operations), we can obtain a Cholesky factorization of \(\mathbf{M}\), and then taking the product of \(\mathbf{M}^{-1}\) with a vector requires \(O(d^2)\). So our goal is to design sketching matrices \(\mathbf{S}\) such
that $SZ$ is cheap to compute, and for which $\kappa(B, M)$ is bounded by a constant.

There are quite a few sketching distributions proposed in the literature, and most of them are good choices for $S$. For concreteness, we describe a specific choice: the COUNTSKETCH transformation \[11\] \[10\] (although Subsampled Randomized Hadamard Transform (SRHT) \[51\] \[8\] is also a good choice, in particular for dense datasets). COUNTSKETCH is specified by a random hash function $h : \{1, \ldots, d\} \rightarrow \{1, \ldots, s\}$ and random sign function $g : \{1, \ldots, d\} \rightarrow \{-1, +1\}$. Applying $S$ to a vector $x$ is given by the formula

$$\langle Sx \rangle_i = \sum_{j \mid h(j) = i} g(j) x_j.$$

It is easy to see that $S$ is a random matrix in which the $j$th column contains a single nonzero entry $g(j)$ in the $h(j)$th row. Clearly, $SZ$ can be computed using $O(\text{nnz}(Z)) = O(nd)$ arithmetic operations. Thus, it only remains to bound the condition number. The following lemma shows that if the sketch size is large enough, then with high probability the condition number is bounded by a constant.

**Lemma 1.** Assume that $\lambda > 0$ or that $Z \in \mathbb{R}^{n \times d}$ has full column rank. Let $s_\lambda(Z) := \text{Tr} \left( (Z^T Z + \lambda I)^{-1} Z^T Z \right)$. Suppose that $S$ is a COUNTSKETCH matrix with $s \geq 20s_\lambda(Z)^2/\delta$ for some $\delta \in (0, 1)$. Then with probability of at least $1 - \delta$ we have that all the generalized eigenvalues of the pencil $(Z^T Z + \lambda I, Z^T S^T SZ + \lambda I)$ are contained in the interval $[1/2, 3/2]$ and $\kappa(Z^T Z + \lambda I, Z^T S^T SZ + \lambda I) \leq 3$.

**Proof.** The argument is rather standard and appeared in similar forms in the literature. To show that the generalized eigenvalues of the pencil $(Z^T Z + \lambda I, Z^T S^T SZ + \lambda I)$ are contained in the interval $[1/2, 3/2]$ and that $\kappa(Z^T Z + \lambda I, Z^T S^T SZ + \lambda I) \leq 3$ to hold, it is enough to show that

$$\frac{1}{2} (Z^T Z + \lambda I) \leq Z^T S^T SZ + \lambda I \leq \frac{3}{2} (Z^T Z + \lambda I).$$

Let $Z = QR$ be a $\lambda$-QR factorization of $Z$ (see \[3\] for a definition). Multiplying by $R^{-1}$ on both sizes, we find it suffices to show that with probability of at least $1 - \delta$ we have

$$\frac{1}{2} I_d \leq Q^T S^T SQ + \lambda R^{-T} R^{-1} \leq \frac{3}{2} I_d,$$

or, equivalently,

$$\|Q^T S^T SQ + \lambda R^{-T} R^{-1} - I_d\|_2 \leq \frac{1}{2}.$$

Since $Q^T S^T SQ + \lambda R^{-T} R^{-1} - I_d = Q^T S^T SQ - Q^T Q$ \[3\] and the spectral norm is dominated by the Frobenius norm, it is enough to show that

$$\|Q^T S^T SQ - Q^T Q\|_F \leq \frac{1}{2}.$$

It is known \[7\] that for any two fixed matrices $A$ and $B$, and a COUNTSKETCH matrix $S_0$ with $m \geq 5/(\epsilon^2 \delta)$ rows, we have that with probability of at least $1 - \delta$,

$$\|A^T S_0^T S_0 B - A^T B\|_F \leq \epsilon \cdot \|A\|_F \cdot \|B\|_F.$$

Since $\|Q\|_F^2 = s_\lambda(Z)$ \[3\], then with $s \geq 20s_\lambda(Z)^2/\delta$ we have

$$\|Q^T S^T SQ - Q^T Q\|_F \leq \frac{1}{2}$$

with probability of at least $1 - \delta$. □
The last lemma justifies the use of CountSketch to form the preconditioner \( M \). In practice, additional heuristics that improve running time and robustness can be inserted into the construction of randomized preconditioners, and these can improve running considerably; see \[ \text{[?]}. \]

Furthermore, our sketching-based preconditioner construction naturally allows for a warm-start. While this is not captured by our theory, heuristically (and empirically) the Riemannian optimization part of our proposed algorithm converges faster if the starting vectors are close to the optimum. Our sketching approach lets us quickly compute good starting vectors (these are the sketch-and-solve approximations). We demonstrate warm-start numerically in Section \[ \text{[?]} \] for CCA and FDA.

In Table \[ \text{[?]}. \] we detail the computational cost, measured in terms of arithmetic operations, of computing the Riemannian components of Table \[ \text{[?]}. \] for our construction of \( M \) as a preconditioner. Table \[ \text{[?]}. \] is based on \[ \text{[?]} \] Table \[ \text{[?]}. \]. Note that all the costs are for operations in ambient coordinates. In the table, we denote by \( T_{\nabla f} \) and by \( T_{\nabla^2 f} \) the cost of computing the Euclidean gradient and the cost of applying the Euclidean Hessian to a tangent vector. Instead of committing to a specific sketch size, we use \( s \) for sketch size (number of rows), and consider two possible sketching distributions: CountSketch and SRHT.

**Remark 2.** In Table \[ \text{[?]}. \] we assumed, for simplicity, that \( s \geq d \). However, if \( \lambda \) is sufficiently large, it is possible for the prescribed values of \( s (s \geq 20s_3(Z)^2/\delta) \) to be smaller than \( d \). In such cases, we can reduce the \( O(sd^2) \) term in the complexity to \( O(sd \min(s,d)) \) by employing the Woodbury formula. We omit the details.

### 4 Sketched Iterative CCA

CCA, originally introduced by Hotelling in 1936 \[ \text{[?]}. \], is a well-established method in statistical learning with numerous applications (e.g., \[ \text{[?] [?] [?] [?] [?] [?] [?] [?] [?]}. \]). In CCA, the relation between a pair of datasets in matrix form is analyzed, where the goal is to find the directions of maximal correlation between a pair of observed variables. In the language of linear algebra, CCA measures the similarities between two subspaces spanned by the columns of the two matrices, whereas in the geometric point of view, CCA computes the cosine of the principle angles between the two subspaces. We consider a regularized version of CCA defined below:\[ \text{[?]}. \]

\[ \text{Table 2: Summary of the cost of various components for using sketching based Riemannian preconditioning for generalized orthogonality constraints.} \]

| Operation | Cost using CountSketch | Cost using SRHT |
|-----------|------------------------|-----------------|
| Preprocessing: computing \(SZ\) | \(O(\text{nnz}(Z)) = O(nd)\) | \(O(nd \log(n))\) |
| Preprocessing: given \(SZ\) forming the inverse of \(M = Z^T S^T S Z + M_d\) | \(O(sd^2 + d^2)\) | \(O(sd^2 + d^2)\) |
| Retraction | \(O(\text{nnz}(Z)p + dp^2)\) | \(O(\text{nnz}(Z)p + dp^2)\) |
| Inner product on the tangent space (Riemannian metric) | \(O(\text{nnz}(SZ)p + dp)\) | \(O(dsp + dp)\) |
| Orthogonal projections on the tangent/normal space | \(O(\text{nnz}(Z)p + d^2p + dp^2)\) | \(O(\text{nnz}(Z)p + d^2p + dp^2)\) |
| Riemannian gradient | \(O(\text{nnz}(Z)p + d^2p + dp^2 + T_{\nabla f})\) | \(O(\text{nnz}(Z)p + d^2p + dp^2 + T_{\nabla f})\) |
| Applying the Riemannian Hessian to a tangent vector | \(O(\text{nnz}(Z)p + d^2p + \text{nnz}(SZ)p + dp^2 + T_{\nabla f} + T_{\nabla^2 f})\) | \(O(\text{nnz}(Z)p + d^2p + dp + dp^2 + T_{\nabla f} + T_{\nabla^2 f})\) |

The definition is formulated as a linear algebra problem. While the problem can be motivated, and described, in the language of statistics, the linear algebraic formulation is more convenient for our purposes.
Definition 3. Let $X \in \mathbb{R}^{n \times d_x}$ and $Y \in \mathbb{R}^{n \times d_y}$ be two data matrices, and $\lambda_x, \lambda_y \geq 0$ be two regularization parameters. Let $q = \max \left( \text{rank} \left( X^T X + \lambda_x I_{d_x} \right), \text{rank} \left( Y^T Y + \lambda_y I_{d_y} \right) \right)$. The $(\lambda_x, \lambda_y)$-canonical correlations $\sigma_1 \geq \cdots \geq \sigma_q$ and the $(\lambda_x, \lambda_y)$-canonical weights $u_1, \ldots, u_q, v_1, \ldots, v_q$ are the arguments that maximize $\text{Tr} \left( U^T X^T Y V \right)$ subject to

$$U^T (X^T X + \lambda_x I_{d_x}) U = I_q, \quad V^T (Y^T Y + \lambda_y I_{d_y}) V = I_q, \quad U^T X^T Y V = \text{diag} (\sigma_1, \ldots, \sigma_q),$$

where $U = [u_1 \ldots u_q] \in \mathbb{R}^{d_x \times q}$ and $V = [v_1 \ldots v_q] \in \mathbb{R}^{d_y \times q}$.

4.1 CCA as an Optimization Problem on a Product of Generalized Stiefel Manifolds

We focus on finding $\sigma_1, \ldots, \sigma_p, u_1, \ldots, u_p$ and $v_1, \ldots, v_p$, where $p \leq q$ is a parameter, i.e., on finding the top $p$-canonical correlations and the corresponding left and right vectors. For convenience, we use the following notations:

$$\Sigma_{xx} := X^T X + \lambda_x I_{d_x}, \quad \Sigma_{yy} := Y^T Y + \lambda_y I_{d_y}, \quad \Sigma_{xy} := X^T Y.$$ 

With these notations, we can reformulate the problem of finding the top $p$-canonical correlations succinctly in the following way:

$$\max \text{Tr} \left( U^T \Sigma_{xy} V \right) \quad \text{s.t.} \quad U^T \Sigma_{xx} U = I_p, \quad V^T \Sigma_{yy} V = I_p, \quad U^T \Sigma_{xy} V \text{ is diagonal with non-increasing diagonal}$$

Notice that without the last constraint, Problem (4.1) is a maximization over the product of two generalized Stiefel manifolds. However, without this constraint the solution is not unique. The reason for that is that the trace operator and the constraint set are invariant to multiplication by orthonormal matrices, and so there are optimal values that are non-diagonal (and so additional steps are needed to extract the canonical correlations from such values). In order to circumvent this issue, we use a well-known method to modify such problems so to make the solution unique. The modification is based on the von Neumann cost function $54$. That is, we replace the objective function $\text{Tr} \left( U^T \Sigma_{xy} V \right)$ with $\text{Tr} \left( U^T \Sigma_{xy} VN \right)$ where $N = \text{diag} (\mu_1, \ldots, \mu_p)$ and we take arbitrary $\mu_1, \ldots, \mu_p$ such that $\mu_1 > \cdots > \mu_p > 0$. In other words, the problem we wish to solve is

$$\max \text{Tr} \left( U^T \Sigma_{xy} VN \right) \quad \text{s.t.} \quad U^T \Sigma_{xx} U = I_p, \quad V^T \Sigma_{yy} V = I_p.$$ 

In the next subsection, we detail the Riemannian components which allow to solve the CCA problem. We show that critical points of the corresponding objective function consist of coordinated left and right canonical correlation vectors not necessarily on the same phase. In particular, the optimal solutions are critical points consisting of coordinated left and right top $p$-canonical correlation vectors on the same phase.

4.2 Preconditioned Riemannian Components for CCA

In this subsection we derive the Riemannian components associated with the CCA problem. The CCA problem is a constrained maximization problem on the product of two generalized Stiefel manifolds: $\text{St}_{\Sigma_{xx}} (p, d_x)$ and $\text{St}_{\Sigma_{yy}} (p, d_y)$. We denote the search space by $\mathbb{S}_{xy} := \text{St}_{\Sigma_{xx}} (p, d_x) \times \text{St}_{\Sigma_{yy}} (p, d_y)$. We consider the use of Riemannian optimization for solving the CCA problem, while exploiting the geometry of the preconditioned generalized Stiefel manifold and use the notion of product manifold. To make the calculations easier, we denote $d = d_x + d_y$ and $Z := \left[ U^T \ V^T \right]^T \in \mathbb{R}^{d \times p}$ where $U \in \text{St}_{\Sigma_{xx}} (p, d_x)$ and $V \in \text{St}_{\Sigma_{yy}} (p, d_y)$. Henceforth, we abuse notation and view $\mathbb{S}_{xy}$ as a subset of $\mathbb{R}^{d \times p}$ given by this coordinate split, and also write $Z = (U, V)$ as a shorthand for $Z = \left[ U^T \ V^T \right]^T$. With these conventions, the optimization problem can be rewritten in the following way:
min \sum_{Z \in S_{xy}} f_{CCA}(Z), \ f_{CCA}(Z) := -\frac{1}{2} \text{Tr} \left( Z^T \left[ \Sigma_{xy}^{T} \Sigma_{xy} \right] Z \right) \tag{4.1}

For a product of disjoint Generalized Stiefel manifolds, if the number of columns of the matrices that belong to each of the manifolds is the same, the various Riemannian components can be computed separately on each of the manifolds and then stacked on top of each other. We use some SPD matrices \(M^{(xx)}\) and \(M^{(yy)}\) to define Riemannian metrics on \(S_{\Sigma_{xx}}(p, d_x)\) and \(S_{\Sigma_{yy}}(p, d_y)\) (respectively), and these, in turn, define a Riemannian metric on \(S_{xy}\) via 
\[
M := \text{blkdiag}(M^{(xx)}, M^{(yy)})
\]
For \(U \in S_{\Sigma_{xx}}(p, d_x)\), let \(\Pi_U(\cdot)\) denote the projection on \(T_U S_{\Sigma_{xx}}(p, d_x)\), and similarly for \(\Pi_V(\cdot)\) where \(V \in S_{\Sigma_{yy}}(p, d_y)\). Similarly, let \(\Pi_U^{\perp}(\cdot)\) and \(\Pi_V^{\perp}(\cdot)\) be the projections on the corresponding normal spaces. Given \(Z \in S_{xy}\) the orthogonal projection on the tangent space \(T_Z S_{xy}\) is \(\Pi_Z(\xi Z) = (\Pi_U(\xi U), \Pi_V(\xi V))\) where \(\xi Z := (\xi U, \xi V) \in \mathbb{R}^{d \times p}\).

Let \(f_{CCA}\) be extended smoothly to be defined on \(\mathbb{R}^{d \times p}\) where \(f_{CCA}\) is defined by Eq. (4.1) as well. The following are analytical expressions for the Riemannian gradient and the Riemannian Hessian in ambient coordinates:

\[
\nabla f_{CCA}(Z) = \Pi_Z \left( M^{-1} \nabla f_{CCA}(Z) \right) = -\left[ \begin{array}{c}
\Pi_U \left( (M^{(xx)})^{-1} \Sigma_{xy} VN \right) \\
\Pi_V \left( (M^{(yy)})^{-1} \Sigma_{xy}^T UN \right)
\end{array} \right], \tag{4.2}
\]

\[
\nabla^2 f_{CCA}(Z) = \Pi_Z \left( M^{-1} \left[ -\Sigma_{xy}^2 f_{CCA} \xi Z N + \Sigma \left[ \xi U \Sigma_{xy} VN + \xi V \Sigma_{xy} ^T UN \right] \right. \right.
\]
\[
\left. \left. + \Sigma \left[ \xi U \Sigma_{xy} VN \xi V \Sigma_{xy} ^T UN \right] \right) \right)
\]

along with formulas for the retraction and vector transport, various Riemannian optimization algorithms can be applied to solve Problem (4.1). In the next theorem, we summarize the critical points. In the theorem statement, a pair of left and right canonical correlation vectors \(u\) and \(v\) are on the same phase if \(u^T X^T Y v \geq 0\).

**Theorem 4.** A point \(Z = (U, V) \in S_{xy}\) is a critical point of \(f_{CCA}(Z)\) on \(S_{xy}\) if and only if the columns of \(U\) and \(V\) are left and right canonical correlation vectors not necessarily on the same phase.

The optimal solutions of minimizing \(f_{CCA}(Z)\) on \(S_{xy}\) are critical points \(Z\) such that the columns of \(U\) and \(V\) are coordinated left and right top \(p\)-canonical correlation vectors on the same phase. Moreover, the optimal solution is unique up to sign of the columns of \(U\) and \(V\) if \(\sigma_1 > \sigma_2 > ... > \sigma_{p+1} \geq 0\).

**Proof.** Recall that critical points are ones in which the Riemannian gradient is zero, and as such, whether a point is a critical point or not does not depend on the choice of Riemannian metric (see [1] Eq. 3.31). Thus, for the sake of identifying the critical points, we can use \(M = \Sigma\) and get a simplified form for the Riemannian gradient (Eq. (4.2)):

\[
\nabla f_{CCA}(Z) = -\left[ \begin{array}{c}
\Sigma_{xx}^{-1} \Sigma_{xy} VN - \text{Usym} \left( U^T \Sigma_{xx}^{-1} \Sigma_{xy} VN \right) \\
\Sigma_{yy}^{-1} \Sigma_{xy}^T UN - \text{Vsym} \left( V^T \Sigma_{yy}^{-1} \Sigma_{xy}^T UN \right)
\end{array} \right]
\]

\[
= -\left[ \begin{array}{c}
(I_{d_x} - U U^T \Sigma_{xx}) \Sigma_{xx}^{-1} \Sigma_{xy} VN + \text{Uskew}(U^T \Sigma_{xy} VN) \\
(I_{d_y} - V V^T \Sigma_{yy}) \Sigma_{yy}^{-1} \Sigma_{xy}^T UN + \text{Vskew}(V^T \Sigma_{xy}^T UN)
\end{array} \right].
\]
There is a connection between the canonical correlations and the singular value decomposition of $\mathbf{R} := \Sigma_{xx}^{-1/2} \Sigma_{xy} \Sigma_{yy}^{-1/2}$ [50]: a pair of vectors $\mathbf{u}$ and $\mathbf{v}$ are canonical correlation vectors corresponding to the same canonical correlation if and only if $\tilde{\mathbf{u}} = \Sigma_{xx}^{1/2} \mathbf{u}$ and $\tilde{\mathbf{v}} = \Sigma_{yy}^{1/2} \mathbf{v}$ are left and right singular vectors of $\mathbf{R}$ corresponding to the same singular value.

Canonical correlation vectors are the columns of $\mathbf{U}$ and $\mathbf{V}$ it and only if the columns of $(\tilde{\mathbf{U}}, \tilde{\mathbf{V}}) = (\Sigma_{xx}^{1/2} \mathbf{U}, \Sigma_{yy}^{1/2} \mathbf{V})$ are $p$ left and right coordinated singular vectors of the matrix $\mathbf{R}$. Thus, we use this relation to prove this theorem.

To show that all $\mathbf{Z} \in \mathbb{S}_{xy}$ such that the columns of $\mathbf{U}$ and $\mathbf{V}$ are left and right coordinated canonical correlation vectors not necessarily on the same phase are critical points, let $\alpha_1, \ldots, \alpha_p$ be some singular values of $\mathbf{R}$, and let $\tilde{\mathbf{u}}_1, \ldots, \tilde{\mathbf{u}}_p, \tilde{\mathbf{v}}_1, \ldots, \tilde{\mathbf{v}}_p$ be the corresponding left and right singular vectors not necessarily on the same phase. Writing $\tilde{\mathbf{u}}_i, \ldots, \tilde{\mathbf{u}}_p$ as the columns of $\mathbf{U}$ and and $\tilde{\mathbf{v}}_1, \ldots, \tilde{\mathbf{v}}_p$ as the columns of $\mathbf{V}$, and defining $\mathbf{U} = \Sigma_{xx}^{-1/2} \tilde{\mathbf{U}}, \mathbf{V} = \Sigma_{xx}^{-1/2} \tilde{\mathbf{V}}$, the following two equations hold:

$$\Sigma_{xy} \mathbf{V} = \Sigma_{xx} \mathbf{U} \mathbf{A}, \quad \Sigma_{xy}^T \mathbf{U} = \Sigma_{yy} \mathbf{V} \mathbf{A}$$

where $\mathbf{A} := \text{diag} (\beta_1, \ldots, \beta_p)$ such that $|\beta_i| = \alpha_i$ for $i = 1, \ldots, p$. Letting $\mathbf{Z} = (\mathbf{U}, \mathbf{V}) \in \mathbb{S}_{xy}$, we have

$$\text{grad}_{\text{CCA}}(\mathbf{Z}) = -\begin{bmatrix} \mathbf{U} \mathbf{A} - \mathbf{U} \text{sym} \left( \mathbf{U}^T \Sigma_{xx} \mathbf{A} \right) \\ \mathbf{V} \mathbf{A} - \mathbf{V} \text{sym} \left( \mathbf{V}^T \Sigma_{yy} \mathbf{A} \right) \end{bmatrix} = \begin{bmatrix} 0_{dx \times p} \\ 0_{dy \times p} \end{bmatrix}$$

where the last line is true since $\mathbf{A} \mathbf{N}$ is diagonal.

To show the other side, note that if the Riemannian gradient nullifies, then

$$\begin{bmatrix} (\mathbf{I}_{dx} - \mathbf{U} \mathbf{U}^T \Sigma_{xx}) \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{V} \mathbf{N} + \text{Uskew}(\mathbf{U}^T \Sigma_{xy} \mathbf{V} \mathbf{N}) \\ (\mathbf{I}_{dy} - \mathbf{V} \mathbf{V}^T \Sigma_{yy}) \Sigma_{yy}^{-1} \Sigma_{xy} \mathbf{U} \mathbf{N} + \text{Vskew}(\mathbf{V}^T \Sigma_{xy} \mathbf{U} \mathbf{N}) \end{bmatrix} = \begin{bmatrix} 0_{dx \times p} \\ 0_{dy \times p} \end{bmatrix}.$$

By using similar reasoning as in [1] Subsection 4.8.2, $(\mathbf{I}_{dx} - \mathbf{U} \mathbf{U}^T \Sigma_{xx}) \Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{V} \mathbf{N} = 0_{dx \times p}$ we get $\Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{V} = \mathbf{U} (\mathbf{U}^T \Sigma_{xy} \mathbf{V})$, since $\mathbf{N}$ is an invertible matrix. Also, since $\mathbf{U} \in \text{St}_{\Sigma_{xx}}(p, dx)$ it is a full (column) rank matrix then $\text{Uskew}(\mathbf{U}^T \Sigma_{xy} \mathbf{V} \mathbf{N})$ vanishes if and only if $\text{skew}(\mathbf{U}^T \Sigma_{xy} \mathbf{V} \mathbf{N})$ vanishes, which leads to $(\mathbf{U}^T \Sigma_{xy} \mathbf{V}) \mathbf{N} = \mathbf{N} (\mathbf{U}^T \Sigma_{xy} \mathbf{V})$. This implies that $\mathbf{U}^T \Sigma_{xy} \mathbf{V}$ is diagonal because any rectangular matrix that commutes with a diagonal matrix with distinct entries is diagonal. Thus, we have

$$\Sigma_{xx}^{-1} \Sigma_{xy} \mathbf{V} = \mathbf{U} \mathbf{D}, \quad \text{(4.4)}$$

where $\mathbf{D} = \mathbf{U}^T \Sigma_{xy} \mathbf{V}$ is diagonal. Similarly, we have

$$\Sigma_{xy}^{-1} \Sigma_{yy}^T \mathbf{U} = \mathbf{V} \mathbf{D}, \quad \text{(4.5)}$$

where $\mathbf{D} = \mathbf{V}^T \Sigma_{xy}^T \mathbf{U} = \mathbf{U}^T \Sigma_{xy} \mathbf{V}$ is diagonal. From Eq. (4.4) and Eq. (4.5) we get

$$\mathbf{R} \Sigma_{yy}^{1/2} \mathbf{V} = \Sigma_{xx}^{1/2} \mathbf{UD}, \quad \mathbf{R}^T \Sigma_{xx}^{1/2} \mathbf{U} = \Sigma_{yy}^{1/2} \mathbf{VD}.$$

This implies that the columns of $(\tilde{\mathbf{U}}, \tilde{\mathbf{V}}) = (\Sigma_{xx}^{1/2} \mathbf{U}, \Sigma_{yy}^{1/2} \mathbf{V})$ are some $p$ left and right singular vectors of $\mathbf{R}$ not necessarily on the same phase, but corresponding to the same singular values.

Finally, to identify the optimal solutions, note that at the critical points the objective function is the sum of the canonical correlations multiplied by a diagonal element of $\mathbf{N}$, and a sign corresponding to the canonical
correlation vectors in the columns of $U$ and $V$ and the correspondence of their phase. Thus, the optimal solutions that minimize $f_{\text{CCA}}(Z)$ on $S_{xy}$ are $Z = (U, V) \in S_{xy}$ such that the columns of $U$ and $V$ correspond to the top $p$-canonical correlations on the same phase. Otherwise, we can increase the value of the objective function either by flipping the sign of one of the vectors or by replacing a canonical vector with another that corresponds to a smaller canonical correlation. Moreover, if we assume that $\sigma_1 > \sigma_2 > ... > \sigma_{p+1} \geq 0$, then for the aforementioned $Z = (U, V) \in S_{xy}$, the columns of $(U, V)$ belong each to a one dimensional singular left and right space and so do the columns of the corresponding $(U, V)$, i.e., unique solution up the the signs of the columns of $(U, V)$. In the case where some $\sigma_i = \sigma_j$ for $1 \leq i, j \leq p$, permutations of the columns of $U$ and $V$ associated with $\sigma_i$ keep the solution optimal making it non-unique. 

Naturally, we want our proposed optimization algorithm to converge to an optimal point. In Theorem 4 we characterized all the critical points of $f_{\text{CCA}}(Z)$ on $S_{xy}$. In general, a typical guarantee for Riemannian optimization algorithms is that for a sequence of iterates, all the accumulation points of the sequence are critical points (e.g. [1] Theorem 4.3.1]). Unfortunately, this guarantee does not specify to which of the critical points the convergence is to. However, we can utilize the fact that in practice, for a sufficiently close initial guess, Riemannian optimization methods converge to the stable critical points and do not converge to unstable critical points [1] Section 4.4. We analyze the stability of the various critical points of $f_{\text{CCA}}(Z)$ on $S_{xy}$ in Appendix A and show that under mild assumptions the solutions of Problem (4.1) are asymptotically stable, while other critical points are unstable.

4.3 The Effect of Preconditioning on the Convergence

The following theorem allows us to reason about the quality of a preconditioner for the CCA problem. In this theorem, we bound the condition number at the optimum based on how well the preconditioner approximates a specific matrix ($\Sigma$). Due to the length of the proof, we delegate it to Appendix C.1.

**Theorem 5.** Consider using Riemannian optimization to minimize $f_{\text{CCA}}(Z)$ subject to $Z \in S_{xy}$, where we use the Riemannian metric defined by $M = \text{blkdiag}(M^{(xx)}, M^{(yy)})$ where $M^{(xx)} \in \mathbb{R}^{d_x \times d_x}$ and $M^{(yy)} \in \mathbb{R}^{d_y \times d_y}$ are given preconditioners matrices. Also assume that $\sigma_1 > \sigma_2 > ... > \sigma_{p+1} \geq 0$ and that $\Sigma$ is a SPD matrix. Then at the global minimizer of $f_{\text{CCA}}(Z)$ subject to $Z \in S_{xy}$, denoted by $Z^* = (U^*, V^*)$, the following bound on the condition number of the Riemannian Hessian at $Z^*$ holds

$$\kappa(\text{Hess} f_{\text{CCA}}(Z^*)) \leq \kappa_{\text{CCA}}^* \cdot \kappa(\Sigma, M)$$

where

$$\kappa_{\text{CCA}}^* := \frac{\max \{\mu_p(\sigma_1 + \sigma_p + 1), \frac{1}{2}(\mu_1 + \mu_2)(\sigma_1 + \sigma_2)\}}{\min \{\mu_p(\sigma_p - \sigma_{p+1}), \min_{1 \leq j < p} \frac{1}{2} (\mu_j - \mu_{j+1})(\sigma_j - \sigma_{j+1})\}}$$

and $\mu_1 > ... > \mu_p > 0$. If $M = \Sigma$ then $\kappa(\text{Hess} f_{\text{CCA}}(Z^*)) = \kappa_{\text{CCA}}^*$.

4.4 Randomized Preconditioning for CCA

The condition number bound in Theorem 5 separates two factors: $\kappa_{\text{CCA}}^*$ and $\kappa(\Sigma, M)$. The first, $\kappa_{\text{CCA}}^*$, depends on the gap between the $p + 1$ largest canonical correlations and on the differences between the values in $N$, which are parameters for the CCA problem as a Riemannian optimization problem. The dependence on the gap almost always appears in problems of this form, since the more the singular values are distinct it is easier to distinguish between them. The second component, $\kappa(\Sigma, M)$, measures how close the preconditioner, which defines the Riemannian metric, approximates $\Sigma$. The preconditioner that minimizes the bound in Theorem 5 is $M = \Sigma$. However, using that preconditioner, requires explicitly computing a
Theorem 5 provides an argument in favor of our proposed randomized preconditioner, i.e., easy to factorize \( M \) such that \( \kappa(\Sigma, M) \) is bounded. In order to achieve this goal, the preconditioners \( M^{(xx)} \) and \( M^{(yy)} \) should approximate \( \Sigma_{xx} = X^T X + \lambda_x I_{d_x} \) and \( \Sigma_{yy} = Y^T Y + \lambda_y I_{d_y} \) respectively as described in Section 3 (i.e., using sketching for \( X \) and \( Y \) correspondingly). A pseudocode description of an end-to-end randomized preconditioned CCA algorithm with warm-start appears in Algorithm 1. The following corollary summarizes our theoretical results regarding the proposed algorithm. We remark that COUNTSKETCH can possibly be replaced with other sketching transforms (such as SRHT), and Riemannian CG can be replaced with other Riemannian optimization methods, although the bounds in the corollary might change.

**Corollary 6.** Consider Algorithm 1. Let \( \delta \in (0, 1) \) and denote \( s_\lambda = \max(s_{\lambda_x}(X), s_{\lambda_y}(Y)) \). If \( s = \max([0.4 s_\lambda^2/\delta], d) \), then with probability of at least \( 1 - \delta \), the condition number of the Riemannian Hessian at the optimum is bounded by \( 3 c_{\text{CCA}} / s \), regardless of the condition number of \( \Sigma_{xx} \) and \( \Sigma_{yy} \). Furthermore, assuming we use Riemannian CG, all computations are done in ambient \( \mathbb{R}^{d_x \times p} \) coordinates, then the preprocessing steps take \( O(n \text{nnz}(X) + n \text{nnz}(Y)) = O(nd) \) and \( O(nd^2 + d^2) \). Assuming a bounded number of line-search steps in each iteration then each iteration takes \( O(p (n \text{nnz}(X) + n \text{nnz}(Y)) + dp^2 + d^2 p) \).

**Proof.** The condition number bound follows from Lemma 4 and Theorem 5 with one additional argument. From Lemma 4 we know that with probability of at least \( 1 - \delta \) we have that all the generalized eigenvalues of the pencil \( (\Sigma_{xx}, M^{(xx)}) \) are contained in the interval \([1/2, 3/2]\), and the same is true for the pencil \( (\Sigma_{yy}, M^{(yy)}) \). Recall that all the generalized eigenvalues of the pencil \( (\Sigma_{xx}, M^{(xx)}) \) are also generalized eigenvalues of the pencil \( (\Sigma, M) \), and the same is true for the generalized eigenvalues of \( (\Sigma_{yy}, M^{(yy)}) \). Indeed, after an appropriate padding with zeros each generalized eigenvector of \( (\Sigma_{xx}, M^{(xx)}) \) or \( (\Sigma_{yy}, M^{(yy)}) \) is a generalized eigenvector of \( (\Sigma, M) \). Thus, since \( (\Sigma_{xx}, M^{(xx)}) \) and \( (\Sigma_{yy}, M^{(yy)}) \) have \( d_x \) and \( d_y \) generalized eigenvalues and corresponding eigenvectors, they characterize all the generalized eigenvalues and corresponding eigenvectors of \( (\Sigma, M) \). Thus, also the eigenvalues of the pencil \( (\Sigma, M) \) are contained in the interval \([1/2, 3/2]\), and subsequently \( \kappa(\Sigma, M) \leq 3 \). Using Theorem 5 we get the require bound for the condition number.

The costs are evident from Table 2, once we observe that none of the operations require forming \( \Sigma_{xx}, \Sigma_{yy} \) or \( \Sigma_{xy} \), but instead require taking product of these matrices with vectors. These products can be computed in cost proportional to the number of non-zeros in \( X \) and/or \( Y \) by iterated products. In addition, we use the fact that \( SX \) and \( SY \) can be computed in \( O(n \text{nnz}(X)) = O(nd_x) \) and \( O(n \text{nnz}(Y)) = O(nd_y) \) operations. The required preprocessing is to factorize \( M^{(xx)} \) and \( M^{(yy)} \), so we can efficiently take products with \( (M^{(xx)})^{-1} \).
With these notations, we can reformulate the problem of finding the within-class and between-class scatter is minimized. In this paper, we consider a regularized version of FDA as defined below:

Definition 7. [20, Section 4.11] Let \( X^{(i)} \) be samples from \( l \leq d \) different classes, and denote by \( x_1, \ldots, x_n \) the union of the different classes (the entire dataset in a sequential index). For \( i = 1, \ldots, n \), let \( y_i \) label the corresponding to \( x_i \), i.e., \( y_i = k \) if \( x_i = x_j^{(k)} \) for some \( j \). Let \( m_k \), for \( k = 1, \ldots, l \), denote the sample mean of class \( k \) (i.e., \( m_k := \frac{1}{n_k} \sum_{i=1}^{n_k} x_i^{(k)} \)), and \( m := \frac{1}{n} \sum_{i=1}^{n} x_i = \frac{1}{n} \sum_{k=1}^{l} n_k m_k \) denote the dataset sample mean of the entire dataset. Let \( S_B \) and \( S_w \) be the between-class and within-class scatter matrices (respectively):

\[
S_B := \sum_{k=1}^{l} n_k (m_k - m)(m_k - m)^T, \quad S_w := \sum_{i=1}^{n} (x_i - m_y)(x_i - m_y)^T.
\]

Let \( \lambda \geq 0 \) be a regularization parameter. The \( l - 1 \) FDA weight vectors \( w_1, \ldots, w_{l-1} \) are the columns of \( W \in \mathbb{R}^{d \times (l-1)} \) such that \( W \) is the maximizer of the following cost function:

\[
J(W) = \frac{\det(W^T S_B W)}{\det(W^T (S_w + \lambda I_d) W)}.
\]  

5 Sketched Iterative FDA

Fisher’s linear discriminant analysis (FDA), introduced by Fisher in 1936, is a well-known method for classification [22, 38], and more commonly for dimensionality reduction before classification [13]. The latter is achieved by finding an embedding such that simultaneously the between-class scatter is maximized and the within-class scatter is minimized. In this paper, we consider a regularized version of FDA as defined below:

5.1 FDA as an Optimization Problem on a Generalized Stiefel Manifold

It is well known that the solution of maximizing Eq. (5.1) (i.e., finding the FDA weight vectors) is equivalent to finding a matrix \( W \) such that its columns are the leading \( l - 1 \) generalized eigenvectors of the matrix pencil \( (S_B, S_w + \lambda I_d) \) [20, Section 4.11]. Note that this generalized eigenproblem has at most \( l - 1 \) nonzero generalized eigenvalues since the matrix \( S_w + \lambda I_d \) is a SPD matrix, and \( S_B \) is the sum of \( l \) matrices of rank one or less, where only \( l - 1 \) of these are independent, thus, \( S_B \) is of rank \( l - 1 \) or less. We denote the eigenvalues of the matrix pencil \( (S_B, S_w + \lambda I_d) \) with correspondence to the FDA weight vectors by \( \rho_1 \geq \rho_2 \geq \ldots \geq \rho_l \geq 0 \).

We focus on finding the \( p \) leading FDA weight vectors, i.e., \( w_1, \ldots, w_p \) corresponding to \( \rho_1 \geq \rho_2 \geq \ldots \geq \rho_p \), where \( p \leq l - 1 \). For the purpose of describing and analyzing our algorithm, it is useful to write:

\[
S_w = \hat{X}^T \hat{X}, \quad \hat{X} := X - \hat{Y}, \quad S_B = \hat{Y}^T \hat{Y},
\]

where \( \hat{X} \in \mathbb{R}^{n \times d} \) is a matrix such that each \( i \)-th row of \( \hat{X} \) is \( (x_i - m_y)^T \), \( \hat{Y} \in \mathbb{R}^{n \times d} \) is a matrix such that each \( i \)-th row of \( \hat{Y} \) is of the form \( m_y \), (thus, there are at most \( l \) different rows in \( \hat{Y} \)), and \( \hat{Y} \in \mathbb{R}^{l \times d} \) is a matrix such that each \( k \)-th row of \( \hat{Y} \) is \( \sqrt{\rho_k}(m_k - m)^T \). With these notations, we can reformulate the problem of finding the \( p \) leading FDA weight vectors as a

\[2\] For \( l = 2 \) the matrix \( S_B \) is defined by \( S_B = (m_1 - m_2)(m_1 - m_2)^T \). The definitions coincide after multiplying \( S_B = (m_1 - m_2)(m_1 - m_2)^T \) by \( 2 (n_1 n_2) / n \).
Riemannian optimization problem on the generalized Stiefel manifold (see [23 Section 10.2, Eq. 10.5]), i.e., finding the generalized eigenvalues of the matrix pencil $(S_B, S_w + \lambda I_d)$. We use the Brockett cost function [10] and obtain the following optimization problem

$$\max_{W \in \mathbb{R}^{d \times p}} \text{Tr} \left( W^T Y^T Y \right), \quad \text{s.t. } W^T (X^T X + \lambda I_d) W = I_p,$$  \hspace{1cm} (5.2)

where $N = \text{diag}(\mu_1, ..., \mu_p)$ where we take arbitrary $\mu_1, ..., \mu_p$ such that $\mu_1 > ... > \mu_p > 0$.

**Remark 8.** Problem (5.2) is actually a relaxation of the trace-ratio problem [55, 43], which provides superior results in various tasks (e.g., classification and clustering [55]). We focus on Problem (5.2) since it is amenable to our preconditioning strategy.

In the next subsection, we detail the Riemannian components which allow to solve the FDA problem. We show that critical points of the corresponding objective function are matrices $W$ such that the columns are some $p$ FDA weight vectors. In particular, the optimal solutions are critical points consisting of the $p$ leading FDA weight vectors. We further show that if $p_1, \ldots, p_{p+1}$ are distinct, the optimal solution is unique up to sign of the columns of $W$.

### 5.2 Preconditioned Riemannian Components for FDA

We first transform Problem (5.2) into a minimization problem:

$$\min_{\text{St}(S_w + \lambda I_d)(p, d)} f_{\text{FDA}}(W), \quad f_{\text{FDA}}(W) := -\frac{1}{2} \text{Tr} \left( W^T S_B W \right).$$  \hspace{1cm} (5.3)

We use of the components of the generalized Stiefel manifold with a Riemannian metric defined by a SPD matrix $M \in \mathbb{R}^{d \times d}$ to apply Riemannian optimization to solve Problem (5.3).

Let $\tilde{f}_{\text{FDA}}$ be $f_{\text{FDA}}$ extended smoothly to be defined on $\mathbb{R}^{d \times p}$ where $f_{\text{FDA}}$ is defined by Eq. (5.3) as well. For $W \in \text{St}(S_w + \lambda I_d)(p, d)$, let $\Pi_W(\cdot)$ denote the projection on $T_W \text{St}(S_w + \lambda I_d)(p, d)$. Similarly, let $\Pi_{\tilde{W}}(\cdot)$ be the projection on the corresponding normal space. The following are analytical expressions for the Riemannian gradient and Hessian in ambient coordinates:

$$\nabla f_{\text{FDA}}(W) = \Pi_W (M^{-1} \nabla \tilde{f}_{\text{FDA}}(W)) - \Pi_W (M^{-1} S_B W),$$  \hspace{1cm} (5.4)

$$\text{Hess} f_{\text{FDA}}(W)[\xi_W] = \Pi_W (M^{-1} [-S_B \xi_W + (S_w + \lambda I_d) \xi_W (W^T S_B W + \nabla f(W))]).$$  \hspace{1cm} (5.5)

Along with formulas for the retraction and vector transport, various Riemannian optimization algorithms can be applied to solve Problem (5.3). In the next theorem we summarize the critical points. The proof is almost the same as the proof of Theorem 4 thus delegated to Appendix D.1.

**Theorem 9.** A point $W \in \text{St}(S_w + \lambda I_d)(p, d)$ is a critical point of $f_{\text{FDA}}(W)$ on $\text{St}(S_w + \lambda I_d)(p, d)$ if and only if the columns of $W$ are some $p$ FDA weight vectors.

The optimal solutions of minimizing $f_{\text{FDA}}(W)$ on $\text{St}(S_w + \lambda I_d)(p, d)$ are critical points $W$ such that the columns are the $p$ leading FDA weight vectors. Moreover, the optimal solution is unique up to sign of the columns if $p_1 > p_2 > ... > p_{p+1} \geq 0$.

In the FDA problem, we want any optimization algorithm to converge to an optimal point. In Theorem 9 we prove that the critical points of $f_{\text{FDA}}(W)$ on $\text{St}(S_w + \lambda I_d)(p, d)$ are matrices $W \in \text{St}(S_w + \lambda I_d)(p, d)$ such that the columns are some $p$ FDA weight vectors. Similarly to the CCA problem, we analyze the stability of the critical points and show that under mild assumptions the optimal solutions of Problem (5.3) are asymptotically stable while other critical points are unstable (see Appendix B).
5.3 The Effect of Preconditioning on the Convergence

The following theorem provides a bound on the condition number of the Riemannian Hessian at the optimum based on how well the preconditioner approximates a specific matrix $(S_w + \lambda I_d)$. This theorem provides a general guideline in designing a Riemannian preconditioner via the Riemannian metric, and in particular motivates our proposed approach detailed in Subsection 5.4. The proof uses the same arguments as the proof of Theorem 5, though they are simplified considerably since only a single generalized Stiefel manifold is considered. In order to streamline this paper, we delegate the proof to Appendix D.3.

**Theorem 10.** Consider using Riemannian optimization to minimize $f_{\text{FDA}}(W)$ subject to $W \in \mathcal{S}t_{(S_w + \lambda I_d)}(p, d)$, where we use the Riemannian metric defined by $M \in \mathbb{R}^{d \times d}$, which is a given preconditioner matrix. Assume that $\rho_1 > \rho_2 > \ldots > \rho_{p+1} \geq 0$ and that $S_w + \lambda I_d$ is a SPD matrix. Let $W^\star$ denote the global minimizer of $f_{\text{FDA}}(W)$ subject to $W \in \mathcal{S}t_{(S_w + \lambda I_d)}(p, d)$. Then,

$$\kappa(\text{Hess}_{\text{FDA}}(W^\star)) \leq \kappa_{\text{FDA}}^\star \cdot \kappa(S_w + \lambda I_d, M)$$

where

$$\kappa_{\text{FDA}}^\star := \frac{\mu_1 (\rho_1 - \rho_d)}{\min\{\rho_p (\rho - \rho_{p+1}), \min_{1 \leq j < p} \frac{1}{2} (\mu_j - \mu_{j+1}) (\rho_j - \rho_{j+1})\}}$$

and $\mu_1 > \cdots > \mu_p > 0$. If $M = S_w + \lambda I_d$ then $\kappa(\text{Hess}_{\text{FDA}}(W^\star)) = \kappa_{\text{FDA}}^\star$.

5.4 Randomized Preconditioning for FDA

The bound on the condition number in Theorem 10 decomposes two components: the first, $\kappa_{\text{FDA}}^\star$, depends only on the FDA problem (and its formulation as an Riemannian optimization problem), and $\kappa_{\text{FDA}}^\star$ depends both on the gap between the $p + 1$ largest generalized eigenvalues, and on the diagonal elements of $N$, which are parameters of the optimization problem. The dependence on the gap almost always appears in problems of this form, since the more the generalized eigenvalues associated with the FDA weight vectors we search for are distinct it is easier to distinguish between them. The second component, $\kappa(S_w + \lambda I_d, M)$, measures how close the preconditioner defined metric approximates the natural metric for the constraints. The preconditioner, which minimizes the bound is $M = S_w + \lambda I_d$. However, using $M = S_w + \lambda I_d$ requires explicitly computing $S_w$ which costs $O(nd^2)$ arithmetic operations. As for the CCA problem, direct methods for solving FDA require $\Theta(nd^2)$ arithmetic operations as well (exact solution requires finding the inverse of $S_w + \lambda I_d$ and then finding the eigenvalues and corresponding eigenvectors of $(S_w + \lambda I_d)^{-1}S_B$). Thus, we want $M$ to approximate $S_w + \lambda I_d$, while allowing a cheap factorization which is satisfied by our proposed randomized preconditioning approach.

We propose to design the preconditioner in the following way: $M$ approximates $S_w + \lambda I_d = \hat{X}^T \hat{X} + \lambda I_d$ via a matrix sketching procedure for $\hat{X}$ as described in Section 3. A full description of a randomized preconditioned algorithm for FDA with warm-start appears in Algorithm 2. The following corollary summarize our theoretical results regarding the proposed algorithm. Note that COUNTSKETCH can possibly be replaced with other sketching transforms, and Riemannian CG can be replaced with any other Riemannian optimization methods, although the bound in the corollary might change. We delegate the proof to Appendix D.5.

**Corollary 11.** Consider Algorithm 2. Let $\delta \in (0, 1)$. If $s = \max\{\left[20s_\lambda(\hat{X})^2 / \delta^2\right], d\}$, then with probability of at least $1 - \delta$, the condition number of the Riemannian Hessian at the optimum is bounded by $3\kappa_{\text{FDA}}^\star$, regardless of the condition number of $S_w + \lambda I$. Furthermore, assuming we use Riemannian CG, $n \geq d \geq p$, and all computations are done in ambient $\mathbb{R}^{d \times p}$ coordinates, then the preprocessing steps take $O(\text{nnz}(\hat{X})) = O(nd)$ and $O(sd^2 + d^2)$. Assuming a bounded number of line-search steps in each iteration then each iteration takes $O(p (\text{nnz}(\hat{X}) + ld) + \text{nnz}(\hat{X})p + d^2p + dp^2)$. 

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work by Gonen et al. [27], which we term as Riemannian CG and Riemannian Trust-Region. Our aim is to show the effectiveness of our randomized preconditioning approach. We experiment with both the preconditioned CCA and FDA algorithms presented in Sections 4 and 5. Our experiments are not designed to be exhaustive; we use a prototype MATLAB implementation. In particular we present experiments with our proposed preconditioned Riemannian optimization algorithms. The experiments we present here are with \(\Sigma_w + \lambda I_d\) for FDA, by approximating \(X, Y\) and \(\hat{X}\) correspondingly. We briefly summarize that method: suppose \(A \in \mathbb{R}^{d \times d}\) be some SPD matrix, and let \(A = U \Lambda U^T\) be an eigendecomposition, with the diagonal entries in \(\Lambda\) sorted in descending order. Given \(k\), let us denote by \(U_k\) the first \(k\) columns of \(U\), \(\Lambda_k\) denote the leading \(k \times k\) minor of \(\Lambda\), and \(\lambda_k\) the \(k\)-th largest eigenvalue of \(A\). The \(k\)-dominant subspace preconditioner of \(A + \lambda I_d\) is \(U (\Lambda - \lambda_k I) U^T + (\lambda_k + \lambda) I_d\). The dominant subspace can be found using a sparse SVD solver (we use MATLAB’s svds).

We use MATLAB for our implementations. We use the manopt library for Riemannian optimization. In the manopt library we implemented the generalized Stiefel manifold with a non-standard metric. The experiments we present here are with \(p = 3\) and \(N = \text{diag}(3, 2.75, 2)\). We also achieved similar results for other choices of \(p\) as well (which we do not include in the text).

We did not optimize the implementation, so clock time is not an appropriate metric for performance, and instead we use alternative metrics. In Riemannian Trust-Region Method, different iterations do a variable amount of passes over the data, so we measure products with the data matrices, as this is the dominant cost of our algorithm. As for Riemannian CG, the manopt solver restricts the number of line-search steps in each iteration to 25, otherwise the step is rejected. In practice, in our experiments the number of products in different iterations is between 6 to 26 for CCA and between 3 to 13 for FDA, so we report the number of iterations. Against the iterations or passes we plot the suboptimality of the current iterate: \(|\sum_{i=1}^p \sigma_i \mu_i + f_{\text{CCA}}(Z)| / \sum_{i=1}^p \sigma_i \mu_i\) for CCA and \(|\sum_{i=1}^p \rho_i \mu_i + f_{\text{FDA}}(W)| / \sum_{i=1}^p \rho_i \mu_i\) for FDA. We use manopt’s default stopping criteria: the optimization process terminates if the norm of the Riemannian gradient drops below \(10^{-6}\). We cap the number of iterations by 1000.

We use in our experiments three popular datasets: MNIST (Figures 6.1 and 6.2), MEDIANILL (Figure 6.3), and MNIST MEDIANILL (Figure 6.4).

Algorithm 2 Sketched Riemannian Iterative FDA with warm-start.

1. **Input**: \(X \in \mathbb{R}^{n \times d}, y \in \mathbb{N}^n, s \geq d, \lambda \geq 0\).
2. Compute matrices \(S_B\) and \(\hat{X}\).
3. **Generate random** \(h : \{1, \ldots, d\} \rightarrow \{1, \ldots, s\}\) and \(g : \{1, \ldots, d\} \rightarrow \{-1, +1\}\). Let \(S\) denote the corresponding COUNTSKETCH matrix.
4. \(X_S \leftarrow S X\).
5. \(W \leftarrow \text{exact - fda}(X_S)\).
6. \(M \leftarrow X_S^T X_S + \lambda I_d\).
7. **Notation**: \(S_w = \hat{X}^T \hat{X}\). Do not compute this matrix (algorithms only require taking products with it).
8. **Choose**: any \(N = \text{diag}(\mu_1, \ldots, \mu_p)\) s.t. \(\mu_1 > \ldots > \mu_p > 0\).
9. Using Riemannian CG, solve \(\max \text{Tr}(W^T S_B W N)\) s.t. \(W \in S_{S_w + \lambda I}(p, d)\). Use \(M\) for the metric.

Start the iteration from \(q f_{S_w + \lambda I}(\hat{W})\).

6 Numerical Experiments

We report experiments with our proposed preconditioned Riemannian optimization algorithms. The experiments are not designed to be exhaustive; we use a prototype MATLAB implementation. In particular we present experiments with the preconditioned CCA and FDA algorithms presented in Sections 4 and 5. Our aim is to show the effectiveness of our randomized preconditioning approach. We experiment with both Riemannian CG and Riemannian Trust-Region.

In addition to Algorithms 1 and 2, we experiment with an additional preconditioning strategy based on work by Gonen et al. [27], which we term as Dominant Subspace Preconditioning. This preconditioner was designed to approximate of the empirical correlation matrix so that it can be used to speed up SVRG for ridge regression problems. We use MATLAB’s svds. In our experiments we use this method to precondition \(\Sigma_{xx}\) and \(\Sigma_{yy}\) for CCA, and \(S_w + \lambda I_d\) for FDA, by approximating \(X, Y\) and \(X\) correspondingly. We briefly summarize that method: suppose \(A \in \mathbb{R}^{d \times d}\) be some SPD matrix, and let \(A = U \Lambda U^T\) be an eigendecomposition, with the diagonal entries in \(\Lambda\) sorted in descending order. Given \(k\), let us denote by \(U_k\) the first \(k\) columns of \(U\), \(\Lambda_k\) denote the leading \(k \times k\) minor of \(\Lambda\), and \(\lambda_k\) the \(k\)-th largest eigenvalue of \(A\). The \(k\)-dominant subspace preconditioner of \(A + \lambda I_d\) is \(U (\Lambda - \lambda_k I) U^T + (\lambda_k + \lambda) I_d\). The dominant subspace can be found using a sparse SVD solver (we use MATLAB’s svds).

We use MATLAB for our implementations. In the manopt library we implemented the generalized Stiefel manifold with a non-standard metric. The experiments we present here are with \(p = 3\) and \(N = \text{diag}(3, 2.75, 2)\). We also achieved similar results for other choices of \(p\) as well (which we do not include in the text).

We did not optimize the implementation, so clock time is not an appropriate metric for performance, and instead we use alternative metrics. In Riemannian Trust-Region Method, different iterations do a variable amount of passes over the data, so we measure products with the data matrices, as this is the dominant cost of our algorithm. As for Riemannian CG, the manopt solver restricts the number of line-search steps in each iteration to 25, otherwise the step is rejected. In practice, in our experiments the number of products in different iterations is between 6 to 26 for CCA and between 3 to 13 for FDA, so we report the number of iterations. Against the iterations or passes we plot the suboptimality of the current iterate: \(|\sum_{i=1}^p \sigma_i \mu_i + f_{\text{CCA}}(Z)| / \sum_{i=1}^p \sigma_i \mu_i\) for CCA and \(|\sum_{i=1}^p \rho_i \mu_i + f_{\text{FDA}}(W)| / \sum_{i=1}^p \rho_i \mu_i\) for FDA. We use manopt’s default stopping criteria: the optimization process terminates if the norm of the Riemannian gradient drops below \(10^{-6}\). We cap the number of iterations by 1000.

We use in our experiments three popular datasets: MNIST (Figures 6.1 and 6.2), MEDIANILL (Figure 6.3), and MNIST MEDIANILL (Figure 6.4)
Figure 6.1: Results for CCA on MNIST.

6.3) and COVTYPE\textsuperscript{4} (Figure 6.4). MNIST is used for testing CCA and FDA, where for CCA we try to correlate the left side of the image to the right side of the image. MEDIANILL (43,907 examples) is a multilabel dataset, so we use it to test CCA. COVTYPE is a large (581,012 examples) labeled dataset, and we use it to test FDA.

Consider Figure 6.1 (CCA on MNIST). For Riemannian CG the number of products per iteration is never bigger than 20. As a reference, for CCA the number of iterations required for CG and Trust-Region with $M = \Sigma$ is 218 and 15 correspondingly, whereas without a preconditioner ($M = I_d$) the CG did not converge even after 1000 iterations and the Trust-Region required 21 iterations to converge. We clearly see the direct correspondence between sketch quality (as measured by the sketch size $s$) and number of iterations. Furthermore, the number of iterations is close to optimal after sketching to only $s = 2000$ (there are 60,000 examples in the original dataset) or using only 40 singular vectors for the dominant subspace preconditioner (there are 784 features in the dataset)\textsuperscript{5}.

Next, consider Figure 6.2 (FDA on MNIST). For Riemannian CG the number of products per iteration is never bigger than 9. As a reference, for FDA the number of iterations required for CG and Trust-Region

\textsuperscript{4}Datasets were downloaded for LIBSVM’s website: https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/

\textsuperscript{5}Interestingly, with $s \geq 500$ the subspace embedding preconditioner uses less iterations than the optimal preconditioner. This is because of the use of sketching based warm-start.
with $M = S_w + \lambda I_d$ is 95 and 11 correspondingly, whereas without a preconditioner ($M = I_d$) the CG did not converge even after 1000 iterations and the Trust-Region required 20 iterations to converge, so again we see that the sketching reduces the number of iterations.

Consider Figure 6.3 (CCA on MEDIANILL). For Riemannian CG the number of products per iteration is never bigger than 20. As a reference, the number of iterations required for CG and Trust-Region with $M = \Sigma$ is 107 and 15 correspondingly, whereas without a preconditioner ($M = I_d$) the number of iterations for CG is 550 and for Trust-Region is 23. The dataset has 30,993 examples and 221 features, so again we see that we can sketch to relatively small size ($s = 2000$ or $k = 40$) and get an effective preconditioner.

Consider Figure 6.4 (FDA on COVTYPE). For Riemannian CG the number of products per iteration is never bigger than 10. As a reference, the number of iterations required for CG and Trust-Region with $M = S_w + \lambda I_d$ is 71 and 19 correspondingly, whereas without a preconditioner ($M = I_d$) the CG did not converge even after 1000 iterations and the Trust-Region required 44 iterations to converge. Considering that the dataset has over half a million examples, subspace embedding preconditioning is highly effective, as it sketches the data to a comparatively very small size. The dataset has only 50 features, so dominant subspace preconditioning is less effective for this data set.
A Stability of the Critical Points of $f_{\text{CCA}}$

In the following theorem, we show that under reasonable assumptions the critical points which solve Problem (4.1) are asymptotically stable. Moreover, we show that critical points which are saddle points or local maximizers of Problem (4.1) are unstable.

We use [1, Proposition 4.4.1] and [1, Proposition 4.4.2]. First, recall the definition of a descent mapping from [1, Chapter 4.4]: we say that $F$ is a descent mapping for a cost function $f$ on $\mathcal{M}$ if $f(F(x)) \leq f(x)$ for all $x \in \mathcal{M}$. Now, [1, Proposition 4.4.1] shows that if we use any Riemannian algorithm that induces a descent mapping, and for which for every starting point the series of points generated by the algorithm has only accumulation points that are critical points, then any critical point which is not a local minimum with a compact neighborhood where the cost function achieves the same value for all other critical points is unstable. Additionally, [1, Proposition 4.4.2] shows that if the same conditions hold, and the distance on the manifold between iterations goes to zero as the algorithm approaches a local minimum, then if this minimum is an isolated critical point, it is an asymptotically stable critical point.

**Theorem 12.** Consider using Riemannian optimization to minimize $f_{\text{CCA}}(Z)$ subject to $Z \in S_{xy}$, and assume that the mapping defined by the algorithm is a descent mapping. Assume that $\sigma_1 > \sigma_2 > \ldots > \sigma_{p+1} \geq 0$, then $Z$ that minimize $f_{\text{CCA}}(Z)$ on $S_{xy}$ are asymptotically stable. Furthermore, critical points which are
Figure 6.4: Results for FDA on COVTYPE.

not a local minimum of Problem (4.1) are unstable.

**Proof.** To prove the asymptotic stability of $Z = (U, V)$ that minimize $f_{CCA}(Z)$ on $S_{xy}$, we use [1, Proposition 4.4.2]. Recall from Theorem 4 that $Z$ that solve Problem (4.1) are unique up the the signs of the columns of $U$ and $V$, making these points isolated global (and consequently local) minimizers of $f_{CCA}(Z)$ on $S_{xy}$. According to [1, Proposition 4.4.2], such points $Z$ are asymptotically stable.

Suppose $Z$ is a critical point of $f_{CCA}(Z)$ on $S_{xy}$ which is not a local minimum. Then, there exists compact neighborhoods with either no other critical points, if there are no multiplicities of the canonical correlations, or where all other critical point achieve the same value for the cost function, if there are multiplicities. Thus, according to [1, Proposition 4.4.1], such $Z$ are unstable.

**Remark 13.** Consider the case that one or more of the top $p$-canonical correlations is not simple, i.e., some $\sigma_i = \sigma_j$ for $1 \leq i, j \leq p$. Then there is no longer an isolated minima of the form $Z = (U, V) \in S_{xy}$ such that the columns of $U$ and $V$ are the left and right top $p$-canonical vectors, because permutations and linear combinations of the columns of $U$ and $V$ associated with $\sigma_i$ which maintain the phase do not change the optimal value. In such case, we can still guarantee that there exists a neighborhood of the space of the left and right top $p$-canonical correlation spaces for which all the starting points converge. Indeed, any neighborhood of these spaces contains a sublevel set of $f_{CCA}$ for which the only critical points of $f_{CCA}$
in this sublevel set belong to the space of the left and right top $p$-canonical correlation spaces. Thus, if a Riemannian optimization algorithm which induces a descent mapping is started with an initial point within such a sublevel set, and assuming all accumulation points are critical points of $f_{\text{CCA}}$, then it converges to the space of the left and right top $p$-canonical correlation spaces.

In the next theorem, we show that under certain assumptions, critical points which do not solve Problem (11) are saddle points or local maximizers. Furthermore, the algorithm is likely to converge to the desired global minimizer since under some assumptions it is the only local minimizer (up to the signs of the columns) among the critical points, thus making it the only asymptotically stable critical point. The proof is delegated to Appendix D.2 since it relies on the proof of Theorem 5.

**Theorem 14.** Consider using Riemannian optimization to minimize $f_{\text{CCA}}(Z)$ subject to $Z \in S_{xy}$, where we use the Riemannian metric defined by $M = \text{blkdiag} \left( M^{(xx)}, M^{(yy)} \right)$ where $M^{(xx)} \in \mathbb{R}^{d_x \times d_x}$ and $M^{(yy)} \in \mathbb{R}^{d_y \times d_y}$ are given preconditioners matrices. Assume that for all $i = 1, \ldots, q$ the values $\sigma_i$ are distinct, and that $\Sigma$ is a SPD matrix. Then the global minimizer of $f_{\text{CCA}}(Z)$ subject to $Z \in S_{xy}$, denoted by $Z^* = (U^*, V^*)$, is the only (strict) local minimizer of $f_{\text{CCA}}(Z)$ on $S_{xy}$, up to the signs of the columns, and all other critical points are either saddle points or global maximizers. Thus, $Z^*$ is the only asymptotically stable critical point, and all other critical points are unstable.

**B Stability of the Critical Points of $f_{\text{FDA}}$**

To analyze the stability of the critical points, we use [11 Proposition 4.4.1] and [11 Proposition 4.4.2]. The following theorem shows that under reasonable assumptions the critical points which solve Problem (5.3) are asymptotically stable and critical points which are saddle points of Problem (5.3) are unstable. The proof is analogous to the proof of Theorem 14 so we delegate it to Appendix D.2.

**Theorem 15.** Consider using Riemannian optimization to minimize $f_{\text{FDA}}(W)$ subject to $W \in \text{St}(S_w + \lambda I_d)(p, d)$, and assume that the mapping defined by the algorithm is a descent mapping. Assume that $\rho_1 > \rho_2 > \ldots > \rho_{p+1} \geq 0$, then $W \in \text{St}(S_w + \lambda I_d)(p, d)$ such that the columns are the $p$ leading FDA weight vectors are asymptotically stable. Furthermore, critical points which are not a local minimum of Problem (5.3) are unstable.

**Remark 16.** Consider the case that one or more of the $p$-dominant generalized eigenvalues of the matrix pencil $(S_B, S_w + \lambda I_d)$ is not simple, i.e., some $\rho_i = \rho_j$ for $1 \leq i, j \leq p$. Then there is no longer an isolated minima of the form $W \in \text{St}(S_w + \lambda I_d)(p, d)$ such that the columns are the $p$ leading FDA weight vectors, because permutations and linear combinations of the columns of $W$ associated with $\rho_i$ do not change the optimal value. In such case, we can still guarantee that there exists a neighborhood of the space of the $p$-dominant generalized eigenspaces for which all the starting points converge to the space of the $p$-dominant generalized eigenspaces. Indeed, any neighborhood of these generalized eigenspaces contains a sublevel set of $f_{\text{FDA}}$ for which the only critical points of $f_{\text{FDA}}$ in this sublevel set belong to the space of the $p$-dominant generalized eigenspaces. Thus, if a Riemannian optimization algorithm which induces a descent mapping is started with an initial point within such a sublevel set, and assuming all accumulation points are critical points of $f_{\text{FDA}}$, then it converges to the space of the $p$-dominant generalized eigenspaces.

**Theorem 17.** Consider using Riemannian optimization to minimize $f_{\text{FDA}}(W)$ subject to $W \in \text{St}(S_w + \lambda I_d)(p, d)$, where we use the Riemannian metric defined by $M \in \mathbb{R}^{d \times d}$, which is a given preconditioner matrix. Assume that for all $i = 1, \ldots, d$ the values $\rho_i$ are distinct and that $S_w + \lambda I_d$ is a SPD matrix. Let $W^*$ denote the global minimizer of $f_{\text{FDA}}(W)$ subject to $W \in \text{St}(S_w + \lambda I_d)(p, d)$. Then $W^*$ is the only (strict) local minimizer of $f_{\text{FDA}}(W)$ on $\text{St}(S_w + \lambda I_d)(p, d)$, up to the signs of the columns, and all other critical points are either saddle points or strict local maximizers. Thus, $W^*$ is the only asymptotically stable critical point, and all other critical points are unstable.
C Omitted Proofs Regarding Section 4

C.1 Proof of Theorem 5

Proof. In order to bound the condition number of the Riemannian Hessian at \( Z^* \in S_{xy} \), we need to bound its maximal and minimal eigenvalues. Thus, to prove the theorem we analyze the eigenvalues of the Riemannian Hessian at some critical point \( Z \in S_{xy} \) (in particular at \( Z^* \in S_{xy} \)) using the Courant-Fischer Theorem (also called the minimax principle, see [31] Chapter 1, Section 6.10) for the compact self-adjoint linear operator \( \text{Hess}_{CCA}(Z)[\cdot]: T_Z S_{xy} \to T_Z S_{xy} \) over the finite dimensional vector space \( T_Z S_{xy} \):

\[
\lambda_k(\text{Hess}_{CCA}(Z)) = \min_{U, \dim(U) = k - 1} \max_{0 \neq \xi \in U^\perp} R(\xi), \\
\lambda_k(\text{Hess}_{CCA}(Z)) = \max_{U, \dim(U) = k} \min_{0 \neq \xi \in U} R(\xi),
\]

where

\[
R(\xi) := \frac{g_Z(\xi, \text{Hess}_{CCA}(Z)[\xi])}{g_Z(\xi, \xi)},
\]

In the above, \( \lambda_k(\text{Hess}_{CCA}(Z)) \) is the \( k \)th largest eigenvalue (i.e., eigenvalues are ordered in a descending order) of \( \text{Hess}_{CCA}(Z) \), and \( U \) is a linear subspace of \( T_Z S_{xy} \). In particular, the maximal and minimal eigenvalues are given by the formulas

\[
\lambda_{\max}(\text{Hess}_{CCA}(Z)) = \max_{0 \neq \xi \in T_Z S_{xy}} R(\xi), \\
\lambda_{\min}(\text{Hess}_{CCA}(Z)) = \min_{0 \neq \xi \in T_Z S_{xy}} R(\xi).
\]

We begin by simplifying the quotient \( R(\xi) \). Recall that any critical point of \( f_{CCA} \) is a matrix \( Z = (U, V) \in S_{xy} \) such that the columns of \( (\tilde{U}, \tilde{V}) = (\Sigma_{xx}^{1/2} U, \Sigma_{yy}^{1/2} V) \) are \( p \) left and right singular vectors (not necessarily on the same phase) of the matrix \( R := \Sigma_{xx}^{-1/2} \Sigma_{xy} \Sigma_{yy}^{-1/2} \) (see Theorem 4). Let \( \alpha_1, \ldots, \alpha_p \) be some singular values of the matrix \( R \), and let \( \tilde{u}_1, \ldots, \tilde{u}_p, \tilde{v}_1, \ldots, \tilde{v}_p \) be the corresponding left and right singular vectors (not necessarily on the same phase). Writing \( \tilde{u}_1, \ldots, \tilde{u}_p \) as the columns of \( \tilde{U} \) and and \( \tilde{v}_1, \ldots, \tilde{v}_p \) as the columns of \( \tilde{V} \), and defining \( U = \Sigma_{xx}^{-1/2} U, V = \Sigma_{xx}^{-1/2} V \), the following two equations hold:

\[
\Sigma_{xy} V = \Sigma_{xx} U A \\
\Sigma_{xy}^T U = \Sigma_{xy} V A
\]

where \( A := \text{diag}(\beta_1, \ldots, \beta_p) \) such that \( |\beta_i| = \alpha_i \) for \( i = 1, \ldots, p \). Letting \( Z = (U, V) \in S_{xy} \), plugging in the ambient coordinates formula for the Riemannian Hessian (Eq. (4.3)), the Riemannian gradient nullifies (see Theorem 4) and we have

\[
\text{Hess}_{CCA}(Z)[\xi] = \Pi_Z(M^{-1}[-\Sigma_{w^2}_{CCA} \xi N + \Sigma \left( \xi U^T \Sigma_{xy} Y N \right) \Sigma V^T \Sigma_{xy}^T U N] + \Sigma \left( \xi U^T \xi V^T M_{grad f_{CCA}(Z)}[\xi] \right) = \Pi_Z \left( M^{-1} \left[ -\Sigma_{w^2}_{CCA} \xi + \xi N \right] + \Sigma \xi A \right) N.
\]

Plugging in the formula for the Riemannian Hessian at a critical point (Eq. (4.7)), the quotient \( R(\xi) \) is reduced to

\[
R(\xi) = \frac{\text{Tr} \left( \xi^T M \Pi_Z \left( M^{-1} \left[ -\Sigma_{w^2}_{CCA} \xi + \xi N \right] + \Sigma \xi A \right) N \right)}{\text{Tr} \left( \xi^T M \xi \right)}.
\]
Now, using the fact that the projection to the tangent space is self-adjoint with respect to the Riemannian metric and that for any $\xi \in T_Z S_{xy}$ we have $\mathbf{P}_Z (\xi_Z) = \xi_Z$, we further see that

$$\frac{\text{Tr} (\xi_Z^T \mathbf{M} \mathbf{P}_Z (\mathbf{M}^{-1} [-\Sigma \nabla^2_{f_{CCA}} \xi_Z + \Sigma \xi_Z A] N))}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)} = \frac{\text{Tr} (\xi_Z^T (-\Sigma \nabla^2_{f_{CCA}} \xi_Z + \Sigma \xi_Z A) N)}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)}.$$ 

Obviously, we can also write

$$\frac{\text{Tr} (\xi_Z^T (-\Sigma \nabla^2_{f_{CCA}} \xi_Z + \Sigma \xi_Z A) N)}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)} = \frac{\text{Tr} (\xi_Z^T (-\Sigma \nabla^2_{f_{CCA}} \xi_Z + \Sigma \xi_Z A) N)}{\text{Tr} (\xi_Z^T \Sigma \xi_Z)} \cdot \frac{\text{Tr} (\xi_Z^T \Sigma \xi_Z)}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)}.$$ (C.8)

Using Eq. (C.8), a simplified form of the quotient $R(\xi_Z)$, we can estimate upper and lower bounds on $R(\xi_Z)$ where $\mathbf{0} \neq \xi_Z \in T_Z S_{xy}$ in order to bound the condition number of the Riemannian Hessian at $Z^* \in S_{xy}$. Since for $\xi_Z \neq \mathbf{0}$ the term $\frac{\text{Tr} (\xi_Z^T \Sigma \xi_Z)}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)} > 0$, then the upper and lower bounds on

$$\frac{\text{Tr} (\xi_Z^T (-\Sigma \nabla^2_{f_{CCA}} \xi_Z + \Sigma \xi_Z A) N)}{\text{Tr} (\xi_Z^T \Sigma \xi_Z)} \cdot \frac{\text{Tr} (\xi_Z^T \Sigma \xi_Z)}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)}.$$ (C.9)

together with the upper and lower bounds of $\frac{\text{Tr} (\xi_Z^T \Sigma \xi_Z)}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)} > 0$ bound the condition number of the Riemannian Hessian at $Z^* \in S_{xy}$.

We begin by estimating the term $\frac{\text{Tr} (\xi_Z^T \Sigma \xi_Z)}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)} > 0$. We use the vectorization operator, and the Kronecker product to rewrite it in the following form

$$\frac{\text{Tr} (\xi_Z^T \Sigma \xi_Z)}{\text{Tr} (\xi_Z^T \mathbf{M} \xi_Z)} = \frac{\text{vec} (\xi_Z)^T (\mathbf{I}_p \otimes \Sigma) \text{vec} (\xi_Z)}{\text{vec} (\xi_Z)^T (\mathbf{I}_p \otimes \mathbf{M}) \text{vec} (\xi_Z)}.$$ (C.10)

Eq. (C.10) is the generalized Rayleigh quotient for the matrix pencil $(\mathbf{I}_p \otimes \Sigma, \mathbf{I}_p \otimes \mathbf{M})$. Note that $\mathbf{I}_p \otimes \Sigma$ and $\mathbf{I}_p \otimes \mathbf{M}$ are both SPD matrices, thus the generalized eigenvalues of the matrix pencil $(\mathbf{I}_p \otimes \Sigma, \mathbf{I}_p \otimes \mathbf{M})$ are equivalent to the eigenvalues of the matrix $(\mathbf{I}_p \otimes \mathbf{M})^{-1} (\mathbf{I}_p \otimes \Sigma) = \mathbf{I}_p \otimes \Sigma^{-1}$. According to [39, Section 2] the eigenvalues $\mathbf{I}_p \otimes \Sigma^{-1}$ are $p$ copies of each of the eigenvalues of $\Sigma^{-1}$. Thus, the maximal and minimal eigenvalues of the matrix pencil $(\mathbf{I}_p \otimes \Sigma, \mathbf{I}_p \otimes \mathbf{M})$ denoted by $\lambda_{\text{max}}$ and $\lambda_{\text{min}}$ are equivalent to the maximal and minimal generalized eigenvalues of the matrix pencil $(\Sigma, \mathbf{M})$, and so is the corresponding condition number

$$\kappa (\mathbf{I}_p \otimes \Sigma, \mathbf{I}_p \otimes \mathbf{M}) = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} = \kappa (\Sigma, \mathbf{M}).$$

Recall the definition of the generalized eigenvalues. The generalized eigenvalues of the matrix pencil $(\mathbf{A}, \mathbf{B})$, where $\mathbf{A} \in \mathbb{R}^{d \times d}$ and $\mathbf{B} \in \mathbb{R}^{d \times d}$ is a symmetric positive semi-definite matrix such that $\ker (\mathbf{B}) \subseteq \ker (\mathbf{A})$, are defined as follows: if for $\lambda \in \mathbb{R}$ and $\mathbf{v} \notin \ker (\mathbf{B})$ it holds that $\mathbf{A} \mathbf{v} = \lambda \mathbf{B} \mathbf{v}$ then $\lambda$ is a generalized eigenvalue and $\mathbf{v}$ is a generalized eigenvector of the matrix pencil $(\mathbf{A}, \mathbf{B})$. The generalized eigenvalues are denoted by $\lambda_1 (\mathbf{A}, \mathbf{B}) \geq \lambda_2 (\mathbf{A}, \mathbf{B}) \geq \cdots \geq \lambda_{\text{rank} (\mathbf{B})} (\mathbf{A}, \mathbf{B})$. Therefore, using the Courant-Fischer Theorem for
the matrix pencil \((I_p \otimes \Sigma, I_p \otimes M)\) we have
\[
\hat{\lambda}_{\text{max}} := \lambda_{\text{max}}(I_p \otimes \Sigma, I_p \otimes M)
\]
\[
= \max_{0 \neq \xi \in \mathbb{R}^{d_x \times p}} \text{vec} (\xi)^T (I_p \otimes \Sigma) \text{vec} (\xi)
\]
\[
\geq \max_{0 \neq \xi \in T^2S_{xy}} \text{vec} (\xi)^T (I_p \otimes \Sigma) \text{vec} (\xi)
\]
\[
= \max_{0 \neq \xi \in T^2S_{xy}} \frac{\text{Tr} (\xi^T \Sigma \xi)}{\text{Tr} (\xi^T M \xi)}
\]
and
\[
\hat{\lambda}_{\text{min}} := \lambda_{\text{min}}(I_p \otimes \Sigma, I_p \otimes M)
\]
\[
= \min_{0 \neq \xi \in \mathbb{R}^{d_x \times p}} \frac{\text{vec} (\xi)^T (I_p \otimes \Sigma) \text{vec} (\xi)}{\text{vec} (\xi)^T (I_p \otimes M) \text{vec} (\xi)}
\]
\[
\leq \min_{0 \neq \xi \in T^2S_{xy}} \frac{\text{vec} (\xi)^T (I_p \otimes \Sigma) \text{vec} (\xi)}{\text{vec} (\xi)^T (I_p \otimes M) \text{vec} (\xi)}
\]
\[
= \min_{0 \neq \xi \in T^2S_{xy}} \frac{\text{Tr} (\xi^T \Sigma \xi)}{\text{Tr} (\xi^T M \xi)}
\]

Next, we analyze Eq. \([C.9]\). Recall that \(\xi = (\xi_U, \xi_V) \in T_{2S_{xy}} \Sigma_{xx} (p, d_x)\) and \(\xi_V \in T_{V \Sigma_{xy}} (p, d_y)\), thus we can rewrite the tangent vectors in the following form:
\[
\xi_U = U \Omega_U + U \Sigma_{xx} \perp K_U, \quad \xi_V = V \Omega_V + V \Sigma_{yy} \perp K_V,
\]
where \(U \Sigma_{xx} \perp\) is \(\Sigma_{xx}\)-orthogonal to \(U\) so that the union of the columns of \(U\) and \(U \Sigma_{xx} \perp\) is a basis to \(\mathbb{R}^{d_x}\), and similarly \(V \Sigma_{yy} \perp\) is \(\Sigma_{yy}\)-orthogonal to \(V\) so that the union of the columns of \(V\) and \(V \Sigma_{yy} \perp\) is a basis to \(\mathbb{R}^{d_y}\), \(\Omega_U = -\Omega_U^T \in \mathbb{R}^{p \times p}\), \(\Omega_V = -\Omega_V^T \in \mathbb{R}^{p \times p}\), \(K_U \in \mathbb{R}^{(d_x - p) \times p}\) and \(K_V \in \mathbb{R}^{(d_y - p) \times p}\). Note that we can always make the choice of the columns of \(U \Sigma_{xx} \perp\) and \(V \Sigma_{yy} \perp\) to be such that \(\Sigma_{xx} \Sigma_{xx} \perp, \Sigma_{yy} \Sigma_{yy} \perp\) are some \(\min \{d_x - p, d_y - p\}\) left and right singular vectors not necessarily on the same phase of the matrix \(R\) belonging to the same singular values. Without loss of generality suppose \(d_x \geq d_y\). With this choice we have
\[
\Sigma_{xy} V \Sigma_{yy} \perp = \Sigma_{xx} U \Sigma_{xx} \perp \hat{A}, \quad \Sigma_{xx} U \Sigma_{xx} \perp \Sigma_{yy} V \Sigma_{yy} \perp = \Sigma_{yy} V \Sigma_{yy} \perp \hat{A}^T,
\]
and
\[
U^T \Sigma_{xx} \Sigma_{xy} V \Sigma_{yy} \perp = \hat{A} \in \mathbb{R}^{(d_x - p) \times (d_y - p)}, \quad V^T \Sigma_{xy} \Sigma_{yy} \Sigma_{xx} \perp = \hat{A}^T \in \mathbb{R}^{(d_y - p) \times (d_x - p)}
\]
where \(\hat{A}\) is a diagonal matrix (but not necessarily a square matrix), with the corresponding values on the diagonal \(\beta_{p+1}, ..., \beta_{d_y}\), which satisfy \(|\beta_i| = \alpha_i\) for \(i = p + 1, ..., d_y\).

Now,
\[
\xi_U^T \Sigma \xi = \begin{bmatrix} \Omega_U & \Omega_V \end{bmatrix} \begin{bmatrix} \Omega_U & \Omega_V \end{bmatrix} + \begin{bmatrix} K_U & K_V \end{bmatrix} \begin{bmatrix} K_U & K_V \end{bmatrix}
\]
and
\[
\xi_V^T \Sigma \xi = \begin{bmatrix} \Omega_U & \Omega_V \end{bmatrix} \begin{bmatrix} \Omega_U & \Omega_V \end{bmatrix} + \begin{bmatrix} K_U & K_V \end{bmatrix} \begin{bmatrix} K_U & K_V \end{bmatrix}
\]
Let
\[
m_z := \text{vec} \left( \begin{bmatrix} \Omega_U \\ \Omega_V \end{bmatrix} \right), \quad k_z := \text{vec} \left( \begin{bmatrix} K_U \\ K_V \end{bmatrix} \right)
\]
Then,
\[ \text{Tr} \left( \xi_k^T \Sigma \xi_k \right) = m_k^T m_k + k_k^T k_k, \]

\[ \text{Tr} \left( -[ \Omega_U \quad \Omega_V ] \left[ \begin{array}{cc} A & 2 \\ \Omega_U & \Omega_V \end{array} \right] N + [ \Omega_U \quad \Omega_V ] \right) \]

\[ \text{Tr} \left( -[ K_U^T \quad K_V^T ] \left[ \begin{array}{cc} A & 2 \\ K_U & K_V \end{array} \right] N + [ K_U^T \quad K_V^T ] \right) \]

\[ = m_k^T \left( \text{AN} \otimes \text{I}_{2p} - \text{N} \otimes \left[ A \quad A \right] \right) m_k + k_k^T \left( \text{AN} \otimes \text{I}_{2p} - \text{N} \otimes \left[ A^2 \quad A \right] \right) k_k \]

thus,
\[ \frac{\text{Tr} \left( \xi_k^T \left( -\Sigma_{\text{CCA}} \xi_k + \Sigma \xi_k \right) \right) \text{N}}{\text{Tr} \left( \xi_k^T \Sigma \xi_k \right)} \]

Recalling that \( \Omega_U = -\Omega_U^T \) and \( \Omega_V = -\Omega_V^T \), and both are real matrices (so the elements of the main diagonals are 0), we have
\[ m_k^T m_k = 2 \left( \sum_{1 \leq j < i \leq p} (\Omega_U)_{ij}^2 + \sum_{1 \leq j < i \leq p} (\Omega_V)_{ij}^2 \right), \quad \text{C.11} \]

and
\[ m_k^T \left( \text{AN} \otimes \text{I}_{2p} - \text{N} \otimes \left[ A \quad A \right] \right) m_k = \sum_{1 \leq j < i \leq p} \left[ (\mu_i \beta_i + \mu_j \beta_j) \left( \Omega_U \right)_{ij}^2 + (\Omega_V)_{ij}^2 \right] - 2 (\beta_i \mu_j + \beta_j \mu_i) (\Omega_U)_{ij} (\Omega_V)_{ij}, \quad \text{C.12} \]

Thus, only the \( p(p-1)/2 \) entries below the diagonal of \( \Omega_U \) and the \( p(p-1)/2 \) entries below the diagonal of \( \Omega_V \) determine the values of Eq. (C.11) and Eq. (C.12). Let us now denote by \( \bar{m}_Z \) the column stack of \( (\Omega_U, \Omega_V) \), but only with the subdiagonal entries of \( \Omega_U \) and of \( \Omega_V \) (i.e., \( m_k \) “purged” of the superdiagonal elements). We then have,
\[ m_k^T m_k = \bar{m}_Z^T \bar{m}_Z \]

and
\[ m_k^T \left( \text{AN} \otimes \text{I}_{2p} - \text{N} \otimes \left[ A \quad A \right] \right) m_k = \bar{m}_Z^T \Psi \bar{m}_Z \]

where \( \Psi \in \mathbb{R}^{p(p-1) \times p(p-1)} \) is a matrix defined as follows: \( \Psi \) is a block diagonal matrix, where the blocks are of descending order: \( 2(p-1), 2(p-2), \ldots, 2 = 2 \). The \( j \)th \( (1 \leq j \leq p - 1) \) block, denoted by \( \Psi_j \), is of the order \( 2(p-j) \) and has following form:
\[ \Psi_j := \left[ \begin{array}{cc} D_j & -T_j \\ -T_j & D_j \end{array} \right] \]
where
\[ D_j = \text{diag} \left( \mu_{j+1} \beta_{j+1}, \mu_{j} \beta_{j}, \mu_{j+2} \beta_{j+2}, \ldots, \mu_{p} \beta_{p} + \mu_{j} \beta_{j} \right), \]
and
\[ T_j = \text{diag} \left( \beta_{j+1} \mu_{j+1}, \beta_{j} \mu_{j+1}, \beta_{j+2} \mu_{j}, \beta_{j} \mu_{j+2}, \ldots, \beta_{p} \mu_{j} + \beta_{j} \mu_{p} \right). \]

We make the following change of variables: \( \tilde{d}_z := \sqrt{2} \hat{m}_z \). Finally, Eq. (C.9) is rewritten in the following way
\[
\frac{\text{Tr} \left( \xi_z^T \left( -\Sigma \text{CCA} \xi_z + \Sigma \xi_z A \right) N \right)}{\text{Tr} \left( \xi_z^T \Sigma \xi_z \right)} = \begin{bmatrix} \tilde{d}_z^T & k_z^T \end{bmatrix} \text{blkdiag} \left( \frac{1}{2} \Psi, AN \otimes I_{d-2p} - N \otimes \begin{bmatrix} \hat{A}^T & \hat{A} \end{bmatrix} \right) \begin{bmatrix} \tilde{d}_z \\ k_z \end{bmatrix}.
\]

(C.13)

Note that the mapping \( \varphi(\cdot) : T_Z \mathbb{S}_x y \to \mathbb{R}^{pd-p(p+1)} \) defined by
\[
\varphi(\xi_z) := \begin{bmatrix} \tilde{d}_z \\ k_z \end{bmatrix},
\]
is a coordinate chart of the elements of \( T_Z \mathbb{S}_x y \), since \( \varphi(\cdot) \) is a bijection (one-to-one correspondence) of the elements of \( T_Z \mathbb{S}_x y \) onto \( \mathbb{R}^{pd-p(p+1)} \). Indeed, \( k_z \) is a column stack of \( (K_U, K_V) \), thus we can retract the matrices \( K_U \) and \( K_V \). Similarly \( \tilde{d}_z \) is proportional to \( \hat{m}_z \) which is a column stack of \( (\Omega_U, \Omega_V) \), but only with the subdiagonal entries of \( \Omega_U \) and \( \Omega_V \). Since \( \Omega_U \) and \( \Omega_V \) are skew-symmetric matrices, we can retract \( \Omega_U \) and \( \Omega_V \). With the matrices \( K_U, K_V, \Omega_U \) and \( \Omega_V \) at hand, we can fully retract \( \xi_z = (\xi_U, \xi_V) \).

The eigenvalues and corresponding eigenvectors of any linear operator over a finite dimensional vector space do not depend on the choice of coordinate chart and basis, thus the eigenvalues and eigenvectors of \( \text{Hess}_{\text{CCA}}(Z) \) \([\cdot] : T_Z \mathbb{S}_x y \to T_Z \mathbb{S}_x y \) which are computed using the Courant-Fischer Theorem for compact self-adjoint linear operators (Eq. (C.1) and Eq. (C.2)), can be also computed by the Courant-Fischer Theorem for symmetric matrices [28, Theorem 4.2.6] after applying \( \varphi(\cdot) \). In particular, Eq. (C.13) determines the signs of the eigenvalues of the Riemannian Hessian at any \( Z \in \mathbb{S}_x y \) (in the special case \( M = \Sigma \), the eigenvalues of Eq. (C.14) are the eigenvalues of the Riemannian Hessian at a critical point \( Z \in \mathbb{S}_x y \)), and the bounds of Eq. (C.13) together with the bounds of the term \( \text{Tr} \left( \xi_z^T \Sigma \xi_z \right) / \text{Tr} \left( \xi_z^T M \xi_z \right) \) bound the condition number of the Riemannian Hessian at \( Z^* \in \mathbb{S}_x y \).

To that end, we perform the following computation. The right-hand side of Eq. (C.13) is a Rayleigh quotient, so according to the Courant-Fischer Theorem for symmetric matrices the eigenvalues of the \( pd - p(p + 1) \times pd - p(p + 1) \) symmetric matrix
\[
\text{blkdiag} \left( \frac{1}{2} \Psi, AN \otimes I_{d-2p} - N \otimes \begin{bmatrix} \hat{A}^T & \hat{A} \end{bmatrix} \right),
\]
are determined by critical values of Eq. (C.13). The set of eigenvalues of the matrix in Eq. (C.14) is equal to the union of the set of eigenvalues of \( \frac{1}{2} \Psi \) and
\[
\Phi := AN \otimes I_{d-2p} - N \otimes \begin{bmatrix} \hat{A}^T & \hat{A} \end{bmatrix}.
\]
The matrix \( \Phi \) is a \( p(d-2p) \times p(d-2p) \) block diagonal matrix, where all the blocks are \( p \times p \), and the \( j \)th block is
\[
\mu_j \beta_j I_{d-2p} - \mu_j \begin{bmatrix} \hat{A}^T & \hat{A} \end{bmatrix}.
\]
Thus, the eigenvalues of $\Phi$ are $\mu_j (\beta_j \pm \beta_i)$ and $\mu_j \beta_j$ for $j = 1, \ldots, p$ and $i = p + 1, \ldots, d_y$. In summary, we have $p(d_y - p)$ eigenvalues of the form $\mu_j (\beta_j + \beta_i)$, similarly $p(d_y - p)$ eigenvalues of the form $\mu_j (\beta_j - \beta_i)$, and $p(d_x - d_y)$ eigenvalues of the form $\mu_j \beta_j$. From the definition of $\Phi$, we see that the eigenvalues of $\frac{1}{2} \Psi$ are: $\frac{1}{2} [(\mu_j \beta_j + \mu_i \beta_i) \pm (\beta_j \mu_j + \beta_i \mu_i)]$ for $1 \leq j < i \leq p$. These eigenvalues can also be rewritten as: $\frac{1}{2} (\mu_j + \mu_i) (\beta_j + \beta_i)$ and $\frac{1}{2} (\mu_j - \mu_i) (\beta_j - \beta_i)$.

Now, we have all the eigenvalues of the matrix in Eq. (C.14): $p(d_y - p)$ eigenvalues of the form $\mu_j (\beta_j + \beta_i)$ where $j = 1, \ldots, p$ and $i = p + 1, \ldots, d_y$, $p(d_y - p)$ eigenvalues of the form $\mu_j (\beta_j - \beta_i)$ where $j = 1, \ldots, p$ and $i = p + 1, \ldots, d_y$, $p(d_x - d_y)$ eigenvalues of the form $\mu_j \beta_j$ where $j = 1, \ldots, p$, $p(p - 1)/2$ eigenvalues of the form $\frac{1}{2} (\mu_j + \mu_i) (\beta_j + \beta_i)$ where $1 \leq j < i \leq p$, and $p(p - 1)/2$ eigenvalues of the form $\frac{1}{2} (\mu_j - \mu_i) (\beta_j - \beta_i)$ where $1 \leq j < i \leq p$.

Finally, we bound the condition number of the Riemannian Hessian at $Z^* = (U^*, V^*) \in S_{XY}$. In such case, $\beta_1 = \sigma_1 > \ldots > \beta_p = \sigma_p$. Without loss of generality, we can always choose $U_{\Sigma_{xx, \perp}}$ and $V_{\Sigma_{yy, \perp}}$ such that $\beta_{p+1} = \sigma_{p+1} \geq \ldots \geq \beta_d = \sigma_d$. Then, we have that Eq. (C.9) is bounded by the minimal and maximal eigenvalues of Eq. (C.14). Thus,

$$0 < \max_{0 \neq \xi \in T_{Z^*}S_{XY}} \frac{\text{Tr} (\xi^T \left(-\Sigma_{\Sigma_{CA}} \xi + \Sigma_{\Sigma^*} A \right) N)}{\text{Tr} (\xi^T \Sigma_{\Sigma^*} \xi)} = \max \left\{ \mu_1 (\sigma_1 + \sigma_{p+1}), \frac{1}{2} (\mu_1 + \mu_2)(\sigma_1 + \sigma_2) \right\},$$

and

$$\min_{0 \neq \xi \in T_{Z^*}S_{XY}} \frac{\text{Tr} (\xi^T \left(-\Sigma_{\Sigma_{CA}} \xi + \Sigma_{\Sigma^*} A \right) N)}{\text{Tr} (\xi^T \Sigma_{\Sigma^*} \xi)} = \min \left\{ \mu_p (\sigma_p - \sigma_{p+1}), \min_{1 \leq j < i \leq p} \frac{1}{2} (\mu_j - \mu_i) (\sigma_j - \sigma_i) \right\} > 0.$$
In the special case $\mathbf{M} = \Sigma$, the bound on the condition number of the Riemannian Hessian at $\mathbf{Z}^* = (\mathbf{U}^*, \mathbf{V}^*) \in S_{xy}$ is reduced to an equality

$$\kappa(\text{Hess}f_{\text{CCA}}(\mathbf{Z}^*)) = \kappa_{\text{CCA}}.$$ 

### C.2 Proof of Theorem 14

**Proof.** We prove that the global minimizer of $f_{\text{CCA}}(\mathbf{Z})$ subject to $\mathbf{Z} \in S_{xy}$, denoted by $\mathbf{Z}^*$, is the only (strict) local minimum of $f_{\text{CCA}}(\mathbf{Z})$ and all other critical points are either saddle points or strict local maximizers.

Eq. (C.8) helps to determine the signs of the eigenvalues of the Riemannian Hessian at any critical point $\mathbf{Z} \in S_{xy}$ and in particular at $\mathbf{Z}^*$: the matrices $\Sigma$ and $\mathbf{M}$ are both SPD matrices, therefore for $\xi_\mathbf{z} \neq 0$ the term $\text{Tr} (\xi_\mathbf{z}^2 \Sigma_\mathbf{z}) / \text{Tr} (\xi_\mathbf{z}^2 \mathbf{M}_\mathbf{z}) > 0$, thus only Eq. (C.9), where $0 \neq \xi_\mathbf{z} \in T_\mathbf{z}S_{xy}$ determines the signs. In addition, at a critical point $\mathbf{Z} \in S_{xy}$, Eq. (C.9) equals to the quotient $R(\xi_\mathbf{z})$ for the choice $\mathbf{M} = \Sigma$, since Proposition 5.5.6 and Eq. 5.35] show that at a critical point the term $g_\mathbf{z}(\xi_\mathbf{z}. \text{Hess} f_{\text{CCA}}(\mathbf{Z})(\xi_\mathbf{z}))$, which is the numerator of $R(\xi_\mathbf{z})$, does not depend on the choice of Riemannian metric. Thus, the optimal values of Eq. (C.9) satisfying Eq. (C.1) or Eq. (C.2) are the eigenvalues of the Riemannian Hessian at $\mathbf{Z} \in S_{xy}$ with the choice $\mathbf{M} = \Sigma$. Obviously, classification of the critical points does not depend on the Riemannian metric. Therefore, we can classify the critical points using the signs of the eigenvalues of the Riemannian Hessian at any critical point $\mathbf{Z} \in S_{xy}$ with the choice $\mathbf{M} = \Sigma$.

Recall from the proof of Theorem 5 that in the special case $\mathbf{M} = \Sigma$, the eigenvalues of Eq. (C.14) are also the eigenvalues of the Riemannian Hessian at a critical point $\mathbf{Z} \in S_{xy}$. The eigenvalues are: $p(d_y - p)$ eigenvalues of the form $\mu_j (\beta_j + \beta_i)$ where $j = 1, \ldots, p$ and $i = p + 1, \ldots, d_y$, $p(d_y - p)$ eigenvalues of the form $\mu_j (\beta_j - \beta_i)$ where $j = 1, \ldots, p$ and $i = p + 1, \ldots, d_y$, $p(p-1)/2$ eigenvalues of the form $(\mu_j - \mu_i) (\beta_j + \beta_i)$ where $1 \leq j < i \leq p$, and $p(p-1)/2$ eigenvalues of the form $(\mu_j - \mu_i) (\beta_j - \beta_i)$ where $1 \leq j < i \leq p$, and $p - p' > 0$ for $i = 1, \ldots, p$, and $p - p' > 0$ for $j < i$. Also $|\beta_i| = \sigma_i$ for $i = 1, \ldots, p$. Thus, the signs of the eigenvalues of the matrix in Eq. (C.14) are only determined by $\beta_j$, $\beta_j + \beta_i$ and $\beta_j - \beta_i$, where $\beta_j$ are up to their sign the $p$ singular values of the matrix $\mathbf{R} := \Sigma_{xx}^{-1/2} \Sigma_{xy} \Sigma_{yy}^{-1/2}$ corresponding to left and right singular vectors which are the columns of $(\tilde{\mathbf{U}}, \tilde{\mathbf{V}}) = (\Sigma_{xx}^{1/2} \mathbf{U}, \Sigma_{yy}^{1/2} \mathbf{V})$. In particular, for an optimal $\mathbf{Z}^* = (\mathbf{U}^*, \mathbf{V}^*) \in S_{xy}$ such that the columns of $(\tilde{\mathbf{U}}, \tilde{\mathbf{V}}) = (\Sigma_{xx}^{1/2} \mathbf{U}, \Sigma_{yy}^{1/2} \mathbf{V})$ are ordered left and right $p$-dominant singular vectors of the matrix $\mathbf{R}$ on the same phase, then we have that $\beta_1 = \sigma_1 > \ldots > \beta_p = \sigma_p$. We conclude that $\beta_i$ such that $i = p + 1, \ldots, d_y$ satisfies $|\beta_i| = \sigma_i$, which leads to $\beta_j > 0$, $\beta_j + \beta_i > 0$ and $\beta_j - \beta_i > 0$ where $j = 1, \ldots, p$ and $i = p + 1, \ldots, d_y$ or $1 \leq j < i \leq p$. Therefore, in this case all the eigenvalues of the matrix Eq. (C.14) are strictly positive, the matrix Eq. (C.14) is SPD, and consequently the eigenvalues of the Riemannian Hessian at $\mathbf{Z}^* \in S_{xy}$ are all strictly positive. This proves that $\mathbf{Z}^*$ is a strict local minimum of $f_{\text{CCA}}(\mathbf{Z})$ on $S_{xy}$ (see [2 Proposition 6.2.]).

If we prove that $\mathbf{Z}^*$ is the only (strict) local minimum (up to the signs of the columns of $\mathbf{U}^*$ and $\mathbf{V}^*$), then $\mathbf{Z}^*$ is the only asymptotically stable critical point following Theorem 12. In order to prove it we further assume that for all $i = 1, \ldots, q$ the values $\sigma_i$ are distinct, then we can conclude the following. Suppose $\mathbf{Z} = (\mathbf{U}, \mathbf{V})$ is any other critical point differs from $\mathbf{Z}^*$ at the optimal value, i.e., such that the columns of $(\tilde{\mathbf{U}}, \tilde{\mathbf{V}}) = (\Sigma_{xx}^{1/2} \mathbf{U}, \Sigma_{yy}^{1/2} \mathbf{V})$ are left and right singular vectors corresponding to some $p$ singular values of the matrix $\mathbf{R}$ not necessarily on the same phase, so that Eq. (C.5) and Eq. (C.6) hold, and there exists at least one $1 \leq j \leq p$ for which $\beta_j \neq \sigma_j$. We consider the different cases:

1. Suppose $\beta_1, \ldots, \beta_p$ are not ordered in any particular order (possible for $p \geq 3$), then there exists $j$ such that $\beta_j$ is larger than some $\beta_k$ and smaller than $\beta_m$ where $j < k, m \leq p$, then $\beta_j - \beta_k > 0$ and $\beta_j - \beta_m < 0$. In this case there are both strictly positive and strictly negative eigenvalues of the Riemannian Hessian at $\mathbf{Z}$ for the choice $\mathbf{M} = \Sigma$, therefore, $\mathbf{Z}$ is a saddle point.

2. Suppose $\beta_1, \ldots, \beta_p$ are ordered in a descending order. Since $\mathbf{Z}$ is not an optimal solution of Problem (4.4), then there exists at least one $1 \leq j \leq p$ for which $\beta_j \neq \sigma_j$. Thus, on the one hand
for the sake of identifying the critical points, we can assume that
point is a critical point or not does not depend on the choice of Riemannian metric (see [1, Eq. 3.31]). Thus,

Proof.

D.1 Proof of Theorem 9

for the Riemannian gradient:

\[ \alpha \]
columns of \( A \) where \( A \)

In all cases, \( Z \) is not a local minimizer. Thus, \( Z^* \) is the only (strict) local minimum (up to the signs of the columns of \( U^* \) and \( V^* \)). According to Theorem 12 all the other critical points are unstable. □

D Omitted Proofs Regarding Section 5

D.1 Proof of Theorem 9

Proof. Recall that critical points are ones in which the Riemannian gradient is zero, and as such, whether a point is a critical point or not does not depend on the choice of Riemannian metric (see [11 Eq. 3.31]). Thus, for the sake of identifying the critical points, we can assume that \( M = S_w + \lambda I_d \) and use a simplified form for the Riemannian gradient:

\[
\text{grad}_{\text{FDA}}(W) = \Pi_W ((S_w + \lambda I_d)^{-1} \nabla_{\text{FDA}}(W))
\]

\[
= -\Pi_W ((S_w + \lambda I_d)^{-1} S_B WN)
\]

\[
= -{(S_w + \lambda I_d)^{-1} S_B WN - W \text{sym } (W^T S_B WN)}
\]

\[
= -{[I_d - WW^T (S_w + \lambda I_d)] (S_w + \lambda I_d)^{-1} S_B WN + W \text{skew } (W^T S_B WN)}.
\]

Let \( \alpha_1, \ldots, \alpha_p \) be some generalized eigenvalues of the matrix pencil \( (S_B, S_w + \lambda I_d) \), and let \( w_1, \ldots, w_p \) be the corresponding generalized eigenvectors (making them some \( p \) FDA weight vectors). Writing \( w_1, \ldots, w_p \) as the columns of \( W \), the following equation holds:

\[
S_B W = (S_w + \lambda I_d) W A
\]

where \( A = \text{diag} (\alpha_1, \ldots, \alpha_p) \). Letting \( W \in \text{St}(S_w + \lambda I_d)(p,d) \), we have

\[
\text{grad}_{\text{FDA}}(W) = -{(S_w + \lambda I_d)^{-1} S_B WN - W \text{sym } (W^T S_B WN)}
\]

\[
= -{WAN - W \text{sym } (AN)} = 0_{d \times p}.
\]

To show the other side, note that if the Riemannian gradient nullifies, then

\[
[(I_d - WW^T (S_w + \lambda I_d)) (S_w + \lambda I_d)^{-1} S_B WN + W \text{skew } (W^T S_B WN)] = 0_{d \times p}.
\]
By using similar reasoning as in [1] Subsection 4.8.2, \((I_d - WW^T(S_w + \lambda I_d)) (S_w + \lambda I_d)^{-1} S_B \text{WN} \) belongs to the orthogonal complement of the column space of \(W\) (with respect to the matrix \((S_w + \lambda I_d)\), and \(\text{Wskew} (W^T S_B \text{WN}) \) belongs to the column space of \(W\). Thus, we get that the gradient vanishes if and only if the following two formulas hold:

\[
(I_d - WW^T(S_w + \lambda I_d)) (S_w + \lambda I_d)^{-1} S_B \text{WN} = 0_{d \times p}, \tag{D.1}
\]

and

\[
\text{Wskew} (W^T S_B \text{WN}) = 0_{d \times p}. \tag{D.2}
\]

From Eq. \((D.1)\) we get

\[
(S_w + \lambda I_d)^{-1} S_B W = W (W^T S_B W),
\]

since \(N\) is an invertible matrix. Also, since \(W \in \text{St}_{(S_w + \lambda I_d)}(p, d)\) it is a full (column) rank matrix then Eq. \((D.2)\) vanishes if and only if

\[
\text{skew} (W^T S_B \text{WN}) = 0_p,
\]

which leads to \((W^T S_B W) N = N (W^T S_B W)\). This implies that \((W^T S_B W)\) is diagonal because any rectangle matrix that commutes with a diagonal matrix with distinct entries is diagonal. Finally we get

\[
(S_w + \lambda I_d)^{-1} S_B W = WD,
\]

where \(D = W^T S_B W\) is a diagonal matrix. This implies that the columns of \(W\) correspond to some \(p\) generalized eigenvectors the matrix pencil \((S_B, S_w + \lambda I_d)\), thus, making the columns some \(p\) FDA weight vectors.

Finally, to identify the optimal solutions, note that at the critical points the objective function is a sum of the generalized eigenvalues corresponding to the columns of \(W\) multiplied by a diagonal element of \(N\). Thus, the optimal solutions that minimize \(f_{FDA}(W)\) on \(\text{St}_{(S_w + \lambda I_d)}(p, d)\) are \(W \in \text{St}_{(S_w + \lambda I_d)}(p, d)\) such that the columns correspond to the \(p\) leading FDA weight vectors. Otherwise, we can increase the value of the objective function by replacing a weight vector with another that corresponds to a smaller generalized eigenvalue. Moreover, if we assume that \(\rho_1 > \rho_2 > ... > \rho_{p+1} \geq 0\), then for the aforementioned \(W\), the columns belong each to a one dimensional generalized eigenspace, i.e., unique solution up the the signs of the columns. In the case where some \(\rho_i = \rho_j\) for \(1 \leq i, j \leq p\), permutations of the columns of \(W\) associated with \(\rho_i\) keep the solution optimal making it non-unique.

\[\Box\]

D.2 Proof of Theorem 15

**Proof.** To prove the asymptotic stability of \(W \in \text{St}_{(S_w + \lambda I_d)}(p, d)\) such that the columns are the \(p\) leading FDA weight vectors we use [1] Proposition 4.4.2. Recall from Theorem ?? that \(W\) that solve Thus, in such case points \(W\) that solve Problem \((5.3)\) are unique up the the signs of the columns of \(W\), making these point isolated global (and consequently local) minimizers of \(f_{FDA}\) on \(\text{St}_{(S_w + \lambda I_d)}(p, d)\). According to [1] Proposition 4.4.2, such points \(W\) are asymptotically stable.

Suppose \(W\) is a critical point of \(f_{FDA}(W)\) on \(\text{St}_{(S_w + \lambda I_d)}(p, d)\) which is not a local minimum. Then, there exists compact neighborhoods with either no other critical points, if there are no multiplicities of the generalized eigenspaces, or where all other critical point achieve the same value for the cost function, if there are multiplicities of the generalized eigenspaces. Thus, according to [1] Proposition 4.4.1, such \(W\) are unstable.

\[\Box\]

D.3 Proof of Theorem 10

**Proof of Theorem 10** The proof is similar to the proof of Theorem 3. In order to bound the condition number of the Riemannian Hessian at \(W^*\), we need to bound its maximal and minimal eigenvalues. Thus,
to prove the theorem we analyze the eigenvalues of the Riemannian Hessian at some critical point \( W \in St(S_w + \lambda I_d) \) (in particular at \( W^* \)) using the Courant–Fischer Theorem for the compact self-adjoint linear operator \( \text{Hess}_{\text{FDA}}(W) \) \( : T_W St(S_w + \lambda I_d) \rightarrow T_W St(S_w + \lambda I_d) \) over the finite dimensional vector space \( T_W St(S_w + \lambda I_d) \) (see Chapter 1, Section 6.10):

\[
\lambda_k(\text{Hess}_{\text{FDA}}(W)) = \min_{U, \dim(U) = k-1} \max_{0 \neq \xi_W \in U^\perp} R(\xi_W), \quad (D.3)
\]

\[
\lambda_k(\text{Hess}_{\text{FDA}}(W)) = \max_{U, \dim(U) = k} \min_{0 \neq \xi_W \in U} R(\xi_W), \quad (D.4)
\]

where

\[
R(\xi_W) := \frac{g_W(\xi_W, \text{Hess}_{\text{FDA}}(W)[\xi_W])}{g_W(\xi_W, \xi_W)},
\]

\( \lambda_k(\text{Hess}_{\text{FDA}}(W)) = \rho_k \) is the \( k \)th largest eigenvalue (in a descending order) of \( \text{Hess}_{\text{FDA}}(W) \), and \( U \) is a linear subspace of \( T_W St(S_w + \lambda I_d) \). In particular, the maximal and minimal eigenvalues are given by the formulas:

\[
\lambda_{\max}(\text{Hess}_{\text{FDA}}(W)) = \max_{0 \neq \xi_W \in T_W St(S_w + \lambda I_d)(p, d)} R(\xi_W), \quad (D.5)
\]

\[
\lambda_{\min}(\text{Hess}_{\text{FDA}}(W)) = \min_{0 \neq \xi_W \in T_W St(S_w + \lambda I_d)(p, d)} R(\xi_W). \quad (D.6)
\]

We begin by simplifying the quotient \( R(\xi_W) \). Recall that any critical point of \( f_{\text{FDA}}(\cdot) \) is a matrix \( W \in St(S_w + \lambda I_d) \) such that the columns are some \( p \) generalized eigenvectors of the matrix pencil \( (S_B, S_w + \lambda I_d) \) (see Theorem 9). Let \( \alpha_1, \ldots, \alpha_p \) be some generalized eigenvalues of the matrix pencil \( (S_B, S_w + \lambda I_d) \), and let \( w_1, \ldots, w_p \) be the corresponding generalized eigenvectors. Writing \( w_1, \ldots, w_p \) as the columns of \( W \), the following equation holds:

\[
S_B W = (S_w + \lambda I_d)W A
\]

where \( A = \text{diag}(\alpha_1, \ldots, \alpha_p) \). Letting \( W \in St(S_w + \lambda I_d) \), plugging in the ambient coordinates formula for the Riemannian Hessian (Eq. 5.5), the Riemannian gradient nullifies (see Theorem 9), and we have

\[
\text{Hess}_{\text{FDA}}(W)[\xi_W] = \Pi_W \left( M^{-1} [-S_B \xi_W N + (S_w + \lambda I_d) \xi_W (W^T S_B WN + \text{grad}_W f)] \right)
\]

\[
= \Pi_W \left( M^{-1} [-S_B \xi_W N + (S_w + \lambda I_d) \xi_W (W^T (S_w + \lambda I_d) WAN)] \right)
\]

\[
= \Pi_W (M^{-1} [-S_B \xi_W + (S_w + \lambda I_d) \xi_W A N]). \quad (D.7)
\]

Plugging in the formula for the Riemannian Hessian at a critical point (Eq. 6.7), the quotient \( R(\xi_W) \) reduces to

\[
R(\xi_W) = \frac{\text{Tr} \left( \xi_W^T M \Pi_W \left( M^{-1} [-S_B \xi_W + (S_w + \lambda I_d) \xi_W A N] \right) \right)}{\text{Tr} \left( \xi_W^T M^2 \xi_W \right)}.
\]

Now using the fact that the projection to the tangent space is self-adjoint with respect to the Riemannian metric, and that for any \( \xi_W \in T_W St(S_w + \lambda I_d)(p, d) \) we have \( \Pi_W (\xi_W) = \xi_W \), we further see that

\[
\frac{\text{Tr} \left( \xi_W^T M \Pi_W \left( M^{-1} [-S_B \xi_W + (S_w + \lambda I_d) \xi_W A N] \right) \right)}{\text{Tr} \left( \xi_W^T M \xi_W \right)} = \frac{\text{Tr} \left( \xi_W^T [-S_B \xi_W + (S_w + \lambda I_d) \xi_W A N] \right)}{\text{Tr} \left( \xi_W^T M \xi_W \right)}
\]
Obviously, we can also write
\[
\frac{\text{Tr} \left( \xi_W^T \left[ -S_B \xi_W + (S_w + \lambda I_d) \xi_W A \right] N \right)}{\text{Tr} \left( \xi_W^T M \xi_W \right)} = \frac{\text{Tr} \left( \xi_W^T \left[ -S_B \xi_W + (S_w + \lambda I_d) \xi_W A \right] N \right)}{\text{Tr} \left( \xi_W^T (S_w + \lambda I_d) \xi_W \right)} \cdot \frac{\text{Tr} \left( \xi_W^T (S_w + \lambda I_d) \xi_W \right)}{\text{Tr} \left( \xi_W^T M \xi_W \right)}. \tag{D.8}
\]

Using Eq. (D.8), a simplified form of the quotient \( R(\xi_W) \), we can estimate upper and lower bounds on \( R(\xi_W) \) where \( 0 \neq \xi_W \in T_{W^*} \text{St}(S_w + \lambda I_d)(p, d) \) in order to bound the condition number of the Riemannian Hessian at \( W^* \). Since for \( \xi_W \neq 0 \) the term \( \frac{\text{Tr} \left( \xi_W^T (S_w + \lambda I_d) \xi_W \right)}{\text{Tr} \left( \xi_W^T M \xi_W \right)} > 0 \), then the upper and lower bounds on
\[
\frac{\text{Tr} \left( \xi_W^T \left[ -S_B \xi_W + (S_w + \lambda I_d) \xi_W A \right] N \right)}{\text{Tr} \left( \xi_W^T (S_w + \lambda I_d) \xi_W \right)}, \tag{D.9}
\]
together with the upper and lower bounds of \( \frac{\text{Tr} \left( \xi_W^T (S_w + \lambda I_d) \xi_W \right)}{\text{Tr} \left( \xi_W^T M \xi_W \right)} \) bound the condition number of the Riemannian Hessian at \( W^* \).

We begin by estimating the term \( \frac{\text{Tr} \left( \xi_W^T (S_w + \lambda I_d) \xi_W \right)}{\text{Tr} \left( \xi_W^T M \xi_W \right)} \). We use the vectorization operator and the Kronecker Product to rewrite it in the following form
\[
\frac{\text{Tr} \left( \xi_W^T (S_w + \lambda I_d) \xi_W \right)}{\text{Tr} \left( \xi_W^T M \xi_W \right)} = \frac{\text{vec} \left( \xi_W \right)^T (I_p \otimes (S_w + \lambda I_d)) \text{vec} \left( \xi_W \right)}{\text{vec} \left( \xi_W \right)^T (I_p \otimes M) \text{vec} \left( \xi_W \right)}. \tag{D.10}
\]

The righthand side of Eq. (D.10) is the generalized Rayleigh quotient for the matrix pencil \((I_p \otimes (S_w + \lambda I_d), I_p \otimes M)\). Note that \((I_p \otimes (S_w + \lambda I_d), I_p \otimes M)\) and \((I_p \otimes M)\) are both SPD matrices, thus the eigenvalues of the matrix pencil \((I_p \otimes (S_w + \lambda I_d), I_p \otimes M)\) are equivalent to the eigenvalues of the matrix \((I_p \otimes M)^{-1} (I_p \otimes (S_w + \lambda I_d)) = I_p \otimes M^{-1} (S_w + \lambda I_d)\) and all positive. According to [39 Section 2] the eigenvalues \(I_p \otimes M^{-1} (S_w + \lambda I_d)\) are \(p\) copies of each of the eigenvalues of \(M^{-1} (S_w + \lambda I_d)\). Thus, the maximal and minimal eigenvalues of the matrix pencil \((I_p \otimes (S_w + \lambda I_d), I_p \otimes M)\) denoted by \(\lambda_{\text{max}}\) and \(\lambda_{\text{min}}\) are equivalent to the maximal and minimal eigenvalues of the matrix pencil \((S_w + \lambda I_d, M)\), and so is the corresponding condition number
\[
\kappa \left( I_p \otimes (S_w + \lambda I_d), I_p \otimes M \right) = \frac{\lambda_{\text{max}}}{\lambda_{\text{min}}} = \kappa \left( (S_w + \lambda I_d), M \right).
\]

Therefore, using the Courant-Fischer Theorem
\[
\lambda_{\text{max}} = \lambda_{\text{max}} \left( I_p \otimes (S_w + \lambda I_d), I_p \otimes M \right)
= \max_{0 \neq \xi_W \in \mathbb{R}^{d \times p}} \frac{\text{vec} \left( \xi_W \right)^T (I_p \otimes (S_w + \lambda I_d)) \text{vec} \left( \xi_W \right)}{\text{vec} \left( \xi_W \right)^T (I_p \otimes M) \text{vec} \left( \xi_W \right)}
\geq \max_{0 \neq \xi_W \in T_{W^*} \text{St}(S_w + \lambda I_d)(p, d)} \frac{\text{vec} \left( \xi_W \right)^T (I_p \otimes (S_w + \lambda I_d)) \text{vec} \left( \xi_W \right)}{\text{vec} \left( \xi_W \right)^T (I_p \otimes M) \text{vec} \left( \xi_W \right)}
\]
and
\[
\lambda_{\text{min}} = \lambda_{\text{min}} \left( I_p \otimes (S_w + \lambda I_d), I_p \otimes M \right)
= \min_{0 \neq \xi_W \in \mathbb{R}^{d \times p}} \frac{\text{vec} \left( \xi_W \right)^T (I_p \otimes (S_w + \lambda I_d)) \text{vec} \left( \xi_W \right)}{\text{vec} \left( \xi_W \right)^T (I_p \otimes M) \text{vec} \left( \xi_W \right)}
\leq \min_{0 \neq \xi_W \in T_{W^*} \text{St}(S_w + \lambda I_d)(p, d)} \frac{\text{vec} \left( \xi_W \right)^T (I_p \otimes (S_w + \lambda I_d)) \text{vec} \left( \xi_W \right)}{\text{vec} \left( \xi_W \right)^T (I_p \otimes M) \text{vec} \left( \xi_W \right)}
\]
Next, we consider Eq. (D.9). Recall that we can rewrite any tangent vector, \( \xi_W \in T_{\mathbf{St}_{(S_w + \lambda I_d)}}(p,d) \), in the following form:

\[
\xi_W = W \Omega_W + W_{(S_w + \lambda I_d)} \perp K_W,
\]

where \( W_{(S_w + \lambda I_d)} \perp \) is \((S_w + \lambda I_d)\)-orthogonal to \( W \) so that the union of the columns of \( W \) and \( W_{(S_w + \lambda I_d)} \perp \) is a basis to \( \mathbb{R}^d \), and \( \Omega_W = -\Omega_W^T \in \mathbb{R}^{p \times p} \). Note that we can always make the choice of the columns of \( W_{(S_w + \lambda I_d)} \perp \) to be some \( d - p \) generalized eigenvalues of the matrix pencil \((S_B, S_w + \lambda I_d)\). With this choice we have

\[
S_B W_{(S_w + \lambda I_d)} \perp = (S_w + \lambda I_d) W_{(S_w + \lambda I_d)} \perp \tilde{A}, \quad W_{(S_w + \lambda I_d)} \perp S_B W_{(S_w + \lambda I_d)} \perp = \tilde{A},
\]

where \( \tilde{A} \in \mathbb{R}^{(d-p) \times (d-p)} \) is a diagonal matrix with the corresponding generalized eigenvalues on the diagonal \( \alpha_{p+1}, ..., \alpha_d \).

Now, we have

\[
\xi_W^T (S_w + \lambda I_d) \xi_W = \Omega_W^T \Omega_W + K_W^T K_W
\]

and

\[
\xi_W^T S_B \xi_W = \Omega_W^T A \Omega_W + K_W^T \tilde{A} K_W.
\]

Substitute these computations into Eq. (D.9)

\[
\frac{\text{Tr} \left( \xi_W^T [-S_B \xi_W + (S_w + \lambda I_d) \xi_W A] N \right)}{\text{Tr} \left( \xi_W^T (S_w + \lambda I_d) \xi_W \right)} = \frac{\text{Tr} \left( \left( \Omega_W^T A \Omega_W + K_W^T \tilde{A} K_W \right) N + (\Omega_W^T \Omega_W + K_W^T K_W) A N \right)}{\text{Tr} \left( \Omega_W^T \Omega_W + K_W^T K_W \right)}
\]

\[
= \frac{\text{vec}(\Omega_W)^T D_1 \text{vec}(\Omega_W) + \text{vec}(K_W)^T D_2 \text{vec}(K_W)}{\text{vec}(\Omega_W)^T \text{vec}(\Omega_W) + \text{vec}(K_W)^T \text{vec}(K_W)},
\]

where

\[
D_1 := AN \otimes I_p - N \otimes A, \quad D_2 := AN \otimes I_{d-p} - N \otimes \tilde{A}.
\]

Recall that \( \Omega_W = -\Omega_W^T \in \mathbb{R}^{p \times p} \), and both are real matrices (so the elements of the main diagonals are 0), we have

\[
\text{vec}(\Omega_W)^T \text{vec}(\Omega_W) = 2 \sum_{p \geq i > j} (\Omega_W)_{ij}^2 \quad \text{(D.11)}
\]

and

\[
\text{vec}(\Omega_W)^T (AN \otimes I_p - N \otimes A) \text{vec}(\Omega_W) = \sum_{1 \leq j < i \leq p} (\Omega_W)_{ij}^2 (\mu_j - \mu_i) (\alpha_j - \alpha_i) \quad \text{(D.12)}
\]

Thus, only the \( p(p-1)/2 \) entries below the diagonal of \( \Omega_W \) determine the values of Eq. (D.11) and Eq. (D.12). Let us now denote by \( \mathbf{m}_W \) the column stack of \( \Omega_W \), but only with the subdiagonal entries of \( \Omega_W \) (i.e., \( \text{vec}(\Omega_W) \) purged of the superdiagonal elements). We then have

\[
\text{vec}(\Omega_W)^T \text{vec}(\Omega_W) = 2 \mathbf{m}_W^T \mathbf{m}_W
\]

and

\[
\text{vec}(\Omega_W)^T (AN \otimes I_p - N \otimes A) \text{vec}(\Omega_W) = \mathbf{m}_W^T \Psi \mathbf{m}_W
\]

where \( \Psi \in \mathbb{R}^{p(p-1)/2 \times p(p-1)/2} \) is a block diagonal matrix, where the blocks are of descending order from \( p - 1, p - 2, ..., 1 \), and each block is a diagonal matrix as well. The \( j \)th \( (1 \leq j \leq p - 1) \) block, denoted by \( \Psi_j \), is of order \( p - j \) and has the following form

\[
\Psi_j = \text{diag} ((\mu_j - \mu_{j+1}) (\alpha_j - \alpha_{j+1}), (\mu_j - \mu_{j+2}) (\alpha_j - \alpha_{j+2}), ..., (\mu_j - \mu_p) (\alpha_j - \alpha_p))
\]

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Now, we make the following change of variables: \( d_W := \sqrt{2} m_W \), \( k_W := \text{vec}(K_W) \). Finally, Eq. (D.9) is rewritten in the following way:

\[
\frac{\text{Tr} \left( \xi_W^T [-S_{\omega} \xi_W + (S_w + \lambda d) \xi_W A] N \right)}{\text{Tr} \left( \xi_W^T (S_w + \lambda d) \xi_W \right)} = \frac{\begin{bmatrix} d_w^T & k_w^T \end{bmatrix} \text{blkdiag} \left( \frac{1}{2} \Psi \cdot AN \otimes I_{d-p} - N \otimes \tilde{A} \right) \begin{bmatrix} d_w \\ k_w \end{bmatrix}}{\begin{bmatrix} d_w^T & k_w^T \end{bmatrix} \begin{bmatrix} d_w \\ k_w \end{bmatrix}}. \tag{D.13}
\]

Note that the mapping \( \varphi(\cdot) : T_{W^*} L_{(S_w + \lambda d)}(p, d) \rightarrow \mathbb{R}^{pd - p(p + 1)/2} \) defined by

\[
\varphi(\xi_W) := \begin{bmatrix} d_W \\ k_W \end{bmatrix},
\]

is a coordinate chart of the elements of \( T_{W^*} L_{(S_w + \lambda d)}(p, d) \), since \( \varphi(\cdot) \) is a bijection (one-to-one correspondence) of the elements of \( T_{W^*} L_{(S_w + \lambda d)}(p, d) \) onto \( \mathbb{R}^{pd - p(p + 1)/2} \). Indeed, \( k_W \) is a column stack of \( K_W \), thus we can retract the matrices \( K_W \). Similarly \( d_W \) is proportional to \( m_W \) which is a column stack of \( \Omega_W \), but only with the the subdiagonal entries of \( \Omega_W \). Since \( \Omega_W \) is a skew-symmetric matrix, we can retract \( \Omega_W \). With the matrices \( K_W \) and \( \Omega_W \) at hand, we can fully retract \( \xi_W \).

The eigenvalues and corresponding eigenvectors of any linear operator over a finite dimensional vector space do not depend on the choice of coordinate chart and basis, thus the eigenvalues and eigenvectors of \( \text{Hess}_{FDA}(W)[\cdot] : T_{W^*} L_{(S_w + \lambda d)}(p, d) \rightarrow T_{W^*} L_{(S_w + \lambda d)}(p, d) \) which are computed using the Courant Fischer Theorem for compact self-adjoint linear operators (Eq. (D.3) and Eq. (D.4)), can also be computed by the Courant Fischer Theorem for symmetric matrices \[28, \text{Theorem 4.2.6}] after applying \( \varphi(\cdot) \). In particular, Eq. (D.9) determines the signs of the eigenvalues of the Riemannian Hessian at any \( W \in L_{(S_w + \lambda d)}(p, d) \) (in the special case \( M = S_w + \lambda d \), the eigenvalues of Eq. (D.14) are the eigenvalues of the Riemannian Hessian at \( W \in L_{(S_w + \lambda d)}(p, d) \)), and the bounds of Eq. (D.9) together with the bounds of the term \( \text{Tr} \left( \xi_W^T (S_w + \lambda d) \xi_W \right) / \text{Tr} \left( \xi_W^T M \xi_W \right) \) bound the condition number of the Riemannian Hessian at \( W^* \in L_{(S_w + \lambda d)}(p, d) \).

To that end, we perform the following computation. The right-hand side of Eq. (D.13) is a Rayleigh quotient, so according to the Courant-Fischer Theorem for symmetric matrices the eigenvalues (in particular, the maximal and the minimal) of the \( pd - p(p + 1)/2 \times pd - p(p + 1)/2 \) symmetric matrix

\[
\text{blkdiag} \left( \frac{1}{2} \Psi \cdot AN \otimes I_{d-p} - N \otimes \tilde{A} \right), \tag{D.14}
\]

are determined by optimal (in particular the maximal and the minimal) values of Eq. (D.13). The set of eigenvalues of Eq. (D.14) is equal to the union of the set of eigenvalues of \( \frac{1}{2} \Psi \cdot AN \otimes I_{d-p} - N \otimes \tilde{A} \). Since Eq. (D.14) is a diagonal matrix, its eigenvalues are simply the diagonal elements:

\[
\frac{1}{2} (\mu_j - \mu_i) (\alpha_j - \alpha_i), \quad 1 \leq j < i \leq p,
\]

and

\[
\mu_j (\alpha_j - \alpha_i), \quad j = 1, \ldots, p, \quad i = p + 1, \ldots, d.
\]

Finally, we bound the condition number of the Riemannian Hessian at \( W^* \in L_{(S_w + \lambda d)}(p, d) \). In such case, \( \alpha_1 = \rho_1 > \ldots > \alpha_p = \rho_p \). Without loss of generality, we can always choose \( W_{(S_w + \lambda d)} \) such that the corresponding eigenvalues to its columns are in a descending order, thus, \( \alpha_{p+1} = \rho_{p+1} \geq \ldots \geq \alpha_d = \rho_d \geq 0 \). Then, we have that Eq. (D.9) is bounded by the minimal and maximal eigenvalues of (D.14). Thus,

\[
0 < \max_{0 \neq \xi_W \in T_{W^*} L_{(S_w + \lambda d)}(p, d)} \frac{\text{Tr} \left( \xi_{W^*}^T [-S_{B} \xi_{W^*} + (S_w + \lambda d) \xi_{W^*} A] N \right)}{\text{Tr} \left( \xi_{W^*}^T (S_w + \lambda d) \xi_{W^*} \right)} \leq \mu_1 (\rho_1 - \rho_d),
\]

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and
\[
\min_{0 \neq \xi_{W} \in T_{W} \cdot St_{(S_{w} + \lambda I_{d})}(p, d)} \frac{\text{Tr} \left( \xi_{W}^{T} \left[ -S_{R} \xi_{W} + (S_{w} + \lambda I_{d}) \xi_{W} A \right] N \right)}{\text{Tr} \left( \xi_{W}^{T} (S_{w} + \lambda I_{d}) \xi_{W} \right)} \geq \min \left\{ \mu_{p} (\rho_{p} - \rho_{p+1}), \min_{1 \leq j < p} \frac{1}{2} (\mu_{j} - \mu_{j+1}) (\rho_{j} - \rho_{j+1}) \right\} > 0.
\]

We use Eq. (D.5) and Eq. (D.6) to bound the condition number:
\[
\lambda_{\max}(\text{Hess}_{FDA}(W^{*})) = \max_{0 \neq \xi_{W} \in T_{W} \cdot St_{(S_{w} + \lambda I_{d})}(p, d)} \frac{g_{W} \cdot (\xi_{W}, \text{Hess}_{FDA}(W^{*})[\xi_{W}])}{g_{W} \cdot (\xi_{W}, \xi_{W})} \leq \mu_{1} (\rho_{1} - \rho_{d}) \lambda_{\max} ,
\]
and
\[
\lambda_{\min}(\text{Hess}_{FDA}(W^{*})) = \min_{0 \neq \xi_{W} \in T_{W} \cdot St_{(S_{w} + \lambda I_{d})}(p, d)} \frac{g_{W} \cdot (\xi_{W}, \text{Hess}_{FDA}(W^{*})[\xi_{W}])}{g_{W} \cdot (\xi_{W}, \xi_{W})} \geq \min \left\{ \mu_{p} (\rho_{p} - \rho_{p+1}), \min_{1 \leq j < p} \frac{1}{2} (\mu_{j} - \mu_{j+1}) (\rho_{j} - \rho_{j+1}) \right\} \lambda_{\min} .
\]
Finally,
\[
\kappa(\text{Hess}_{FDA}(W^{*})) = \frac{\lambda_{\max}(\text{Hess}_{FDA}(W^{*}))}{\lambda_{\min}(\text{Hess}_{FDA}(W^{*}))} \leq \kappa^{*}_{FDA} \cdot \kappa (S_{w} + \lambda I_{d}, M) ,
\]
where
\[
\kappa^{*}_{FDA} = \min \left\{ \mu_{p} (\rho_{p} - \rho_{p+1}), \min_{1 \leq j < p} \frac{1}{2} (\mu_{j} - \mu_{j+1}) (\rho_{j} - \rho_{j+1}) \right\} .
\]
In the special case \(M = S_{w} + \lambda I_{d}\), the bound on the condition number of the Riemannian Hessian at \(W^{*} \in St_{(S_{w} + \lambda I_{d})}(p, d)\) is reduced to
\[
\kappa(\text{Hess}_{FDA}(W^{*})) = \kappa^{*}_{FDA} .
\]

D.4 Proof of Theorem 17

Proof. To show that \(W^{*}\) is a strict local minimum of \(f_{FDA}(W)\) we show that the eigenvalues of the Riemannian Hessian at \(W^{*}\) are strictly positive (see [7, Proposition 6.2.]). Moreover, under the assumption that for all \(i = 1, \ldots, d\) the values \(\rho_{i}\) are distinct, we prove that \(W^{*}\) is the only local minimum of \(f_{FDA}(W)\) and all other critical points are either saddle points or strict local maximizers.

Eq. (D.8) helps to determine the signs of the eigenvalues of the Riemannian Hessian at any critical point \(W \in St_{(S_{w} + \lambda I_{d})}(p, d)\) and in particular at \(W^{*}\): the matrices \(S_{w} + \lambda I_{d}\) and \(M\) are both SPD matrices, therefore for \(\xi_{W} \neq 0\) the term \(\text{Tr} \left( \xi_{W}^{T} (S_{w} + \lambda I_{d}) \xi_{W} \right) > 0\), thus only Eq. (D.9), where \(0 \neq \xi_{W} \in T_{W} \cdot St_{(S_{w} + \lambda I_{d})}(p, d)\) determines the signs. In addition, at a critical point \(W \in St_{(S_{w} + \lambda I_{d})}(p, d)\) Eq. (D.9) equals to the quotient \(R(\xi_{W})\) for the choice \(M = S_{w} + \lambda I_{d}\), since [1] Proposition 5.5.6 and Eq. (5.25) show that at a critical point the term \(g_{W} \cdot (\xi_{W}, \text{Hess}_{FDA}(W^{*})[\xi_{W}])\) which is the numerator of \(R(\xi_{W})\) do not depend on the choice of Riemannian metric. Thus, the optimal values of Eq. (D.9) satisfying Eq. (D.3) or Eq. (D.4) are the eigenvalues of the Riemannian Hessian at \(W \in St_{(S_{w} + \lambda I_{d})}(p, d)\) with the choice \(M = S_{w} + \lambda I_{d}\). Obviously, classification of the critical points does not depend on the Riemannian metric.

Therefore, we can classify the critical points using the signs of the eigenvalues of the Riemannian Hessian at \(W \in St_{(S_{w} + \lambda I_{d})}(p, d)\) with the choice \(M = S_{w} + \lambda I_{d}\).
Recall from the proof of Theorem [10] that in the special case $M = S_w + \lambda I_d$, the eigenvalues of Eq. (D.14) are also the eigenvalues of the Riemannian Hessian at a critical point $W \in St(S_w + \lambda I_d)(p, d)$. The eigenvalues are:

$$\frac{1}{2} (\mu_j - \mu_i) (\alpha_j - \alpha_i), \quad 1 \leq j < i \leq p,$$

and

$$\mu_j (\alpha_j - \alpha_i), \quad j = 1, ..., p, \quad i = p + 1, ..., d.$$

Now, we can conclude the signs of the eigenvalues of the Riemannian Hessian at any critical point $W \in St(S_w + \lambda I_d)(p, d)$ for the choice $M = S_w + \lambda I_d$, and classify these critical points. Recall that $\mu_i > 0$ for $i = 1, ..., p$, and $\mu_j - \mu_i > 0$ for $j < i$. Also $\alpha_i \geq 0$. Thus, the signs of the eigenvalues of Eq. (D.14) are only determined by the differences between $\alpha_j, j = 1, ..., p$ which are some generalized eigenvalues of the matrix pencil $(S_B, S_w + \lambda I_d)$, corresponding to the generalized eigenvectors on ordered $1 \leq j < i \leq p$, but on the other hand there exists at least one pair of indexes $j = 1, ..., p$ and $i = p + 1, ..., d$ such that $\alpha_j - \alpha_i < 0$, otherwise it contradicts the assumption on the columns of $W$, and the $d - j$ trailing $\alpha_i$’s, i.e., $\alpha_j - \alpha_i$ where $1 \leq j < i \leq p$ or $j = 1, ..., p$ and $i = p + 1, ..., d$.

In particular, for $W^*$ such that the columns are the $p$-dominant generalized eigenvectors of the matrix pencil $(S_B, S_w + \lambda I_d)$, then by the assumption that $\alpha_1 = \rho_1 > ... > \alpha_p = \rho_p$, we have $\alpha_j - \alpha_i > 0$ where $1 \leq j < i \leq p$ or $j = 1, ..., p$ and $i = p + 1, ..., d$. Therefore, in this case all the eigenvalues of Eq. (D.14) are strictly positive, thus the matrix in Eq. (D.14) is SPD, and consequently the eigenvalues of the Riemannian Hessian at $W^*$ are all strictly positive. Thus, $W^*$ is a strict local minimum of $f_{FDA}(W)$ on $St(S_w + \lambda I_d)(p, d)$.

If we prove that $W^*$ it is the only local minimum (up to the signs of the columns), then it is the only asymptotically stable critical point according to Theorem [15]. In order to prove it we further assume that for all $i = 1, ..., d$ the values $\rho_i$ are distinct, then we can conclude the following. Suppose $W$ is any other critical point differs from $W^*$ at the optimal value, i.e., such that the columns of $W$ are ordered generalized eigenvectors corresponding to some $p$ singular values of the matrix pencil $(S_B, S_w + \lambda I_d)$, $\alpha_1, ..., \alpha_p$, which are not the leading $p$ values. We consider the different cases:

1. Suppose $\alpha_1, ..., \alpha_p$ are not ordered in any particular order (possible only for $p \geq 3$), then there exists $j$ such that $\alpha_j$ is larger than some $\alpha_k$ and smaller than $\alpha_m$ where $j < k, m \leq p$, then $\alpha_j - \alpha_k > 0$ and $\alpha_j - \alpha_m < 0$. In this case there are both strictly positive and strictly negative eigenvalues of the Riemannian Hessian at $W$ for the choice $M = S_w + \lambda I_d$, thus $W$ is a saddle point.

2. Suppose $\alpha_1, ..., \alpha_p$ are ordered in a descending order. Since $Z$ is not an optimal solution of Problem (5.3), then there exists at least one $1 \leq j \leq p$ for which $\alpha_j \neq \rho_j$. Thus, on the one hand $\alpha_j - \alpha_i > 0$ where $1 \leq j < i \leq p$, but on the other hand there exists at least one pair of indexes $j = 1, ..., p$ and $i = p + 1, ..., d$ such that $\alpha_j - \alpha_i < 0$, otherwise it contradicts the assumption that there exists at least one $1 \leq j \leq p$ for which $\alpha_j \neq \rho_j$. In this case there are both strictly positive and strictly negative eigenvalues of the Riemannian Hessian at $W$ for the choice $M = S_w + \lambda I_d$, therefore, $W$ is a saddle point.

3. Suppose $\alpha_1, ..., \alpha_p$ are ordered in an ascending order. Then, $\alpha_j - \alpha_i < 0$ where $1 \leq j < i \leq p$. Now, we consider two sub-cases:

(a) There exists at least one $1 \leq j \leq p$ for which $\alpha_j \neq \rho_{d-j+1}$. Then, there exists at least one pair of indexes $j = 1, ..., p$ and $i = p + 1, ..., d$ such that $\alpha_j - \alpha_i > 0$, otherwise it contradicts the assumption that there exists at least one $1 \leq j \leq p$ for which $\alpha_j \neq \rho_{d-j+1}$. In this case there are both strictly positive and strictly negative eigenvalues of the Riemannian Hessian at $W$ for the choice $M = S_w + \lambda I_d$, therefore, $W$ is a saddle point.
(b) Consider the case \( \alpha_1 = \rho_d < \alpha_2 = \rho_{d-1} < \ldots < \alpha_p = \rho_{d-p+1} \). Thus, \( \alpha_j - \alpha_i < 0 \) where \( 1 \leq j < i \leq p \) or \( j = 1, \ldots, p \) and \( i = p+1, \ldots, d \). In this case all the eigenvalues of the Riemannian Hessian at \( W \) are strictly negative for the choice \( M = S_w + \lambda_1 I_d \), thus, \( W \) is a local maximizer. Since it is the only strict local maximizer up to the signs of the columns of \( W \), and it is also the global maximizer.

In all cases, \( W \) is not a local minimizer of \( f_{\text{FDA}}(W) \) on \( St_{(S_w + \lambda I_d)}(p, d) \). Thus, \( W^* \) is the only (strict) local minimum (up to the signs of the columns). According to Theorem 12 all these critical points are unstable.

### D.5 Proof of Corollary 11

**Proof.** The condition number bound follows immediately from Lemma 1 and Theorem 10. For the costs, the same arguments as in the proof of Corollary 6 hold: none of the operations require forming \( S_B \) or \( S_w \), but instead require taking product of these matrices with vectors. These products can be computed in cost proportional to the iterated products of the matrices \( \hat{X} \) and/or \( \hat{Y} \) with vectors. Computing a product of the matrix \( X = X - Y \) with a vector is equivalent to computing the product of the same vector with the matrices \( X \) and \( Y \) and subtracting the result. Computing the product of \( X \) with a vector is proportional number of non-zeros in \( X \), and the cost of the product of \( Y \) with a vector is \( O(ld) \) since \( Y \) has exactly \( l \) distinct rows. Computing a product of the matrix \( \hat{Y} \) with a vector costs \( O(ld) \) since \( \hat{Y} \) is a \( l \times d \) matrix. The preprocessing steps follow from Table 2. Assuming a bounded number of line-search steps in each iteration of Riemannian CG, the costs follows from Table 2 as each iteration requires a bounded number of computations of each of the following: objective function evaluation \( O(p (\text{nnz}(X) + ld)) \), retraction \( O(\text{nnz}(X)p + dp^2) \), vector transport and Riemannian gradient \( O(p(\text{nnz}(X) + ld) + \text{nnz}(\hat{X})p + dp^2 + d^2p) \).

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