Abstract

Covariance operators are fundamental in functional data analysis, providing the canonical means to analyse functional variation via the celebrated Karhunen–Loève expansion. These operators may themselves be subject to variation, for instance in contexts where multiple functional populations are to be compared. Statistical techniques to analyse such variation are intimately linked with the choice of metric on covariance operators, and the intrinsic infinite-dimensionality of these operators. In this paper, we describe the manifold-like geometry of the space of trace-class infinite-dimensional covariance operators and associated key statistical properties, under the recently proposed infinite-dimensional version of the Procrustes metric (Pigoli et al. *Biometrika* 101, 409–422, 2014). We identify this space with that of centred Gaussian processes equipped with the Wasserstein metric of optimal transportation. The identification allows us to provide a detailed description of those aspects of this manifold-like geometry that are important in terms of statistical inference; to establish key properties of the Fréchet mean of a random sample of covariances; and to define generative models that are canonical for such metrics and link with the problem of registration of warped functional data.

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1 Introduction

Background and Contributions Covariance operators play a central role in functional data analysis (Hsing and Eubank, 2015; Ramsay and Silverman, 2005): nonparametric inference on the law of a stochastic process $X$ viewed as a random element of an infinite-dimensional separable Hilbert space $\mathcal{H}$ (most usually $L^2$ or some reproducing kernel Hilbert subspace thereof). In particular, covariance operators serve as the canonical means...
to study the variation of such random functions. Their spectrum provides a singular system separating the stochastic and functional fluctuations of $X$, allowing for optimal finite dimensional approximations and functional PCA via the Karhunen–Loève expansion. And, that same singular system arises as the natural means of regularisation for inference problems (such as regression and testing) which are ill-posed in infinite dimensions (Panaretos and Tavakoli, 2013; Wang et al., 2016).

There are natural statistical applications where covariances may be the main object of interest in themselves, and may present variation of their own. These typically occur in situations where several different “populations” of functional data are considered, and there is strong reason to suspect that each population may present different structural characteristics. Each one of $K$ populations is modelled by a prototypical random function $X_k$, with mean function $\mu_k \in \mathcal{H}$ and covariance operator $\Sigma_k : \mathcal{H} \times \mathcal{H} \to \mathcal{H}$ and we are able to observe $N_k$ realisations from each population: $\{X_k^i : i = 1, \ldots, N_k; k = 1, \ldots, K\}$. Examples of such situations include the two (or potentially more) populations of DNA strands considered in Panaretos et al. (2010), Kraus and Panaretos (2012), and Tavakoli and Panaretos (2016), resulting from different base pair composition of each DNA strand, but clearly extend to much wider contexts.

A classical problem is the case where it is assumed that the different populations differ in their mean structure, leading to what has become known as Functional Analysis of Variance (see Zhang (2013) for an overview). This represents first-order variation across populations, as it can be considered as a model of the form

$$X_k^i(t) = \mu(t) + \mu_k(t) + \varepsilon_i(t),$$

with $\varepsilon_i(t)$ being mean zero and covarying according to some $\Sigma$.

An intriguing further type of variation is second-order variation, which occurs by assuming that the covariance operators vary across populations, $\Sigma_i \neq \Sigma_j$ for $i \neq j$. This type of variation is particularly relevant in functional data, as it represents qualitative differences in the smoothness and fluctuation properties of the different populations. Early contributions in this area were motivated through financial and biophysical applications (Benko et al., 2009; Panaretos et al., 2010). These led to a surge of methods and theory on second-order variation of functional populations, in many directions: Horváth et al. (2013), Paparoditis and Sapatinas (2014), Gabrys et al. (2010), Fremdt et al. (2013), Horváth and Kokoszka (2012), Jarušková (2013), Coffey et al. (2011), Kraus (2015).
What is common to many of these approaches is that the second-order variation is, in a sense, linear. That is, the covariance operators are imbedded in the space of Hilbert–Schmidt operators, and statistical inference is carried out with respect to the corresponding metric. This space is, of course, a Hilbert space, and thus methodology of this form can be roughly thought of as modelling the second order variation via linear perturbations of an underlying covariance operator:

\[ \Sigma_k = \Sigma + E_k. \]

Here \( E_k \) would be a random zero-mean self-adjoint trace-class operator, with spectral constraints to assure the non negative-definiteness of the left hand side. Being a random trace-class self-adjoint operator, \( E \) admits its own Karhunen-Loève expansion, and this is precisely what has been employed in order to extend the linear PCA inferential methods from the case of functions. However, the restriction \( \Sigma + E_k \succeq 0 \) immediately shows that the Hilbert–Schmidt approach has unavoidable weaknesses, as it imbeds covariance operators in a larger linear space, whereas they are not closed under linear operations. Quite to the contrary, covariance operators are fundamentally constrained to obey nonlinear geometries, as they are characterised as the “squares” of Hilbert–Schmidt class operators.

In the multivariate (finite dimensional) literature this problem has been long known, and well-studied, primarily due to its natural connections with: (1) the problem of diffusion tensor imaging (see, e.g., Alexander, 2005; Schwartzman et al., 2008; Dryden et al., 2009) where it is fundamental in problems of smoothing, clustering, extrapolation, and dimension reduction, to name only a few; and (2) the statistical theory of shape (Dryden and Mardia, 1998), where Gram matrices (by definition non-negative) encode the invariant characteristics of Euclidean configurations under Euclidean motions. Consequently, inference for populations of covariance operators has been investigated under a wide variety of possible geometries for the space of covariance matrices (see, e.g., Dryden et al. (2009) or Schwartzman (2006) for an overview). However, many of these metrics are based on quantities that do not lend themselves directly for generalisation to infinite dimensional spaces (e.g., determinants, logarithms and inverses).

Pigoli et al. (2014) were the first to make important progress in the direction of considering second-order variation in appropriate nonlinear spaces, motivated by the problem of cross-linguistic variation of phonetics in Romance languages (where the uttering of a short word is modelled as a random function). They paid particular attention to the generalisation of the
so-called Procrustes size-and-shape metric (which we will call simply Procrustes metric henceforth, for tidiness), and derived some of its basic properties, with a view towards initiating a programme of non-Euclidean analysis of covariance operators. In doing so, they (implicitly or explicitly) generated many further interesting research directions on the geometrical nature of this metric, its statistical interpretation, and the properties of Fréchet means with respect to this metric.

The purpose of this paper is to address some of these questions, and further our understanding of the Procrustes metric and the induced statistical models and procedures, thus placing this new research direction in non-Euclidean statistics on a firm footing. The starting point is a relatively straightforward but quite consequential observation: that the Procurstes metric between two covariance operators on $\mathcal{H}$ coincides with the Wasserstein metric between two centred Gaussian processes on $\mathcal{H}$ endowed with those covariances, respectively (Proposition 3, Section 2). This connection allows us to exploit the wealth of geometrical and analytical properties of optimal transportation, and contribute in two ways. On the one hand, by reviewing and collecting some important aspects of Wasserstein spaces, re-interpreted in the Procrustean context, we elucidate key geometrical (Section 3), topological (Section 4), and computational (Section 8) aspects of the space of covariances endowed with the Procrustes metric. On the other hand, we establish new results related to existence/uniqueness/stability of Fréchet means of covariances with respect to the Procrustes metric (Section 6), tangent space principal component analysis and Gaussian multicoupling (Section 9), and generative statistical models compatible with the Procrustes metric and linking with the problem of warping/registration in functional data analysis (Section 10). We conclude by formulating a conjecture on the regularity of the Fréchet mean that could have important consequences on statistical inference (Conjecture 17), and by posing some additional questions for future research (Section 12). The next paragraph collects the notational conventions employed throughout the paper, while an ancillary section (Section 13) collects some background technical results, for tidiness.

**Notation** Let $\mathcal{H}$ be a real separable Hilbert space with inner product $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{R}$, and induced norm $\| \cdot \| : \mathcal{H} \to [0, \infty)$. Given a bounded linear operator $A : \mathcal{H} \to \mathcal{H}$, we will denote its trace (when defined) by $\text{tr}A$ or $\text{tr}(A)$, its adjoint operator by $A^*$, and its inverse by $A^{-1}$, which in general is only defined on a subspace (often dense) of $\mathcal{H}$. The *kernel* of $A$ will be denoted by $\text{ker}(A) = \{ v \in \mathcal{H} : Av = 0 \}$, and its *range* will be denoted by $\text{range}(A) = \{ Av : v \in \mathcal{H} \}$. We say that a (possibly unbounded) operator $A$...
is self-adjoint if \( \langle Au, v \rangle = \langle u, Av \rangle \) for all \( u, v \) in the domain of definition of \( A \); if \( A \) is bounded, then this is equivalent to \( A = A^* \). A non-negative operator is a self-adjoint, possibly unbounded operator \( A \) such that \( \langle Au, u \rangle \geq 0 \) for all \( u \) in the domain of \( A \). If in addition \( A \) is compact, then there exists a unique non-negative operator whose square equals \( A \), which will be denoted by either \( A^{1/2} \) or \( \sqrt{A} \). For any bounded operator \( A, A^*A \) is non-negative.

The identity operator on \( H \) will be denoted by \( I \). The operator, Hilbert–Schmidt and trace (nuclear) norms will respectively be

\[
\|A\|_\infty = \sup_{\|h\|=1} \|Ah\|, \quad \|A\|_2 = \sqrt{\text{tr}(A^*A)}, \quad \|A\|_1 = \text{tr}(\sqrt{A^*A}).
\]

It is well-known that

\[
\|A\|_\infty \leq \|A\|_2 \leq \|A\|_1
\]

for any bounded linear operator \( A \). When they are all finite, we say that \( A \) is nuclear or trace-class. Covariance operators are well-known to be non-negative and trace-class.

For a pair \( f, g \in H \), the tensor product \( f \otimes g : H \to H \) is the linear operator defined by

\[
(f \otimes g)u = \langle g, u \rangle f, \quad u \in H.
\]

## 2 Procrustes Matching and Optimal Transportation

### 2.1. The Procrustes Distance Between Non-negative Matrices and Operators

In classical statistical shape analysis, one often wishes to compare objects in \( \mathbb{R}^m \) modulo a symmetry group \( G \). To this aim, one chooses a fixed number of \( k \) homologous landmarks on each object, represented by \( k \times m \) matrices \( X_1 \) and \( X_2 \), and contrasts them by the Hilbert–Schmidt (a.k.a. Frobenius) distance of \( X_1 \) to \( X_2 \), optimally matched relative to the group \( G \).

Under suitable conditions, the group \( G \) induces a distance on the orbits of \( X_1 \) and \( X_2 \), the latter called the shapes of \( X_1 \) and \( X_2 \), and usually denoted as \([X_1]\) and \([X_2]\). For instance, if \( G \) is the group of rigid motions on \( \mathbb{R}^m \), one centres the configurations (so that their column sums are zero) and considers the so-called Procrustes shape-and-size distance

\[
\min_{U: U^\top U = I} \|X_1 - X_2 U\|_2 \quad (\text{Dryden and Mardia, 1998, Definition 4.13}),
\]

henceforth abbreviated to Procrustes distance, for simplicity. This distance depends mainly on the Gram matrices \( X_1^\top X_1, X_2^\top X_2 \), which can be thought of as parametrising the shapes \([X_1]\) and \([X_2]\). Since Gram matrices are non-negative, Dryden et al. (2009) considered the Procrustes distance as a metric on covariances \( \mathbb{R}^{k \times k} \ni S_1, S_2 \succeq 0 \),

\[
\Pi(S_1, S_2) = \inf_{U: U^\top U = I} \|S_1^{1/2} - S_2^{1/2} U\|_2. \quad (2.1)
\]
The unique non-negative matrix roots $S_i^{1/2}$ in (2.1) can be replaced by any matrices $Y_i$ such that $S_i = Y_iY_i^\top$, but the former is the canonical choice in the context of covariances (in shape analysis, the $Y_i$ are typically chosen via the Cholesky decomposition, and are thought of as representatives from the corresponding shape equivalence classes).

Covariance operators are trace-class and can be fundamentally seen as “squares” of operators with finite Hilbert–Schmidt norm. In order to analyse linguistic data, Pigoli et al. (2014) considered the generalisation of the Procrustes distance (2.1) to the infinite-dimensional space of covariance operators on the separable Hilbert space $L^2(0,1)$. Their definition applies readily, though, to any separable Hilbert space $\mathcal{H}$, and we give this more general definition here:

**Definition 1 (Procrustes Metric on Covariance Operators).** For any pair of nuclear and non-negative linear operators $\Sigma_1, \Sigma_2 : \mathcal{H} \times \mathcal{H} \to \mathcal{H}$ on the separable Hilbert space $\mathcal{H}$, we define the Procrustes metric as

$$
\Pi(\Sigma_1, \Sigma_2) = \inf_{U : U^*U = \mathcal{I}} \|S_1^{1/2} - \Sigma_2^{1/2}U\|_2,
$$

(2.2)

where $\{U : U^*U = \mathcal{I}\}$ is the set of unitary operators on $\mathcal{H}$.

Their motivation was mainly the construction of a procedure for testing the equality of two covariance operators on the basis of samples from the underlying two populations, tailored to the curved geometry of the space of covariance operators (as opposed to procedures based on embedding covariances in the linear space of trace-class or Hilbert–Schmidt operators). Pigoli et al. (2014) consider the behaviour of $\Pi$ under finite-dimensional projections of the operators in question with progressively increasing dimension, and construct a permutation-based test on the distance between the projections. They also discuss interpolation, geodesic curves and Fréchet means in the space of covariance operators endowed with the distance $\Pi$. In the next three subsections, we show that the distance $\Pi$ can be interpreted as a Wasserstein distance $W$. This observation will allow us not only to shed new light on the results of Pigoli et al., but also to give a more comprehensive description of the geometry of the space as well as to address some questions that were left open in Pigoli et al. (2014).

### 2.2. The Wasserstein Distance and Optimal Coupling

In this subsection, we recall the definition of the Wasserstein distance and review some of its properties that will be used in the paper; we follow Villani (2003). Let $\mu$ and $\nu$ be Borel probability measures on $\mathcal{H}$ and let $\Gamma(\mu, \nu)$ be the set of couplings of $\mu$ and $\nu$. These are Borel probability measures $\pi$ on $\mathcal{H} \times \mathcal{H}$ such
that $\pi(E \times H) = \mu(E)$ and $\pi(H \times F) = \nu(F)$ for all Borel $E, F \subseteq H$. The Wasserstein distance between $\mu$ and $\nu$ is defined as

$$W^2(\mu, \nu) = \inf_{\pi \in \Gamma(\mu, \nu)} \int_{H \times H} \|x - y\|^2 \, d\pi(x, y).$$

The distance is finite when $\mu$ and $\nu$ have a finite second moment, meaning that they belong to the Wasserstein space

$$W(\mathcal{H}) = \left\{ \mu \text{ Borel probability measure on } \mathcal{H} : \int_{\mathcal{H}} \|x\|^2 \, d\mu(x) < \infty \right\}.$$

This optimisation problem is known as the Monge–Kantorovich problem of optimal transportation, and admits a natural probabilistic formulation. Namely, if $X$ and $Y$ are random elements on $\mathcal{H}$ with respective probability laws $\mu$ and $\nu$, then the problem translates to the minimisation problem

$$\inf_{Z_1 \overset{d}{=} X, Z_2 \overset{d}{=} Y} \mathbb{E}\|Z_1 - Z_2\|^2$$

where the infimum is over all random vectors $(Z_1, Z_2)$ in $\mathcal{H} \times \mathcal{H}$ such that $X \overset{d}{=} Z_1$ and $Y \overset{d}{=} Z_2$, marginally. We sometimes write $W(X, Y)$ instead of $W(\mu, \nu)$. We say that a coupling $\pi$ is deterministic if it is manifested as the joint distribution of $(X, T(X))$ for some deterministic map $T : \mathcal{H} \to \mathcal{H}$, called an optimal transportation map (or simply optimal map, for brevity). In such a case $Y$ has the same distribution as $T(X)$ and we write $\nu = T\#\mu$ and say that $T$ pushes $\mu$ forward to $\nu$. If $\mathcal{I}$ is the identity map on $\mathcal{H}$, we can write $\pi$ in terms of $T$ as $\pi = (\mathcal{I}, T)\#\mu$, and we say that $\pi$ is induced from $T$. In order to highlight the fact that the optimal map $T$ transports $\mu$ onto $\nu$, Ambrosio et al. (2008) introduced the notation $T \equiv t^\nu_\mu$, and we will make use of this notation henceforth.

A simple compactness argument shows that the infimum in the Monge–Kantorovich problem is always attained by some coupling $\pi$, for any marginal pair of measures $\mu, \nu \in W(\mathcal{H})$. Moreover, when $\mu$ is sufficiently regular, the optimal coupling is unique and given by a deterministic coupling $\pi = (\mathcal{I}, t^\mu_\nu)\#\mu$ (by symmetry, if $\nu$ is regular then the optimal coupling is unique too and takes the form $(t^\nu_\mu, \mathcal{I})\#\nu$). Furthermore, the optimal map

\footnote{In finite dimensions, it suffices that $\mu$ be absolutely continuous with respect to Lebesgue measure. In infinite dimensions, a Gaussian measure is regular if and only if its covariance operator is injective. For a more general definition, see Ambrosio et al. (2008, Definition 6.2.2).}
$t_\mu^\nu$ is characterised as a gradient of a convex function, a result sometimes referred to as Brenier’s theorem (Brenier, 1991) though it was discovered independently by other authors (Cuesta-Albertos and Matrán, 1989; Knott and Smith, 1984; Rüschendorf and Rachev, 1990). In particular any (finite) non-negative linear combination of optimal transport maps remains optimal, as convexity is preserved under such combinations.

2.3. Optimal Transportation of Gaussian Processes

Despite admitting a useful characterisation as the gradient of a convex function, the optimal transportation map $t_\mu^\nu$ for a regular $\mu$ (and, consequently, the corresponding Wasserstein distance $W(\mu, \nu) = \sqrt{\int_\mathcal{H} \|x - t_\mu^\nu(x)\|^2 \, d\mu(x)}$) rarely admit closed-form expressions. A notable exception is the case where $\mu$ and $\nu$ are Gaussian. Suppose that $\mu \equiv N(m_1, \Sigma_1)$ and $\nu \equiv N(m_2, \Sigma_2)$ are Gaussian measures. Then

$$W^2(\mu, \nu) = \|m_1 - m_2\|^2 + \text{tr}(\Sigma_1) + \text{tr}(\Sigma_2) - 2\text{tr}\sqrt{\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2}}.$$  

See Olkin and Pukelsheim (1982) for a proof in finite dimensions, and Cuesta-Albertos et al. (1996) for any separable Hilbert space.

There is also an explicit expression for the optimal map, but its existence requires some regularity. To simplify the discussion, assume henceforth that the two Gaussian measures $\mu$ and $\nu$ are centered, i.e., $m_1 = m_2 = 0$. When $\mathcal{H} = \mathbb{R}^d$ is finite-dimensional, invertibility of $\Sigma_1$ guarantees the existence and uniqueness of a deterministic optimal coupling of $\mu \equiv N(0, \Sigma_1)$ of $\nu \equiv N(0, \Sigma_2)$, induced by the linear transport map

$$t_{\Sigma_1}^{\Sigma_2} := \Sigma_1^{-1/2}(\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2})^{1/2}\Sigma_1^{-1/2}.$$  

This formula turns out to be (essentially) valid in infinite dimensional Hilbert spaces $\mathcal{H}$, provided that $\Sigma_1$ is “more injective” than $\Sigma_2$, but the statement is a bit more subtle:

**Proposition 2.** Let $\mu \equiv N(0, \Sigma_1)$ and $\nu \equiv N(0, \Sigma_2)$ be centred Gaussian measures in $\mathcal{H}$ and suppose that $\text{ker}(\Sigma_1) \subseteq \text{ker}(\Sigma_2)$ (equivalently, $\text{range}(\Sigma_1) \supseteq \text{range}(\Sigma_2)$). Then there exists a linear subspace of $\mathcal{H}$ with $\mu$-measure 1, on which the optimal map is well-defined and is given by the linear operator

$$t_{\Sigma_1}^{\Sigma_2} = \Sigma_1^{-1/2}(\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2})^{1/2}\Sigma_1^{-1/2}.$$  

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2Recall that a random element $X$ in a separable Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ is Gaussian with mean $m \in \mathcal{H}$ and covariance $\Sigma : \mathcal{H} \times \mathcal{H}$, if $\langle X, h \rangle \sim N(\langle m, h \rangle, \langle h, \Sigma h \rangle)$ for all $h \in \mathcal{H}$; a Gaussian measure is the law of a Gaussian random element.
Proposition 2 is established by Cuesta-Albertos et al. (1996, Proposition 2.2). It is fairly easy to see that this linear subspace includes the range of $\Sigma_1^{1/2}$. In general, the linear map $t_{\Sigma_1}^{\Sigma_2}$ is an unbounded operator and cannot be extended to the whole of $\mathcal{H}$. Note that we have used the obvious switch in notation $t_{\Sigma_1}^{\Sigma_2}$ in lieu of $t_{\nu}^{\mu}$ when $\mu \equiv N(0, \Sigma_1)$ and $\nu \equiv N(0, \Sigma_2)$.

In the special case where $\Sigma_1$ and $\Sigma_2$ commute ($\Sigma_1 \Sigma_2 = \Sigma_2 \Sigma_1$), the proof of Proposition 2 is quite simple, and indeed instructive in highlighting the subtleties involved in infinite dimensions. Assume without loss of generality that $\Sigma_1$ is injective (otherwise replace $\mathcal{H}$ by the closed range of $\Sigma_1$). The domain of definition of $\Sigma_{1/2}$ is the range of $\Sigma_{1/2}$, which is dense in $\mathcal{H}$; however this range has $\mu$-measure zero. The problem is compensated by the compactness of $\Sigma_{1/2}$. Let $\{e_k\}$ be an orthonormal basis of $\mathcal{H}$ composed of the eigenvectors of $\Sigma_1$ and $\Sigma_2$ (they share the same eigenvectors, since they commute) with eigenvalues $a_k$ and $b_k$. Then $t_{\Sigma_1}^{\Sigma_2}$ simplifies to $\Sigma_{1/2} \Sigma_{1/2}$, and is defined for all $x = \sum x_k e_k \in \mathcal{H}$ such that

$$\sum_{k=1}^{\infty} (x_k b_k^{1/2}/a_k^{1/2})^2 = \sum_{k=1}^{\infty} x_k^2 b_k/a_k$$

is finite. If $X \sim N(0, \Sigma_1)$, then $X_k = \langle X, e_k \rangle$ are independent, and by Kolmogorov’s Three Series Theorem (Durrett, 2010, Theorem 2.5.4) the above series converges almost surely because $E(X_k^2) = a_k$ and $\sum E X_k^2 b_k/a_k = \sum b_k = \text{tr}\Sigma_2 < \infty$ because $\Sigma_2$ is trace-class; the other two series in the theorem are also easily verified to converge. We see that $t_{\Sigma_1}^{\Sigma_2}$ is bounded if and only if $b_k/a_k$ is bounded, which may or may not be the case.

2.4. Procrustes Covariance Distance and Gaussian Optimal Transportation We now connect the material in Sections 2.1–2.3, to make the following observation:

**Proposition 3.** The Procrustes distance between two trace-class covariance operators $\Sigma_1$ and $\Sigma_2$ on $\mathcal{H}$ coincides with the Wasserstein distance between two second-order Gaussian processes $N(0, \Sigma_1)$ and $N(0, \Sigma_2)$ on $\mathcal{H}$,

$$\Pi(\Sigma_1, \Sigma_2) = \inf_{R: R^* R = I} \| \Sigma_1^{1/2} - \Sigma_2^{1/2} R \|_2$$

$$= \sqrt{\text{tr}(\Sigma_1) + \text{tr}(\Sigma_2) - 2\text{tr}\sqrt{\Sigma_2^{1/2} \Sigma_1^{1/2}}}$$

$$= W(N(0, \Sigma_1), N(0, \Sigma_2)).$$

**Proof.** Following Pigoli et al. (2014), we write

$$\Pi^2(\Sigma_1, \Sigma_2) = \inf_R \text{tr}[(\sqrt{\Sigma_1} - \sqrt{\Sigma_2 R})^* (\sqrt{\Sigma_1} - \sqrt{\Sigma_2 R})]$$
\[
= \text{tr}\Sigma_1 + \text{tr}\Sigma_2 - 2\sup_R \text{tr}(R^*\Sigma_2^{1/2}\Sigma_1^{1/2}).
\]

Let \( C = (\Sigma_2^{1/2}\Sigma_1^{1/2})^*\Sigma_2^{1/2}\Sigma_1^{1/2} = \Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2} \) and the singular value decomposition \( \Sigma_2^{1/2}\Sigma_1^{1/2} = UC^{1/2}V \) for \( U \) and \( V \) unitary. Then \( \text{tr}(R^*\Sigma_2^{1/2}\Sigma_1^{1/2}) = \text{tr}(VR^*UC^{1/2}) \) is maximised when \( VR^*U \) is the identity (since \( \{VR^*U : R^*R = I\} \) is precisely the collection of unitary operators, and \( C^{1/2} \) is non-negative). We thus have

\[
\Pi^2(\Sigma_1, \Sigma_2) = \text{tr}(\Sigma_1) + \text{tr}(\Sigma_2) - 2\text{tr} \left( \sqrt{\Sigma_2^{1/2}\Sigma_1\Sigma_2^{1/2}} \right),
\]
as desired.

See also Bhatia et al. (2018) who arrive at the same identity in finite dimensions as a variational principle, and who furthermore point out connections to quantum information, where a related quantity is known as the Bures distance. It is worth pointing out that if \( \Sigma_1 \) and \( \Sigma_2 \) happen to commute, then the product \( \Sigma_1^{1/2}\Sigma_2^{1/2} \) is self adjoint, so that \( \sqrt{(\Sigma_1^{1/2}\Sigma_2^{1/2})^*\Sigma_1^{1/2}\Sigma_2^{1/2}} = \Sigma_1^{1/2}\Sigma_2^{1/2} \) and the Wasserstein distance reduces to the Hilbert–Schmidt distance of the covariance roots:

\[
W^2(N(0, \Sigma_1), N(0, \Sigma_2)) = \left\| \Sigma_1^{1/2} \right\|^2_2 + \left\| \Sigma_2^{1/2} \right\|^2_2 - 2\langle \Sigma_1^{1/2}, \Sigma_2^{1/2} \rangle_{\text{HS}}
\]

with the optimal map being \( \Sigma_2^{1/2}\Sigma_1^{-1/2} \) (if \( \ker(\Sigma_1) \subseteq \ker(\Sigma_2) \)).

We shall now take advantage of the wealth of knowledge about optimal transportation theory in order to gain further insight on the geometry and the topology of the space of covariance operators endowed with the Procrustes metric.

### 3 The Tangent Bundle

In this section we review some results from von Renesse and Sturm (2009) and from the book of Ambrosio et al. (2008), where it is shown how the Wasserstein distance \( W \) induces a manifold-like geometry on the Wasserstein space \( \mathcal{W}(\mathcal{H}) \). We then translate these results into geometrical properties of the space of covariance operators, equipped with the Procrusted distance (by identifying the latter with the subspace of \( \mathcal{W}(\mathcal{H}) \) that consists of centred Gaussian measures; see Takatsu (2011) for a detailed description of this...
subspace in the finite dimensional case). Let $\mu \in \mathcal{W}(\mathcal{H})$ and introduce the $L_2$-like space and norm of Borel functions $f : \mathcal{H} \to \mathcal{H}$ by

$$\|f\|_{L_2(\mu)} = \left( \int_{\mathcal{H}} \|f(x)\|^2 \, d\mu(x) \right)^{1/2}, \quad L_2(\mu) = \{f : \|f\|_{L_2(\mu)} < \infty\}.$$

Let $\mu, \nu \in \mathcal{W}(\mathcal{H})$ be such that the optimal map from $\mu$ to $\nu$, $t_{\mu}^{\nu}$, exists. Recalling that $\mathcal{I} : \mathcal{H} \to \mathcal{H}$ is the identity map, we can define a curve

$$\mu_t = [\mathcal{I} + t(t_{\mu}^{\nu} - \mathcal{I})] \# \mu, \quad t \in [0, 1].$$

This curve, known as McCann’s interpolation (McCann, 1997, Equation (7)), is a constant speed geodesic in that $\mu_0 = \mu$, $\mu_1 = \nu$ and

$$W(\mu_t, \mu_s) = (t - s)W(\mu, \nu), \quad 0 \leq s \leq t \leq 1.$$

Considering $\mu$ as a fixed reference measure, any other measure $\nu$ can be identified with the optimal map $t_{\mu}^{\nu}$, provided that this map exists and is unique. By subtracting the identity $\mathcal{I}$, this creates a correspondence between a subset of the Wasserstein space with a subset of the linear space $L_2(\mu)$ in such a way that $\mu$ itself corresponds to $0 \in L_2(\mu)$. This motivates the following definition. The tangent space of $\mathcal{W}(\mathcal{H})$ at $\mu$ is (Ambrosio et al., 2008, Definition 8.5.1)

$$\text{Tan}_\mu = \{t(t - \mathcal{I}) : t \in L_2(\mu); t \text{ optimal between } \mu \text{ and } t \# \mu; t > 0 \}^{L_2(\mu)}.$$

As a subset of $L_2(\mu)$, the tangent space inherits the inner product

$$\langle s, r \rangle_\mu = \int_{\mathcal{H}} \langle s(x), r(x) \rangle \, d\mu(x), \quad s, r \in L_2(\mu).$$

Since optimality of $t$ is independent of $\mu$, the only part of this definition that depends on $\mu$ is this inner product and the corresponding closure operation. Although not obvious from the definition, this is a linear space.\(^3\)

\(^3\)There is an equivalent definition in terms of gradients, in which linearity is clear, see Ambrosio et al. (2008, Definition 8.4.1): when $\mathcal{H} = \mathbb{R}^d$, it is $\text{Tan}_\mu = \{\nabla f : f \in C^\infty_c(\mathbb{R}^d)\}^{L_2(\mu)}$ (compactly supported $C^\infty$ functions). When $\mathcal{H}$ is a separable Hilbert space, one takes $C^\infty_c$ functions that depend on finitely many coordinates, called cylindrical functions (Ambrosio et al., 2008, Definition 5.1.11). The two definitions of the tangent space coincide by Ambrosio et al. (2008, Theorem 8.5.1).
The exponential map \( \exp_\mu : \text{Tan}_\mu \to \mathcal{W} (\mathcal{H}) \) at \( \mu \) is the restriction of the transformation that sends \( r \in \mathcal{L}_2 (\mu) \) to \( (r + \mathcal{I}) \# \mu \in \mathcal{W} (\mathcal{H}) \). Specifically,

\[
\exp_\mu (t(t - \mathcal{I})) = [t(t - \mathcal{I}) + \mathcal{I}] \# \mu = [tt + (1 - t) \mathcal{I}] \# \mu \quad (t \in \mathbb{R}).
\]

Notice that \( \text{Tan}_\mu \) is a strict subset of \( \mathcal{L}_2 (\mu) \). For example, a bounded linear operator \( A \) is always an element of \( \mathcal{L}_2 (\mu) \), but it belongs to the tangent space if and only if \( A \) is self-adjoint.

When \( \mu \) is regular, the log map \( \log_\mu : \mathcal{W} (\mathcal{H}) \to \text{Tan}_\mu \), is well-defined throughout \( \mathcal{W} (\mathcal{H}) \), and given by

\[
\log_\mu (\nu) = t_\mu - \mathcal{I}.
\]

It is the right inverse of the exponential map (which is therefore surjective):

\[
\exp_\mu (\log_\mu (\nu)) = \nu, \quad \nu \in \mathcal{W}, \quad \text{and} \quad \log_\mu (\exp_\mu (t(t - \mathcal{I}))) = t(t - \mathcal{I}) \quad (t \in [0, 1]),
\]

because convex combinations of optimal maps are optimal maps as well (see Section 2.2), and so McCann’s interpolant \( [\mathcal{I} + t(t_\mu - \mathcal{I})] \# \mu \) is mapped bijectively to the line segment \( t(t_\mu - \mathcal{I}) \in \text{Tan}_\mu \) through the log map.

The tangent space as well as the exponential and log maps can be thought of as the Riemannian ones; indeed, the optimal maps arise as minimal tangent vectors to absolutely continuous curves in Wasserstein space. We refer to Ambrosio et al. (2008, Sections 8.4–8.5) for a detailed treatment.

Let us now translate this geometric discussion to the space of covariance operators equipped with the Procrustes metric \( \Pi \) (by implicitly focussing on centred Gaussian measures in \( \mathcal{W} (\mathcal{H}) \)). In this case, writing \( \text{Tan}_\Sigma \) for \( \text{Tan}_{N(0, \Sigma)} \), a unique optimal map \( t \) is a non-negative (Lemma 19), possibly unbounded operator such that \( t \Sigma t \) is trace-class. In other words, \( \Sigma^{1/2} t \) is Hilbert–Schmidt, which is equivalent to \( \Sigma^{1/2} (t - \mathcal{I}) \) being Hilbert–Schmidt. We consequently obtain the description of the tangent space at \( \Sigma \) as

\[
\text{Tan}_\Sigma = \left\{ t(S - \mathcal{I}) : t > 0, S \succeq 0, \| \Sigma^{1/2} (S - \mathcal{I}) \|_2 < \infty \right\}
\]

\[
= \left\{ Q : Q = Q^*, \| \Sigma^{1/2} Q \|_2 < \infty \right\},
\]

where the closure is with respect to the inner product on \( \text{Tan}_\Sigma \), defined as

\[
\langle A, B \rangle_{\text{Tan}_\Sigma} = \int_{\mathcal{H}} \langle Ax, Bx \rangle \, d\mu (x) = \text{tr} (A \Sigma B) = \mathbb{E} [\langle AX, BX \rangle],
\]

where \( X \sim \mu \equiv N (0, \Sigma) \).

For the second equality in the definition of \( \text{Tan}_\Sigma \), notice that if \( Q \) is a bounded self adjoint operator, then \( S = \mathcal{I} + Q/t \) is non-negative when
$t > \| Q \|_\infty$; unbounded $Q$’s can then be approximated. The norm of a self-adjoint operator $Q \in \text{Tan}_\Sigma$ vanishes if and only if $Q \Sigma Q = 0$, which is equivalent to $Q \Sigma = 0$. Quotienting out the equivalence relation $Q \sim Q'$ makes $\text{Tan}_\Sigma$ a Hilbert space (this quotient is the one obtained from the usual identification of functions that equal $N(0, \Sigma)$-almost surely). Note that $\text{Tan}_\Sigma$ certainly contains all (equivalence classes of) bounded self-adjoint operators on $\mathcal{H}$, but also certain unbounded ones. For example, if $\Sigma^{1/3}$ is trace-class, then the tangent space inner product is well defined when taking $A = B = \Sigma^{-1/3}$, even though the latter is an unbounded operator.

The exponential map on $\text{Tan}_\Sigma$ is $\exp_\Sigma(A) = (A + \mathcal{I}) \Sigma (A + \mathcal{I})$. Furthermore, the condition $\ker(\Sigma_0) \subseteq \ker(\Sigma_1)$ (equivalently, $\text{range}(\Sigma_0) \supseteq \text{range}(\Sigma_1)$) is sufficient for the existence of

1. the log map of $\Sigma_1$ at $\Sigma_0$, given by
   \[
   \log_{\Sigma_0} \Sigma_1 = t_0^1 - \mathcal{I} = \Sigma_0^{-1/2} (\Sigma_0^{1/2} \Sigma_1 \Sigma_0^{1/2})^{1/2} \Sigma_0^{-1/2} - \mathcal{I},
   \]
   and defined $N(0, \Sigma)$-almost surely;

2. a unique (unit speed) geodesic from $\Sigma_0$ to $\Sigma_1$ given by
   \[
   \Sigma_t = [(tt_0^1 + (1 - t) \mathcal{I}) \Sigma_0 [tt_0^1 + (1 - t) \mathcal{I}]] = t^2 \Sigma_1
   \]
   \[
   + (1 - t)^2 \Sigma_0 + t(1 - t) [t_0^1 \Sigma_0 + \Sigma_0 t_0^1],
   \]
   where again $t_0^1 = \Sigma_0^{-1/2} (\Sigma_0^{1/2} \Sigma_1 \Sigma_0^{1/2})^{1/2} \Sigma_0^{-1/2}$.

Both points follow from the manifold properties of Wasserstein space discussed earlier in this subsection, by taking $\mu \equiv N(0, \Sigma_0)$ and $\nu \equiv N(0, \Sigma_1)$ and using Proposition 2.

## 4 Topological Properties

The topological properties of the Wasserstein distance between Gaussian measures are well understood, as they related to the topic of weak convergence of Gaussian processes. This knowledge can thus be used in order to characterise the topology induced by the Procrustes distance, and we collect equivalent such characterisations emanating from this knowledge in the next Proposition. Recall that a sequence of measures $\mu_n$ converges to $\mu$ in distribution (or narrowly)$^4$ if $\int f \, d\mu_n \to \int f \, d\mu$ for all continuous bounded $f : \mathcal{H} \to \mathbb{R}$.

$^4$This is often called weak convergence, but we will avoid this terminology in order to avoid confusion: weak convergence of covariance operators is not equivalent to convergence in distribution of the corresponding measures.
Proposition 4 (Procrustes Topology). Let \( \{\Sigma_n\}_{n=1}^{\infty}, \Sigma \) be covariance operators on \( \mathcal{H} \). The following are equivalent:

1. \( N(0, \Sigma_n) \xrightarrow{n \to \infty} N(0, \Sigma) \) in distribution.

2. \( \Pi(\Sigma_n, \Sigma) \xrightarrow{n \to \infty} 0 \).

3. \( \sqrt{\Sigma_n} - \sqrt{\Sigma} \to 0 \).

4. \( \|\Sigma_n - \Sigma\| \xrightarrow{n \to \infty} 0 \).

In particular, a set of covariance operators is pre-compact with respect to \( \Pi \) if and only if the set of corresponding centred Gaussian measures with those covariances is uniformly tight. We also remark that convergence in operator norm is not sufficient for any of (1)-(4): to obtain a counterexample, take \( \Sigma = 0 \) and let \( \Sigma_n \) have \( n \) eigenvalues equal to \( 1/n \) and all the others zero.

**Proof.** Write \( \mu_n \equiv N(0, \Sigma_n) \) and \( \mu \equiv N(0, \Sigma) \) for tidiness and recall that \( \Pi(\Sigma_n, \Sigma) = W(\mu_n, \mu) \). For the implications \( 4 \Rightarrow 1 \Leftrightarrow 3 \) see Examples 3.8.15 and 3.8.13(iii) in Bogachev (1998). By Bogachev (1998, Theorem 3.8.11), if (1) holds, then the measures \( (\mu_n) \) have uniform exponential moments, and by Theorem 7.12 in (Villani, 2003) (1) and (2) are equivalent (see Corollary 23 for a more elementary proof that does not involve Fernique’s theorem). To conclude it suffices to show that (2) yields (4). Let \( X \sim \mu \), \( X_n \sim \mu_n \) (defined on the same probability space) such that \( W^2(\mu_n, \mu) = \mathbb{E}\|X_n - X\|^2 \to 0 \). Notice that \( \Sigma_n = \mathbb{E}X_n \otimes X_n \). Invoking Jensen’s inequality to

\[
\Sigma_n - \Sigma = \mathbb{E}X_n \otimes (X_n - X) + (X_n - X) \otimes X
\]

yields (recall that \( \|f \otimes g\|_1 = \|f\|\|g\| \); see Lemma 20 below)

\[
\|\Sigma_n - \Sigma\|_1 \leq \mathbb{E}\|X_n \otimes (X_n - X)\|_1 + \mathbb{E}\|(X_n - X) \otimes X\|_1 \\
= \mathbb{E}\|X_n\|\|X_n - X\| + \|X_n - X\|\|X\|.
\]

When \( n \) is sufficiently large \( \mathbb{E}\|X_n\|^2 \leq 1 + \mathbb{E}\|X\|^2 \) and then the right-hand side is

\[
\leq \sqrt{\mathbb{E}\|X_n - X\|^2} \left( \sqrt{1 + \mathbb{E}\|X\|^2} + \sqrt{\mathbb{E}\|X\|^2} \right) = C(\Sigma)W(\mu_n, \mu),
\]

where \( C(\Sigma) = \sqrt{1 + \text{tr} \Sigma} + \sqrt{\text{tr} \Sigma} \), and this vanishes as \( n \to \infty \).

More is known about the topology of Wasserstein space; for instance, the exponential and log maps given in Section 3 are continuous, so \( W(\mathcal{H}) \)
is homeomorphic to an infinite-dimensional convex subset of a Hilbert space \( \mathcal{L}_2(\mu) \) (for any regular measure \( \mu \)); see the dissertation Zemel (2017, Lemmas 3.4.4 and 3.4.5) or the forthcoming monograph Panaretos and Zemel (2018).

5 Finite Rank Approximations

Pigoli et al. (2014) considered the validity of approximating the Procrustes distance \( \Pi \) between two infinite-dimensional operators by the distance between finite-dimensional projections thereof (in the sense of convergence of the latter to the former). Though this validity can be obtained from Proposition 4, use of the Wasserstein interpretation of \( \Pi \) provides a straightforward calculation of the projection error and an elementary proof of convergence under projections forming an approximate identity in \( \mathcal{H} \) (whether the projections are finite dimensional or not). If the projections are indeed finite dimensional, one can furthermore establish a stronger form of validity: uniform convergence over compacta.

Let \( \mu \in \mathcal{W}(\mathcal{H}) \) with covariance \( \Sigma \) and \( \mathcal{P} \) be a projection operator (\( \mathcal{P}^* = \mathcal{P} = \mathcal{P}^2 \)). Then by Lemma 19 in Section 13, \( \mathcal{P} \) is an optimal map from \( \mu \) to \( \mathcal{P}\#\mu \) and so

\[
W^2(\mu, \mathcal{P}\#\mu) = \int_{\mathcal{H}} \|x - \mathcal{P}x\|^2 \, d\mu(x) = \text{tr} \left\{ (\mathcal{I} - \mathcal{P})\Sigma(\mathcal{I} - \mathcal{P}) \right\}
\]

\[
= \text{tr} \left\{ (\mathcal{I} - \mathcal{P})\Sigma \right\}.
\]

This is true regardless of \( \mu \) being Gaussian, but taking \( \mu \) to be \( \mathcal{N}(0, \Sigma) \), in particular, yields the explicit error

\[
\Pi^2(\Sigma, \mathcal{P}\Sigma \mathcal{P}) = \text{tr} \left\{ (\mathcal{I} - \mathcal{P})\Sigma \right\},
\]

where \( \mathcal{P}\Sigma \mathcal{P} \) is the projection of \( \Sigma \) onto the range of \( \mathcal{P} \). This indeed converges to zero when \( \mathcal{P}_n \) is an approximate identity, in the sense of \( \mathcal{P}_n \) converging strongly to the identity: a sequence of operators \( T_n \) converges to \( T \) strongly if \( T_n x \to Tx \) for all \( x \in \mathcal{H} \) (Stein and Shakarchi, 2009, p. 198).\(^5\)

**Lemma 5.** Let \( \mathcal{P}_n \) be a sequence of projections that converges strongly to the identity. Then \( \mathcal{P}_n\#\mu \to \mu \) in \( \mathcal{W}(\mathcal{H}) \) for any \( \mu \in \mathcal{W}(\mathcal{H}) \), and consequently \( \Pi(\Sigma, \mathcal{P}_n\Sigma \mathcal{P}_n) \to 0. \)

The setting considered in Pigoli et al. (2014) is indeed a special case of Lemma 5: let \( \{e_j\}_{j \geq 1} \) be an orthonormal basis of \( \mathcal{H} \) and define \( \mathcal{P}_n =\)

---

\(^5\)This is much weaker than convergence in operator norm, but stronger than requiring that \( \langle T_n x, y \rangle \to \langle Tx, y \rangle \) for all \( x, y \in \mathcal{H} \), which is called weak convergence of \( T_n \) to \( T \).
\[ \sum_{j=1}^{n} e_j \otimes e_j \] as the projection onto the span of \( \{e_1, \ldots, e_n\} \). Then \( P_n \) converges strongly to the identity as \( n \to \infty \).

**Proof of Lemma 5.** Since \( P_n x \to x \) for all \( x \) and \( \|P_n x\| \leq \|x\| \), the result that \( P_n \# \mu \to \mu \) in \( \mathcal{W}(\mathcal{H}) \) follows from the dominated convergence theorem. Taking \( \mu \equiv N(0, \Sigma) \) then completes the proof.

When focussing on finite dimensional projections, a stronger statement is possible, if one considers compact sets:

**Proposition 6.** Let \( \{e_j\}_{j \geq 1} \) be an orthonormal basis of \( \mathcal{H} \) and \( P_n = \sum_{j=1}^{n} e_j \otimes e_j \) be the projection on the span of \( \{e_1, \ldots, e_n\} \). Let \( B \) be a collection of non-negative bounded operators satisfying

\[
\sup_{\Sigma \in B} \sum_{j=n+1}^{\infty} \langle \Sigma e_j, e_j \rangle \to 0, \quad \text{as } n \to \infty. \tag{5.1}
\]

Then,

\[
\sup_{\Sigma_1, \Sigma_2 \in B} |\Pi(P_n \Sigma_1 P_n, \Sigma_2 P_n) - \Pi(\Sigma_1, \Sigma_2)| \to 0, \quad n \to \infty.
\]

**Proof.** Let \( \mathcal{K} \subset \mathcal{W}(\mathcal{H}) \) be a collection of measures with \( \Sigma(\mu) \in B \) for all \( \mu \in \mathcal{K} \). It suffices to show that \( W(\mu, \mathcal{P}_n \# \mu) \to 0 \) uniformly and indeed

\[
W^2(\mu, \mathcal{P}_n \# \mu) = \text{tr}(I - \mathcal{P}_n) \Sigma(\mu) = \sum_{j=n+1}^{\infty} \langle \Sigma(\mu) e_j, e_j \rangle
\]

vanishes uniformly as \( n \to \infty \).

The collection \( B \) of covariances of a tight set of centred Gaussian measures satisfies the tail condition (5.1) with respect to any orthonormal basis \( \{e_k\}_{k \geq 1} \) of \( \mathcal{H} \) (Bogachev, 1998, Example 3.8.13(iv)). As per Proposition 4, the tightness condition admits three alternative equivalent formulations in purely operator theory terms. The first is that \( B \) be compact with respect to the distance \( \Pi \). The second is that \( B \) be of the form \( B = \{A^2 : A \in \mathcal{A}\} \) for \( \mathcal{A} \) a compact set of non-negative Hilbert–Schmidt operators. The third is that \( B \) be compact with respect to the trace norm.

In concluding this section, we remark that Rippl et al. (2016) consider stability of the Wasserstein distance under a different setup, where the approximation is in terms of sampling from the corresponding Gaussian measures.

### 6 Existence and Uniqueness of Fréchet Means

The most basic statistical task in a general metric space is that of obtaining a notion of average. If \( \Sigma_1, \ldots, \Sigma_N \) are covariance operators, their
mean can be modelled as a Fréchet mean (Fréchet (1948)) with respect to the Procrustes metric (equivalently, a Wasserstein barycentre of corresponding centred Gaussian measures), defined as the minimiser of the Fréchet functional

\[ F(\Sigma) = \frac{1}{2N} \sum_{i=1}^{N} \Pi^2(\Sigma, \Sigma_i) = \frac{1}{2N} \sum_{i=1}^{N} W^2(N(0, \Sigma), N(0, \Sigma_i)). \]

One can also consider the Fréchet mean of a random covariance operator \( \mathcal{A} \) as the minimiser of \( \Sigma \mapsto F(\Sigma) = \frac{1}{2} \mathbb{E} \Pi^2(\Sigma, \mathcal{A}) \); the empirical case can be recovered from this when \( \mathcal{A} \) has the uniform distribution on the finite set \( \{ \Sigma_1, \ldots, \Sigma_N \} \). See Section 10 for a more thorough discussion of the population case. The Fréchet mean of arbitrary measures in \( \mathcal{W}(\mathcal{H}) \) can be defined in the same way. Unlike the linear mean, existence and uniqueness of Fréchet means in general metric spaces is a rather delicate matter (see, e.g., Bhattacharya and Patrangenaru (2003, 2005) and Karcher (1977)). In the particular case of the Wasserstein space, however, existence and uniqueness can be established under rather mild assumptions. For the finite-dimensional case, such conditions were studied by Agueh and Carlier (2011). Moreover, they show that the Fréchet mean of Gaussian measures is a Gaussian measure, and so there is no ambiguity as to whether we minimise the sum of squared Wasserstein distances over Gaussian measures or arbitrary measures in \( \mathcal{W}(\mathcal{H}) \). This result can be extended to infinite dimensions by approximation using the stability result presented in Section 7 (see Theorem 11 and discussion thereafter, and Theorem 12 for an example of such extension).

Pigoli et al. (2014) also considered the Fréchet mean with respect to \( \Pi \), but working with their formulation \( \Pi(\Sigma_1, \Sigma_2) = \inf_{U: U^*U = \mathcal{A}} \| \Sigma_1^{1/2} - \Sigma_2^{1/2} U \|_2 \) made it difficult to deal with existence and uniqueness. We now show how this can be done easily using the Wasserstein interpretation. We begin with existence, which holds for a general collection of measures. The proof relies upon the notion of multicouplings.

**Definition 7 (Multicoupling).** Let \( \mu_1, \ldots, \mu_N \in \mathcal{W}(\mathcal{H}). \) A multicoupling of \( (\mu_1, \ldots, \mu_N) \) is a Borel measure on \( \mathcal{H}^N \) with marginals \( \mu_1, \ldots, \mu_N. \)

An optimal multicoupling of \( \mu_1, \ldots, \mu_N \) is a multicoupling \( \pi \) that minimises

\[
G(\pi) = \frac{1}{2N^2} \int_{\mathcal{H}^N} \sum_{i<j} \| x_i - x_j \|^2 \, d\pi(x_1, \ldots, x_N)
\]

\[
= \int_{\mathcal{H}^N} \frac{1}{2N} \sum_{i=1}^{N} \| x_i - \overline{x} \|^2 \, d\pi(x).
\]
We shall discuss the probabilistic interpretation of multicouplings in more detail in Section 9; at this stage we merely use them as a tool for deriving analytical properties of Fréchet means. When $N = 2$, multicouplings are simply couplings and finding an optimal multicoupling is the optimal transport problem. On $\mathbb{R}^d$, multicouplings were studied by Gangbo and Święch (1998) (also see Zemel and Panaretos (2017)). In analogy with the optimal transport problem, an optimal multicoupling always exists, and if $\mu_1$ is regular an optimal multicoupling takes the form $(\mathcal{I}, S_2, \ldots, S_N) \# \mu_1$ for some functions $S_i : \mathbb{R}^d \to \mathbb{R}^d$, where

$$(\mathcal{I}, S_2, \ldots, S_N) \# \mu_1(B_1 \times \ldots \times B_N) = \mu_1(\{x \in B_1 : S_2(x) \in B_2, \ldots, S_N(x) \in B_N\})$$

$$= \mu_1 \left( \bigcap_{i=1}^{N} S_i^{-1}(B_i) \right)$$

for any Borel-rectangle $B_1 \times \ldots \times B_N$, and $S_1 = \mathcal{I}$. Agueh and Carlier (2011, Proposition 4.2) show that an optimal coupling yields a Fréchet mean by “averaging”. Although stated in $\mathbb{R}^d$, their argument remains valid in infinite-dimensions, and can also yield necessity, and we reproduce it here in infinite dimensions:

**Lemma 8 (Fréchet means and multicouplings).** Let $\mu^1, \ldots, \mu^N \in \mathcal{W}$. Then $\mu$ is a Fréchet mean of $(\mu^1, \ldots, \mu^N)$ if and only if there exists an optimal multicoupling $\pi \in \mathcal{W}(\mathcal{H}^N)$ of $(\mu^1, \ldots, \mu^N)$ such that

$$\mu = M_N \# \pi, \quad M_N : \mathcal{H}^N \to \mathcal{H}, \quad M_N(x_1, \ldots, x_N) = \bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i.$$

**Proof.** Let $\pi$ be an arbitrary multicoupling of $(\mu^1, \ldots, \mu^N)$ and set $\mu = M_N \# \pi$. Then $(x \mapsto x_i, M_N) \# \pi$ is a coupling of $\mu^i$ and $\mu$, and therefore

$$\int_{\mathcal{H}^N} \|x_i - M_N(x)\|^2 \, d\pi(x) \geq W^2(\mu, \mu_i).$$

Summation over $i$ gives $F(\mu) \leq G(\pi)$ and so $\inf F \leq \inf G$.

For the other inequality, let $\mu \in \mathcal{W}$ be arbitrary. For each $i$ let $\pi^i$ be an optimal coupling between $\mu$ and $\mu^i$. Invoking the gluing lemma (Ambrosio and Gigli, 2013, Lemma 2.1), we may glue all $\pi^i$’s using their common marginal $\mu$. This procedure constructs a measure $\eta$ on $\mathcal{H}^{N+1}$ with marginals $\mu_1, \ldots, \mu_N, \mu$ and its relevant projection $\pi$ is then a multicoupling of $\mu_1, \ldots, \mu_N$. 

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**Procrustes metrics on covariance operators...**
Since $\mathcal{H}$ is a Hilbert space, the minimiser of $y \mapsto \sum \|x_i - y\|^2$ is $y = M_N(x)$. Thus

$$F(\mu) = \frac{1}{2N} \int_{\mathcal{H}^{N+1}} \sum_{i=1}^N \|x_i - y\|^2 \, d\eta(x,y) \\
\geq \frac{1}{2N} \int_{\mathcal{H}^{N+1}} \sum_{i=1}^N \|x_i - M_N(x)\|^2 \, d\eta(x,y) = G(\pi).$$

In particular, $\inf F \geq \inf G$ and combining this with the established converse inequality we see that $\inf F = \inf G$. Observe also that the last displayed inequality holds as equality if and only if $y = M_N(x)$ $\eta$-almost surely, in which case $\mu = M_N \# \pi$. Therefore if $\mu$ does not equal $M_N \# \pi$, then $F(\mu) > G(\pi) \geq F(M_N \# \pi)$, and $\mu$ cannot be optimal. Finally, if $\pi$ is optimal, then

$$F(M_N \# \pi) \leq G(\pi) = \inf G = \inf F$$

establishing optimality of $\mu = M_N \# \pi$ and completing the proof.

**Corollary 9 (Fréchet means and moments).** Any finite collection of measures $\mu^1, \ldots, \mu^N \in \mathcal{W}(\mathcal{H})$ admits a Fréchet mean $\mu$, for all $p \geq 1$

$$\int_{\mathcal{H}} \|x\|^p \, d\mu(x) \leq \frac{1}{N} \sum_{i=1}^N \int_{\mathcal{H}} \|x\|^p \, d\mu_i(x),$$

and when $p > 1$ equality holds if and only if $\mu^1 = \cdots = \mu^N$. In particular, any collection $\Sigma^1, \ldots, \Sigma^N$ of covariance operators admits a Fréchet mean $\Sigma$ with respect to the Procrustes distance $\Pi$, and $\text{tr} \Sigma \leq N^{-1} \sum_{i=1}^N \text{tr} \Sigma^i$.

**Proof.** Let $\pi$ be a multicoupling of $\mu^1, \ldots, \mu^N$ such that $\mu = M_N \# \pi$ (Lemma 8). Then

$$\int_{\mathcal{H}} \|x\|^p \, d\mu(x) = \int_{\mathcal{H}^N} \left( \frac{1}{N} \sum_{i=1}^N x_i \right)^p \, d\pi(x) \leq \frac{1}{N} \sum_{i=1}^N \int_{\mathcal{H}^N} \|x_i\|^p \, d\pi(x) \\\n= \frac{1}{N} \sum_{i=1}^N \int_{\mathcal{H}} \|x\|^p \, d\mu_i(x).$$

The statement about equality follows from strict convexity of $x \mapsto \|x\|^p$ if $p > 1$.

We next turn to uniqueness of Fréchet means. The proof follows from strict convexity of the Fréchet functional $F$ that manifests as soon as enough
non-degeneracy is present. We remark first that if \( \mu \) is a Gaussian measure with covariance \( \Sigma \), then \( \mu \) is regular if and only if \( \Sigma \) is injective, and when this holds, for any \( \nu \in \mathcal{W}(\mathcal{H}) \) (Gaussian or not) the optimal map \( t^\nu \) exists.

**Proposition 10.** Let \( \mu_1, \ldots, \mu_N \in \mathcal{W}(\mathcal{H}) \) and assume that \( \mu_1 \) is regular. Then the Fréchet functional is strictly convex,\(^6\) and the Fréchet mean of \( \mu_1, \ldots, \mu_N \) is unique. In particular, the Fréchet mean of a collection of covariance operators is unique if at least one of the operators is injective.

Uniqueness in fact holds at the population level as well: the condition is that the random covariance operator be injective with positive probability. On \( \mathbb{R}^d \) this was observed by Bigot and Klein (2012) in a parametric setting, and extended to the nonparametric setting by Zemel and Panaretos (2017); the analytical idea dates back to Álvarez-Esteban et al. (2011).

**Proof.** We first establish weak convexity of the squared Wasserstein distance. Let \( \nu_1, \nu_2, \mu \in \mathcal{W}(\mathcal{H}) \) and let \( \pi_i \) be an optimal coupling of \( \nu_i \) and \( \mu \). For any \( t \in (0, 1) \) the linear interpolant \( t\pi_1 + (1-t)\pi_2 \) is a coupling of \( t\nu_1 + (1-t)\nu_2 \) and \( \mu \). This yields the weak convexity

\[
W^2(t\nu_1 + (1-t)\nu_2, \mu) \leq \int_{\mathcal{H}^2} \|x - y\|^2 \, d[t\pi_1 + (1-t)\pi_2](x, y) = tW^2(\nu_1, \mu) + (1-t)W^2(\nu_2, \mu). \tag{6.1}
\]

Now if \( \mu \) is regular, then both couplings \( \pi_i \) are induced by maps \( T_i = t^\nu_i \). If \( \nu_1 \neq \nu_2 \), then \( t\pi_1 + (1-t)\pi_2 \) is not induced from a map, and consequently cannot be the optimal coupling of \( t\nu_1 + (1-t)\nu_2 \) and \( \mu \), as explained in Álvarez-Esteban et al. (2011, Theorem 2.9).\(^7\) Thus the inequality above is strict and \( W^2(\cdot, \mu) \) is strictly convex. The proposition now follows upon noticing that the Fréchet functional is a sum of \( N \) squared Wasserstein distances that are all convex, one of them strictly.

For statistical purposes existence and uniqueness are not sufficient, and one needs to find a constructive way to evaluate the Fréchet mean of a given collection of covariance operators. Pigoli et al. (2014) propose using the classical generalised Procrustes algorithm. The Wasserstein formalism gives rise to another algorithm that can be interpreted as steepest descent in

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\(^6\)Here convexity is to be understood with respect to set-wise addition: if \( \mu \) and \( \nu \) are probability measures, then so is \( t\mu + (1-t)\nu \) for all \( t \in [0, 1] \), where the latter is defined by assigning to a Borel set \( A \) a measure of \( t\mu(A) + (1-t)\nu(A) \). It is with respect to this geometry, rather than the Wasserstein one, that the Fréchet functional is convex.

\(^7\)Álvarez-Esteban et al. (2011) do this in finite dimensions, but their proof works in infinite dimensions. Note that there is no need to work with densities, since in our particular setup \( P_1 = P_2 \) (in the notation of Álvarez-Esteban et al., 2011).
Wasserstein space, while still admitting a Procrustean interpretation (solving successive pairwise transport rather than alignment problems). We will elaborate on these algorithms in Section 8. In practice, implementing these algorithms will require finite-dimensional versions of the operators. This raises the question of stability of the Fréchet mean under projections, which is the topic of the next section.

7 Stability of Fréchet Means

When analysing functional data, one seldom has access to the genuinely infinite-dimensional objects (see, e.g., Hsing and Eubank, 2015; Yao et al., 2005a, b; Descary and Panaretos, 2016). In practice, the observed curves are discretised at some level and the data at hand represent finite-dimensional approximations, potentially featuring some additional level of smoothing. It is therefore important to establish some amount of continuity of any inferential procedure with respect to progressively finer such approximations. In the present context, it is important to verify that the Fréchet mean remains stable as the discretisation becomes finer and finer, and as smoothing parameters decay. Stability of the Procrustes distance itself (as, e.g., in Section 5), does not immediately yield stability of the Fréchet means – the latter amounts to argmin theorems (van der Vaart and Wellner, 1996), whose validity requires further assumptions. Our understanding of the topology of the Wasserstein space, however, allows to deduce this stability of the Fréchet means. We note that the question of convergence of Fréchet–Wasserstein means on locally compact spaces was studied by Le Gouic and Loubes (2017), but their results cannot be applied in our setup, since \( \mathcal{H} \) is not locally compact.

**Theorem 11 (Fréchet means and projections).** Let \( \Sigma^1, \ldots, \Sigma^N \) be covariance operators with \( \Sigma^1 \) injective, and let \( \{\Sigma^i_k : i \leq N, k \geq 1\} \) be sequences such that \( \Sigma^i_k \xrightarrow{k \to \infty} \Sigma^i \) in trace norm (equivalently, in Procrustes distance). Then (any choice of) the Fréchet mean of \( \Sigma^1, \ldots, \Sigma^N \) converges in trace norm to that of \( \Sigma^1, \ldots, \Sigma^N \).

Of course, the result can be phrased in terms of Gaussian measures \( \{N(0, \Sigma^i) : i \leq N\} \) and sequences \( \{N(0, \Sigma^i_k) : i \leq N, k \geq 1\} \), and their Wasserstein barycentres. But, in fact, the result holds far more generally in the space \( \mathcal{W}(\mathcal{H}) \). Let \( \mu^i_k \to \mu^i \) in Wasserstein distance. If for some \( \epsilon > 0 \) and all \( i = 1, \ldots, N \)

\[
\sup_k \int_{\mathcal{H}} \|x\|^{2+\epsilon} \, d\mu^i_k(x) < \infty
\]

then the statement of the theorem holds. The proof follows from modifying the exponent in the definition of \( R^i \) in step 2 to \( 2 + \epsilon \) and noticing that
the resulting moment bound for $\bar{\mu}_k$ supplemented by their tightness yields convergence in Wasserstein distance; see the discussion following Zemel and Panaretos (2017, Equation (5.3)) (and replace 3 by $2 + \epsilon$).

**Proof of Theorem 11.** Denote the corresponding Gaussian measures $\{N(0, \Sigma_i^i) : i \leq N\}$ and sequences $\{N(0, \Sigma_k^i) : i \leq N, k \geq 1\}$ by $\{\mu_i^i : i \leq N\}$ and $\{\mu_k^i : i \leq N, k \geq 1\}$ and let $\bar{\mu}_k$ denote any Fréchet mean of $\mu_1^k, \ldots, \mu_N^k$. Denote the corresponding Fréchet functionals by $F_k$ and $F$.

**Step 1:** tightness of $(\bar{\mu}_k)$. The entire collection $K = \{\mu_k^i\}$ is tight, since all the sequences converge in distribution (Proposition 4). For any $\epsilon > 0$ there exists a compact $K_\epsilon \subset \mathcal{H}$ such that $\mu(K_\epsilon) \geq 1 - \epsilon/N$ for all $\mu \in K$. Replacing $K_\epsilon$ by its closed convex hull (Lemma 21), we may assume it to be convex as well.

Let $\pi_k$ be any multicoupling of $(\mu_1^k, \ldots, \mu_N^k)$. Then the marginal constraints of $\pi_k$ imply that $\pi_k(K_\epsilon^N) \geq 1 - \epsilon$. By Lemma 8, $\bar{\mu}_k$ must take the form $M_N^{-1}\pi_k$ for some multicoupling $\pi_k$. Convexity of $K_\epsilon$ implies that $M_N^{-1}(K_\epsilon) \supseteq K_\epsilon^N$, and so

$$\bar{\mu}_k(K_\epsilon) = \pi_k(M_N^{-1}(K_\epsilon)) \geq \pi_k(K_\epsilon^N) \geq 1 - \epsilon.$$ 

With tightness of $(\bar{\mu}_k)$ established, we may now assume that (up to subsequences) $\bar{\mu}_k$ converge in distribution to a limit $\bar{\mu}$. Since $\bar{\mu}_k$ are Gaussian, they also converge in Wasserstein distance by Proposition 4.

**Step 2:** a moment bound for $\bar{\mu}_k$. Let $\bar{R}^i = \int_{\mathcal{H}}\|x\|^2\,d\mu^i(x)$ denote the second moment of $\mu^i$. Since the second moments can be interpreted as a (squared) Wasserstein distance to the Dirac mass at 0 (or by Theorem 7.12 in Villani, 2003), the second moment of $\mu_k^i$ converges to $\bar{R}^i$ and so for $k$ large it is smaller than $\bar{R}^i + 1$. By Corollary 9, for $k$ large

$$\int_{\mathcal{H}}\|x\|^2\,d\bar{\mu}_k(x) \leq \frac{1}{N} \sum_{i=1}^N \bar{R}^i + 1 \leq \max(\bar{R}^1, \ldots, \bar{R}^N) + 1 := R + 1.$$

**Step 3:** the limit $\bar{\mu}$ is a Fréchet mean of $(\mu^i)$. By the moment bound above, the Fréchet means $\bar{\mu}_k$ can be found (for $k$ large) in the Wasserstein ball

$$B = \{\mu \in \mathcal{W} : W^2(\mu, \delta_0) \leq R + 1\},$$

with $\delta_0$ a Dirac measure at the origin. If $\mu, \nu \in B$ then, since $\mu_k^i \in B$ for $k$ large,

$$|F_k(\mu) - F_k(\nu)| \leq \frac{1}{2N} \sum_{i=1}^N [W(\mu, \mu_k^i) + W(\nu, \mu_k^i)]W(\mu, \nu) \leq 2\sqrt{R + 1} W(\mu, \nu).$$
In other words, all the $F_k$’s are uniformly Lipschitz on $B$. Suppose now that $\mu_k \to \mu$ in $W_L$. Let $\mu \in B$, $\epsilon > 0$ and $k_0$ such that $W(\mu_k, \mu) < \epsilon/(2\sqrt{R} + 1)$ for all $k \geq k_0$. Since $F_k \to F$ pointwise we may assume that $|F(\mu) - F_k(\mu)| < \epsilon$ when $k \geq k_0$ and the same holds for $\mu = \overline{\mu}$. Then for all $k \geq k_0$

$$\epsilon + F(\mu) \geq F_k(\mu) \geq F_k(\mu_k) \geq F_k(\overline{\mu}) - \epsilon \geq F(\overline{\mu}) - 2\epsilon.$$ 

Since $\epsilon$ is arbitrary we see that $\overline{\mu}$ minimises $F$ over $B$ and hence over the entire Wasserstein space $W(\mathcal{H})$.

**Step 4:** conclusion. We have shown or assumed that

- the sequence $(\mu_k)$ is precompact in $W(\mathcal{H})$;
- each of its limits is a minimiser of $F$;
- there is only one minimiser of $F$.

The combination of these three facts implies that $\mu_k$ must converge to the minimiser of $F$.

With this stability established, we can easily lift finite-dimensional results to infinite dimensions. For example, we can deduce that Procrustes averaging produces less “swelling” than linear averaging:

**Theorem 12.** Let $\overline{\Sigma}$ be a unique Fréchet mean of $\Sigma_1, \ldots, \Sigma_n$. Then $(\Sigma_1 + \cdots + \Sigma_n)/n - \overline{\Sigma}$ is non-negative.

**Proof.** For positive operators in finite dimensions, see Bhatia et al. (2018, Theorem 9). If $\Sigma_i$ are merely non-negative (in finite dimensions), let $\overline{\Sigma}_\epsilon$ be the Fréchet mean of the positive operators $\Sigma_i + \epsilon \mathcal{I}$. Then $(\Sigma_1 + \cdots + \Sigma_n)/n + \epsilon \mathcal{I} - \overline{\Sigma}_\epsilon$ is non-negative for all $\epsilon > 0$. Now let $\epsilon \to 0$. This proves the result for finite dimensions.

Now let $\mathcal{P}_k$ be a sequence of finite-dimensional projections that converge strongly to the identity and let $\overline{\Sigma}_k$ be any Fréchet mean of $(\mathcal{P}_k \Sigma_i \mathcal{P}_k)_{i=1}^n$. Any multicoupling assigns probability one to $[\text{range}(\mathcal{P}_k)]^n$ and by Lemma 8 the range of $\overline{\Sigma}_k$ is included in the finite-dimensional space $\text{range}(\mathcal{P}_k)$. The sequence

$$(\mathcal{P}_k \Sigma_1 \mathcal{P}_k + \mathcal{P}_k \Sigma_n \mathcal{P}_k)/n - \overline{\Sigma}_k$$

is non-negative for all $k$. Letting $k \to \infty$ gives the result.

**8 Computation of Fréchet Means: Procrustes Algorithms and Steepest Descent**

Fréchet means rarely admit closed-form expressions, and the Procrustes space of covariances on $\mathcal{H}$ (equivalently, the Wasserstein space of Gaussian
measures on $\mathcal{H}$) is no exception (but see Section 11 for the issue of characterisation). In order to compute the Fréchet mean in practice, one needs to resort to numerical schemes at some level, and such schemes would need to be applied to finite-dimensional versions of the covariances, e.g. covariance operators on some finite dimensional subspace $\mathcal{H}' \subset \mathcal{H}$, resulting from the necessarily discrete nature of observation and/or smoothing.

Let $\Sigma_1, \ldots, \Sigma_N$ be covariance operators on the finite dimensional subspace $\mathcal{H}' \subset \mathcal{H}$, of which one seeks to find a Fréchet mean $\bar{\Sigma}$. Pigoli et al. (2014) suggested an iterative procedure, motivated by generalised Procrustes analysis (Gower, 1975; Dryden and Mardia, 1998), for finding $L = \bar{\Sigma}^{1/2}$, that we summarise as follows. The initial point $L^0$ is the average of $L_i^0 = L_i = \Sigma_i^{1/2}$. At step $k$, one computes, for each $i$, the unitary operator $R_i$ that minimises $\|L_i^{k-1} - L_i^{k-1} R_i\|_2$, and then sets $L_i^k = L_i^{k-1} R_i$. After this, one defines $L^k$ as the average of $\{L_1^k, \ldots, L_N^k\}$ and repeats until convergence. The advantage of this algorithm is that it only involves successively matching pairs of operators (minimising $\|L_i^{k-1} - L_i^{k-1} R_i\|_2$), for which there is an explicit solution in terms of the SVD of the product of the operators in question. Pigoli et al. report good empirical performance of this algorithm (and some of its variants) on discretised versions of the operators if the initial point is chosen as $N^{-1} \sum_{i=1}^N \Sigma_i^{1/2}$, and conjecture that an infinite-dimensional implementation of their algorithm would also exhibit favourable performance. It is not clear whether the algorithm converges, though, when the operators $\{\Sigma_1, \ldots, \Sigma_N\}$ do not commute.

The great advantage of the procedure of Pigoli et al. (2014) is precisely that it only involves successive averaging of solutions of pairwise matching problems until convergence. The Wasserstein formalism allows one to employ a different procedure that is still of Procrustean flavour, but where instead of averaging pairwise SVD matchings, one averages pairwise optimal transport maps:

- Let $\Sigma^0 : \mathcal{H}' \to \mathcal{H}'$ be an injective covariance, serving as the initial point.
- Denote the current iterate at step $k$ as $\Sigma^k$.
- For each $i$ compute the optimal maps from $\Sigma^k$ to each of the prescribed operators $\Sigma_i : \mathcal{H}' \to \mathcal{H}'$, namely
  \[ t_{\Sigma^k}^{\Sigma_i} = (\Sigma^k)^{-1/2} [(\Sigma^k)^{1/2} \Sigma_i (\Sigma^k)^{1/2}]^{1/2} (\Sigma^k)^{-1/2}. \]
- Define their average $T_k = N^{-1} \sum_{i=1}^N t_{\Sigma^k}^{\Sigma_i}$, which is itself a non-negative matrix on $\mathcal{H}'$.  

\[ \text{Procrustes metrics on covariance operators...} \]
• Set the next iterate to $\Sigma^{k+1} = T_k \Sigma^k T_k$ (guaranteed to be injective on $\mathcal{H}'$ if one $\Sigma_i$ is so).

This algorithm has been independently arrived at in this Procrustean form by Zemel and Panaretos (2017) and in the form of a fixed point equation iteration by Álvarez-Esteban et al. (2016). When applied to finite-dimensional\(^8\) covariances, it will provably converge (Álvarez-Esteban et al., 2016; Zemel and Panaretos, 2017) to the unique Fréchet mean $\bar{\Sigma}$ of $\Sigma_1, \ldots, \Sigma_N$ provided one of them is injective, and this independently of the initial point (provided the latter is chosen to be injective). Moreover, Álvarez-Esteban et al. (2016) show $\text{tr} \Sigma^k$ to be increasing in $k$, and Zemel and Panaretos (2017) show that the optimal maps $t_{\Sigma_i}^{\Sigma_k}$ converge uniformly over compacta to $t_{\Sigma_i}^{\Sigma}$ as $k \to \infty$. Though we described the algorithm in the setup of covariance matrices only (i.e., centred Gaussian measures) it can be applied more generally to any finite collection of measures in Wasserstein space.

In terms of the manifold-like geometry of covariances under the Procrustes metric (see Section 3), the algorithm starts with an initial guess of the Fréchet mean; it then lifts all observations to the tangent space at that initial guess via the log map, and averages linearly on the tangent space; this linear average is then retracted onto the manifold via the exponential map, providing the next guess, and iterates. In finite dimensions, the quantity $\left( N^{-1} \sum_{i=1}^{N} t_{\Sigma_i}^{\Sigma_k} - \mathcal{I} \right)$ is precisely the negative gradient of the Fréchet (sum-of-squares) functional (Zemel and Panaretos, 2017, Theorem 1), and so this is a steepest descent in the space of covariances endowed with the Procrustes metric. Compared to the procedure of Pigoli et al. (2014), steepest descent appears to be numerically more stable. For example, we observed through simulations that it is less sensitive to the initial point. Finally, it is worth mentioning that when the covariance operators commute, either algorithm converges to the Fréchet mean after a single iteration.\(^9\)

9 Tangent Space PCA, Optimal Multicoupling, and Amplitude vs Phase Variation

Once a Fréchet mean of a given sample of covariance operators is found, the second order statistical analysis is to understand the variation of the

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\(^8\)i.e. when the operators $\Sigma_1, \ldots, \Sigma_N$ are defined on some finite dimensional subspace $\mathcal{H}' \subset \mathcal{H}$, which will always be the case in practice, as explained in the first paragraph of this section.

\(^9\)In the Wasserstein-inspired algorithm this requires to start from any positive linear combination of the operators themselves, or positive powers thereof.
sample around this mean. The optimal value of the Fréchet functional gives a coarse measure of variance (as a sum of squared distances of the observation from their mean), but it is desirable to find a parsimonious representation for the main sources/paths of variation in the sample, analogous to Principal Component Analysis (PCA) in Euclidean spaces (Jolliffe, 2002) and functional versions thereof in Hilbert spaces (Panaretos and Tavakoli, 2013).

One way of carrying out PCA in non-Euclidean spaces is by working on the tangent space (Huckemann et al., 2010; Fletcher et al., 2004; Dryden et al., 2009). In the setup of covariance operators with the Procrustes distance $\Pi$, this can be done in closed form. Using the log map at $\Sigma$, one lifts the data $\Sigma_1, \ldots, \Sigma_n$ to the points $\log_\Sigma(\Sigma_i) = t_{\Sigma_i} - \mathcal{I} = \Sigma^{-1/2}[\Sigma^{1/2}\Sigma_i\Sigma^{1/2}]^{1/2}\Sigma^{-1/2} - \mathcal{I}$ in the tangent space at the Fréchet mean, $\text{Tan}_\Sigma$ (see Section 3). One can then carry out linear PCA of the data at the level of the tangent space. The resulting components, orthogonal segments in $\text{Tan}_\Sigma$, can then be retracted to the space of covariance operators by means of the exponential map $\exp_\Sigma$. These would give principal geodesics that explain variation in the data; retracting linear combinations of the principal components would result in principal submanifolds.

Since the tangent space is a linear approximation to the manifold, the success of tangent space PCA in explaining the variability of the sample around its mean depends on the quality of the approximation. In finite dimensions, the typical difficulty comes from the cut locus of the manifold; the log map is not defined on the entire manifold, and one often needs to assume that the spread of the observations around the mean is not too large. In the Wasserstein space, this is actually not a problem, since the exponential map is surjective under sufficient injectivity (see Section 3). The difficulty here is of a rather different nature, and amounts precisely to verification that the required injectivity takes place. The issue is that the log map $\log_\Sigma(\Sigma_i)$ at $\Sigma$ is guaranteed to be well-defined if $\ker(\Sigma) \subseteq \ker(\Sigma_i)$ (Proposition 2; equivalently, one requires $\text{range}(\Sigma) \supseteq \text{range}(\Sigma_i)$), but may fail to be defined otherwise. In finite dimensions, we know that if one $\Sigma_i$ is injective (nonsingular), then so is the Fréchet mean, so the log map is well defined. We conjecture that the same result holds in infinite dimensions, and leave this question for future work (see Section 12).

It is important to remark that in practice, the tangent space PCA will only be employed at a discretised level (and thus in finite dimensions), where it is indeed feasible and guaranteed to make sense. The question is whether the procedure remains stable as the dimensionality of the discretisation grows to infinity. The stability of the Wasserstein distance (Section 5) and the
Fréchet mean (Theorem 11) suggests that this should be so, but a rigorous proof amounts to establishing injectivity as in the preceding paragraph.

Tangent space PCA pertains to the collection of observations $\Sigma_1, \ldots, \Sigma_n$ as a whole, and is consequently intimately related to multicoupling of the corresponding measures, admitting a further elegant interpretation. Recall from Section 6 that the problem of optimal multicouplings consists of minimising the functional

$$G(\pi) = \frac{1}{2n^2} \int_{\mathcal{H}^n} \sum_{i<j} ||x_i - x_j||^2 \, d\pi(x_1, \ldots, x_n)$$

over all Borel measures $\pi$ on $\mathcal{H}^n$ having $\mu_1, \ldots, \mu_n$ as marginals. In other words, we seek to multouple (the centred Gaussian measures corresponding to) $\Sigma_1, \ldots, \Sigma_n$ as closely as possible, that is, in such a way that the sum of pairwise squared distances between the covariances is minimal. The probabilistic interpretation is that one is given random variables $X_i \sim \mu_i$ and seeks to construct a random vector $(Y_1, \ldots, Y_n)$ on $\mathcal{H}^n$ such that $Y_i \overset{d}{=} X_i$ marginally, and such that

$$\mathbb{E} \sum_{i<j} ||Y_i - Y_j||^2$$

is minimal.

Intuitively, one wishes to construct a vector on $\mathcal{H}^n$, whose coordinates are maximally correlated, subject to having prescribed marginal distributions. In Lemma 8 we have seen that an optimal multicoupling yields the Fréchet mean. However, as observed in Zemel and Panaretos (2017), the proof actually allows to go in the other direction, and deduce an optimal multicoupling from the Fréchet mean. In the probabilistic terminology, we can write this down formally as follows:

**Lemma 13.** Let $\Sigma_1, \ldots, \Sigma_n$ be covariances on $\mathcal{H}$ with injective Fréchet mean $\overline{\Sigma}$. Let $Z \sim N(0, \overline{\Sigma})$ and define a random Gaussian vector on $\mathcal{H}^n$ by

$$(Y_1, \ldots, Y_n), \quad Y_i = t_{\overline{\Sigma}}^{\Sigma} (Z) = \Sigma^{-1/2} [\Sigma^{1/2} \Sigma_i \Sigma^{1/2}]^{1/2} \Sigma^{-1/2} Z, \quad i = 1, \ldots, n.$$  

Then, the joint law of $(Y_1, \ldots, Y_n)$ is an optimal multicoupling of $N(0, \Sigma_1), \ldots, N(0, \Sigma_n)$.

We can reformulate Lemma 13 as an optimisation problem on the space of covariance operators on the tensor product Hilbert space $\mathcal{H}^n$. Define the coordinate projections $p_i : \mathcal{H}^n \to \mathcal{H}$ by $p_i (h_1, \ldots, h_n) = h_i$. The problem
is to construct a covariance operator $\Sigma$ on $\mathcal{H}^n$ that, under the marginal constraints $p_i^* \Sigma p_i^* = \Sigma_i$, minimises

$$\text{tr} \left[ \sum_{i=1}^{n} p_i \Sigma p_i^* - \sum_{i<j} p_i \Sigma p_j^* \right] = \sum_{i=1}^{n} \text{tr} \Sigma_i - \sum_{i<j} \text{tr} [p_i \Sigma p_j^*].$$

Since the $\Sigma_i$'s are given, one equivalently seeks to maximise the last displayed double sum. According to the lemma, the optimal $\Sigma$ is the covariance operator of the random vector $(Y_1, \ldots, Y_n)$ defined in the statement.

The probabilistic formulation highlights the interpretation of tangent space PCA in terms of functional data analysis, in particular in terms of the problem of phase variation (or warping), and its solution, the process of registration (or synchronisation). Consider a situation where the variation of a random process $X$ arises via both amplitude and phase (see Panaretos and Zemel, 2016, Section 2):

1. First, one generates the realisation of a Gaussian process $X \sim N(0, \Sigma)$, viewed via the Karhunen–Loève expansion as

$$X = \sum_{n=1}^{\infty} \sigma_n^{1/2} \xi_n \varphi_n$$

for $\{\sigma_n, \varphi_n\}$ the eigenvalue/eigenfunction pairs of $\Sigma$, and $\xi_n \overset{iid}{\sim} N(0,1)$ a sequence of real standard normal variables. This is the amplitude variation layer, as corresponds to a superposition of random $N(0, \sigma_n)$ amplitude fluctuations around fixed (deterministic) modes $\varphi_n$.

2. Then, one warps the realisation $X$ into $\tilde{X}$, by applying a (bounded) non-negative operator $T$ (usually uncorrelated with $X$),

$$\tilde{X} = TX = \sum_{n=1}^{\infty} \sigma_n^{1/2} \xi_n T \varphi_n$$

with the condition on $T$ that $\|T \Sigma T\|_1 < \infty$, to guarantee that the resulting $\tilde{X}$ has finite variance. This is the phase variation layer, since it emanates from deformation fluctuations of the modes $\varphi_n$. The term phase comes from the case $\mathcal{H} = L^2[0,1]$, where $\tilde{X}(x) = (TX)(x) = \int_0^1 \tau(x, y) X(y) dy = \sum_{n=1}^{\infty} \sigma_n^{1/2} \xi_n \int_0^1 \tau(x, y) \varphi_n(y) dy$ can be seen to be variation attributable to the “$x$-axis” (ordinate), contrasted to amplitude variation which is attributable to the “$y$-axis” (abcissa).
At the level of covariances, if $T$ is uncorrelated with $X$, then $\tilde{X}$ has covariance $T\Sigma T$ conditional on $T$, which is a geodesic perturbation of $\Sigma$: it corresponds to the retraction (via the exponential map) of a linear perturbation of $\Sigma$ on the tangent space $Tan_\Sigma$. If this perturbation is “zero mean” on the tangent space (i.e. $E[T] = \mathcal{J}$), then one expects $\Sigma$ to be a Fréchet mean of the random operator $T\Sigma T$. So, if one gets to observe multiple such perturbations $\Sigma_k = T_k \Sigma T_k$, the tangent space PCA provides a means of registration of $\{\Sigma_1, \ldots, \Sigma_k\}$: the approximate recovery of $\Sigma$ and $\{T_k\}_{k=1}^n$, allowing for the separation of the amplitude from the phase variation (which, if left unaccounted, would have detrimental effects to statistical inference). This intuition is made precise in the next section, where phase variation is used as a means of suggesting a canonical generative model: a statistical model behind the observed covariances $\{\Sigma_1, \ldots, \Sigma_n\}$ that is naturally compatible with the use of the Procrustes distance.

Before moving on to this, we remark that, in a sense, we have come full circle. The Procrustes distance of Pigoli et al. (2014) is motivated by the Procrustes distance in shape theory, and is thus connected to the optimal simultaneous registration of multiple Euclidean point configurations, subjected to random isometries. And, our interpretation of this distance, shows that it is connected to the optimal simultaneous registration of multiple Gaussian processes, subjected to random transportation deformations.

10 Generative Models, Random Deformations, and Registration

An important question that has not yet been addressed regards the choice of the Procrustes distance for statistical purposes on covariance operators: why would one choose this specific metric rather than another one? As the space of covariance operators is infinite-dimensional, there are naturally many other distances with which one can endow it. For the statistician, the specific choice of metric on a space implicitly assumes a certain data generating mechanism for the sample at hand, and it is therefore of interest to ask what kind of generative model is behind the Procrustes distance. In the Introduction, we noticed that the use of a Hilbert–Schmidt distance on covariances implicitly postulates that second-order variation arises via additive perturbations,

$$\Sigma_k = \Sigma + E_k$$

for $E_k$ being zero mean self adjoint perturbations. Furnished with the insights of the optimal transportation perspective, particularly those gained in the last section (Section 9), we now show that the natural generative model associated with the Procrustes distance is one of random deformations (a.k.a
warping or phase variation), and is intimately related to the registration problem in functional data. Suppose that \( X \) is a Gaussian process with covariance \( \Sigma \) and let \( T \) be a random non-negative bounded operator on \( \mathcal{H} \). Conditional upon \( T \), \( TX \) is a Gaussian process with covariance \( T \Sigma T^* \). It is quite natural (and indeed necessary for identifiability) to assume that \( \Sigma \) is the “correct” (or template) covariance, in the sense that the expected value of \( T \) is the identity. In other words, the covariance of \( TX \) is \( \Sigma \) “on average”. The conjugation perturbations

\[
\Sigma_k = T_k \Sigma T_k^*
\]

then yield a generative model that is canonical for the Procrustes metric, as we now rigorously show:

**Theorem 14 (Generative Model).** Let \( \Sigma \) be a covariance operator and let \( T : \mathcal{H} \to \mathcal{H} \) be a random\(^{10}\) non-negative linear map with \( \mathbb{E} \| T \|_\infty^2 < \infty \) and mean identity. Then the random operator \( T \Sigma T^* \) has \( \Sigma \) as Fréchet mean in the Procrustes metric,

\[
\mathbb{E}[\Pi^2(\Sigma, T \Sigma T^*)] \leq \mathbb{E}[\Pi^2(\Sigma', T \Sigma T^*)],
\]

for all non-negative nuclear operators \( \Sigma' \).

The assumption that \( \mathbb{E} \| T \|_\infty^2 < \infty \) guarantees that the Fréchet functional \( \mathbb{E} \Pi^2(A, T \Sigma T) \) is finite for any covariance (non-negative and nuclear) operator \( \Sigma \). For measures on \( \mathbb{R}^d \) with compact support, the result in Theorem 14 holds in a more general Wasserstein setup, where \( \mu \) is a fixed measure and \( T \) is a random optimal map with mean identity (Bigot and Klein, 2012; Zemel and Panaretos, 2017).

**Proof of Theorem 14.** We use the Kantorovich duality Villani (2003, Theorem 1.3) as in Zemel and Panaretos (2017, Theorem 5). Define the function \( \varphi(x) = \langle Tx, x \rangle / 2 \) and its Legendre transform \( \varphi^*(y) = \sup_{x \in \mathcal{H}} \langle x, y \rangle - \varphi(x) \). We abuse notation for the interest of clarity, and write \( d\Sigma(x) \) for integration with respect to the corresponding measure. The strong and weak Kantorovich duality yield

\[
\frac{1}{2} W^2(N(0, \Sigma), N(0, T \Sigma T)) = \int_{\mathcal{H}} \left( \frac{1}{2} \|x\|^2 - \varphi(x) \right) d\Sigma(x) \\
+ \int_{\mathcal{H}} \left( \frac{1}{2} \|y\|^2 - \varphi^*(y) \right) dT \Sigma T(x);
\]

\(^{10}\)In the sense that \( T \) is Bochner measurable from a probability space \( \Omega \) to \( B(\mathcal{H}) \). In particular, it is separately valued, namely \( T(\Omega) \) is a separable subset of (the nonseparable) \( B(\mathcal{H}) \).
\[
\frac{1}{2} W^2(N(0, \Sigma'), N(0, T \Sigma T)) \geq \int_{\mathcal{H}} \left( \frac{1}{2} \|x\|^2 - \varphi(x) \right) \, d\Sigma'(x)
+ \int_{\mathcal{H}} \left( \frac{1}{2} \|y\|^2 - \varphi^*(y) \right) \, dT \Sigma T(x).
\]

Taking expectations, using Fubini’s theorem and noting that \( \mathbb{E} \varphi(x) = \|x\|^2/2 \) because \( \mathbb{E} T = \mathcal{I} \) formally proves the result; in particular this provides a proof for empirical Fréchet means (when \( T \) takes finitely many values).

To make the calculations rigorous we modify the construction in (Zemel and Panaretos, 2017) to adapt for the unboundedness of the spaces. Let \( \Omega \) be the underlying probability space and \( B(\mathcal{H}) \) the set of bounded operators on \( \mathcal{H} \) with the operator norm topology. We assume that \( T : \Omega \to B(\mathcal{H}) \) is Bochner measurable with (Bochner) mean \( \mathcal{I} \). Then (the measure corresponding to) \( T \Sigma T : \Omega \to \mathcal{W}(\mathcal{H}) \) is measurable because it is a (Lipschitz) continuous function of \( T \). To see this notice that

\[
\int_{\mathcal{H}} \left\| S(x) - T(x) \right\|^2 \, d\Sigma(x) = \text{tr}(S - T) \Sigma (S^* - T^*) \leq \|S - T\|^2 \text{tr} \Sigma.
\]

Similarly,

\[
\left| \int_{\mathcal{H}} \langle (T - S)x, x \rangle \, d\Sigma'(x) \right| = |\text{tr}(T - S)\Sigma'| \leq \|T - S\|_\infty \text{tr} \Sigma'
\]

so the integrals with respect to \( \varphi \) are measurable (from \( \Omega \) to \( \mathbb{R} \)) for all \( \Sigma' \), and integrable because \( \mathbb{E} \|T\|_\infty < \infty \). Since \( W^2(\Sigma', T \Sigma T) \) is measurable and integrable, so are the integrals with respect to \( \varphi^* \) (as a difference between integrable functionals). To conclude the proof it remains to show that for all \( \Sigma' \)

\[
\mathbb{E} \int_{\mathcal{H}} \langle Tx, x \rangle \, d\Sigma'(x) = \int_{\mathcal{H}} \langle (\mathbb{E} T)x, x \rangle \, d\Sigma'(x).
\]

This is clearly true if \( T \) is simple (takes finitely many values). Otherwise, we can find a sequence of simple \( T_n : \Omega \to B(\mathcal{H}) \) such that \( \|T_n - T\|_\infty \to 0 \) almost surely and in expectation. This Fubini equality holds for \( T_n \) and

\[
\left| \mathbb{E} \int_{\mathcal{H}} \langle Tx, x \rangle \, d\Sigma'(x) - \mathbb{E} \int_{\mathcal{H}} \langle T_n x, x \rangle \, d\Sigma'(x) \right| = |\mathbb{E} \text{tr}(T - T_n)\Sigma'| \leq \text{tr} \Sigma' \mathbb{E} \|T - T_n\|_\infty.
\]
\[ \left| \int_{\mathcal{H}} \langle (ET)x, x \rangle \, d\Sigma'(x) - \int_{\mathcal{H}} \langle (ET_n)x, x \rangle \, d\Sigma'(x) \right| = |\text{tr}(ET - ET_n)\Sigma'| \leq \text{tr}\Sigma'\|ET - ET_n\|_{\infty}. \]

By approximation the Fubini equality holds for \( T \), completing the proof.

The reader may have noticed that the proof relies on optimal transport arguments that do not make specific use of linearity of \( T \) or Gaussianity. In the Gaussian case, however, the Fréchet functional can be evaluated explicitly due to the formula of the Wasserstein distance. For the reader’s convenience we outline another, more constructive proof of Theorem 14. The argument is fully rigorous in finite dimensions, and could probably be modified with additional effort to be valid in infinite dimensions.

**Alternative proof of Theorem 14 in finite dimensions.** We first evaluate the term \( \mathbb{E}\text{tr}(T\Sigma T^*) = \mathbb{E}\text{tr}(T\Sigma T) \) in the Wasserstein distance, using \( \mathbb{E}T = \mathcal{I} \), as

\[
\mathbb{E}\text{tr}(T - \mathcal{I})\Sigma(T - \mathcal{I}) + \mathbb{E}(\text{tr}\Sigma T) + \mathbb{E}(\text{tr}T\Sigma) - \mathbb{E}\text{tr}\Sigma = \text{tr}[\text{Cov}(T)\Sigma] + \text{tr}(\Sigma),
\]

where \( \text{Cov}T = \mathbb{E}[(T - \mathcal{I})(T - \mathcal{I})] \). Consequently, the Fréchet functional at \( \Sigma \) equals

\[
\mathbb{E}W^2(T\Sigma T^*, \Sigma) = \text{tr}(\Sigma) + \mathbb{E}\text{tr}(T\Sigma T^*) - 2\mathbb{E}\text{tr}(\Sigma^{1/2}T\Sigma T^*\Sigma^{1/2})^{1/2} = 2\text{tr}(\Sigma) + \text{tr}[\text{Cov}(T)\Sigma] - 2\mathbb{E}\text{tr}(\Sigma^{1/2}T\Sigma^{1/2}) = 2\text{tr}(\Sigma) + \text{tr}[\text{Cov}(T)\Sigma] - 2\text{tr}(\Sigma) = \text{tr}[\text{Cov}(T)\Sigma].
\]

Keeping the above result in mind, we now compute the functional at an arbitrary \( \Sigma' \):

\[
\mathbb{E}W^2(T\Sigma T^*, \Sigma') = \text{tr}(\Sigma') + \mathbb{E}\text{tr}(T\Sigma T^*) - 2\mathbb{E}\text{tr}(\Sigma'^{1/2}T\Sigma T^*\Sigma'^{1/2})^{1/2} = \text{tr}(\text{Cov}(T)\Sigma) + \mathbb{E}\left\{ \text{tr}(\Sigma'^{1/2}T\Sigma'^{1/2}) + \text{tr}(\Sigma^{1/2}T\Sigma^{1/2}) - 2\text{tr}(\Sigma'^{1/2}T\Sigma T\Sigma'^{1/2})^{1/2} \right\}.
\]

To prove that \( F(\Sigma') \geq F(\Sigma) \) it suffices to show that the term inside the expectation is non-negative; we shall do this by interpreting it as the Wasserstein distance between \( B = T^{1/2}\Sigma'T^{1/2} \) and \( A = T^{1/2}\Sigma T^{1/2} \). Write \( B_1 = \)
\(\Sigma^{1/2} T \Sigma^{1/2}, A_1 = \Sigma^{1/2} T \Sigma^{1/2} \). Then the formula for the Wasserstein distance says that 
\[2 \text{tr}(A_1^{1/2} BA_1^{1/2}) \leq \text{tr} A + \text{tr} B = \text{tr} A_1 + \text{tr} B_1.\]
We thus only need to show that \(\text{tr}(A^{1/2} BA^{1/2})^{1/2} = \text{tr}(\Sigma^{1/2} T \Sigma T \Sigma^{1/2})^{1/2}\). Up until now, everything holds in infinite dimensions, but the next argument assumes finite dimensions. In particular, we will establish that 
\(\text{tr}(A^{1/2} BA^{1/2})^{1/2} = \text{tr}(\Sigma^{1/2} T \Sigma T \Sigma^{1/2})^{1/2}\)
by showing that these matrices are conjugate. Assume firstly that \(\Sigma, \Sigma'\) and \(T\) are invertible and write

\[
D = \Sigma^{1/2} T \Sigma T \Sigma^{1/2} = \Sigma^{-1/2} T^{-1/2} [BA] T^{1/2} \Sigma^{1/2} = \Sigma^{-1/2} T^{-1/2} A^{-1/2} [A^{1/2} BA^{1/2}] A^{1/2} T^{1/2} \Sigma^{1/2}.
\]

Thus the non-negative matrices \(D\) and \(A^{1/2} BA^{1/2}\) have the same eigenvalues. This also holds true for their square roots, that consequently have the same trace. Since singular matrices can be approximated by nonsingular ones, this nonnegativity extends to the singular case as well, and so the proof is valid without restriction when \(\mathcal{H} = \mathbb{R}^d\) is finite-dimensional.

When the law of the random deformation \(T\) is finitely supported, we can get a stronger result than that of Theorem 14, without the assumption that \(T\) is bounded. This is not merely a technical improvement, as in many cases the optimal maps will, in fact, be unbounded (see the discussion after Equation (3.1)). This stronger result will also be used in Proposition 16 to obtain a (partial) characterisation of the sample Fréchet mean.

**Theorem 15.** Let \(\Sigma\) be a covariance operator corresponding to a centred Gaussian measure \(\mu \equiv N(0, \Sigma)\) and let \(D \subseteq \mathcal{H}\) be a dense linear subspace of \(\mu\)-measure one. If \(T_1, \ldots, T_n : D \to \mathcal{H}\) are (possibly unbounded) non-negative operators such that \(T_i \in \mathcal{L}_2(\mu)\) for all \(i = 1, \ldots, n\) and \(\sum T_i(x) = nx\) for all \(x \in D\), then \(\Sigma\) is a Fréchet mean of the finite collection \(\{T_i \Sigma T_i : i = 1, \ldots, n\}\).

**Proof.** Straightforward calculations show that the functions \(\varphi_i(x) = \langle T_i x, x \rangle / 2\) are convex on \(D\) and \(T_i x\) is a subgradient of \(\varphi_i\) for any \(i\) and any \(x \in D\). The duality in the previous proof is therefore valid with the integrals involving \(\varphi_i\) taken on \(D\) (rather than on the whole of \(\mathcal{H}\)). These integrals are finite, because \(\varphi\) and \(\varphi^*\) are non-negative functions and the Wasserstein distance is finite. (The integral of \(\|x\|^2 / 2 - \varphi(x)\) with respect to \(\Sigma') may be negative infinite, but this does not hinder the validity of the arguments.) Since there are finitely many integrals, there are no measurability issues and we have \(F(\mu) \leq F(\nu)\) whenever \(\nu(D) = 1\). By continuity considerations, since \(D\) is dense in \(\mathcal{H}\), this means that \(F(\mu) \leq F(\nu)\) for all \(\nu \in \mathcal{W}(\mathcal{H})\), so \(\mu\), that is, \(\Sigma\), is a Fréchet mean.
11 Characterisation of Fréchet Means via an Operator Equation

Knott and Smith (1984) show that, in finite dimensions, a positive definite solution $\Sigma$ to the equation

$$\Sigma = \frac{1}{n} \sum_{i=1}^{n} (\Sigma_{i}^{1/2} \Sigma \Sigma_{i}^{1/2})^{1/2}$$

(11.1)

is a Fréchet mean of $\Sigma_{1}, \ldots, \Sigma_{n}$ (see also Rüschendorf and Uckelmann, 2002.) Later, Agueh and Carlier (2011) proved that (11.1) is in fact a characterisation of the mean in that (if one $\Sigma_{i}$ is invertible) this fixed point equation has a unique invertible solution, which is the Fréchet mean of $\Sigma_{1}, \ldots, \Sigma_{n}$. Part of their results extend easily to infinite dimensions:

**Proposition 16.** Let $\Sigma_{1}, \ldots, \Sigma_{n}$ be covariance operators. Then:

1. Any Fréchet mean $\Sigma$ of $\Sigma_{1}, \ldots, \Sigma_{n}$ satisfies (11.1).

2. If (11.1) holds, and $\ker(\Sigma) \subseteq \bigcap_{i=1}^{n} \ker(\Sigma_{i})$, then $\Sigma$ is a Fréchet mean.

**Proof.** Let $\mathcal{P}_{k}$ be a sequence of finite rank projections that converge strongly to the identity. Then $\mathcal{P}_{k} \Sigma_{i} \mathcal{P}_{k}$ converge to $\Sigma_{i}$ in Wasserstein distance (Section 5) and thus in trace norm by Proposition 4. If $\Sigma_{k}$ is the Fréchet mean of the projected operators, then it satisfies (11.1) by Agueh and Carlier (2011, Theorem 6.1), with $\Sigma_{i}$ replaced by $\mathcal{P}_{k} \Sigma_{i} \mathcal{P}_{k}$. But $\Sigma_{k}$ converges to $\Sigma$ in trace norm (Theorem 11 and Proposition 4) and by continuity (11.1) holds true for $\Sigma$.

Conversely, the kernel conditions means that $T_{i} = t_{\Sigma_{k}}^{i} = \Sigma^{-1/2} (\Sigma_{i}^{1/2} \Sigma \Sigma_{i}^{1/2})^{1/2} \Sigma^{-1/2}$ exists and is defined on a dense subspace $D_{i}$ of $\Sigma$-measure one (Proposition 2). Equation (11.1) yields $\sum T_{i} = n \mathcal{I}$ on $D = \bigcap_{i=1}^{n} D_{i}$, a set of full measure, and by Theorem 15 $\Sigma$ is a Fréchet mean.

In view of Proposition 16, injectivity of the Fréchet mean is equivalent to the existence of an injective solution to the operator equation (11.1).

12 Open Questions and Future Work

We conclude with some open questions. The most important of these is the injectivity (regularity) of the Fréchet mean $\Sigma$. We conjecture that, as in the finite dimensional case,

**Conjecture 17 (Regularity of the Fréchet Mean).** Let $\Sigma_{1}, \ldots, \Sigma_{n}$ be covariances on $\mathcal{H}$ with $\Sigma_{1}$ injective. Then, their Fréchet mean $\tilde{\Sigma}$ with respect to the Procrustes metric $\Pi$ is also injective.

Resolution of the conjecture (in the positive direction) will automatically yield the solution to the multicoupling problem (by virtue of Lemma 13).
and the validity of the geodesic principal component analysis (Section 9),
irrespective of finite-dimensionality. As mentioned in the previous section,
injectivity is equivalent to the existence of an injective solution to the fixed
point equation (11.1); see Proposition 16.

We remark that injectivity indeed holds when the operators in question
commute, because then $\Sigma^{1/2} = n^{-1}(\Sigma_1^{1/2} + \cdots + \Sigma_n^{1/2})$. However, it is not
possible to bound $\Sigma^{1/2}$ in terms of $\Sigma_i^{1/2}$, not even up to constants. More
precisely,

Lemma 18. For all $\Sigma$ of infinite rank and all $n \geq 2$ there exist covariance
operators $\Sigma_1, \ldots, \Sigma_n$ with mean $\Sigma$ and such for any non-negative number $c$,
$\Sigma - c(\Sigma_1 + \cdots + \Sigma_n)$ is not positive.

Proof. Without loss of generality $n = 2$, because if $\Sigma_1$ and $\Sigma_2$ are as
required, then so are $(\Sigma_1, \Sigma_2, \Sigma, \ldots, \Sigma)$. Let $\lambda_k$ and $\mu_k$ be disjoint sequences
of nonzero eigenvalues of $\Sigma$ and such that $\lambda_k / \mu_k > 5^k$ (this is possible since
the eigenvalues go to zero), with corresponding eigenvectors $(e_k)$ and $(f_k)$.

Define an operator $T$ by $T(e_k) = e_k + b_k f_k$, $T(f_k) = b_k e_k + f_k$ (and $T$
is the identity on the orthogonal complement of the $e_k$’s and $f_k$’s). Then $T$
is self-adjoint, and it is non-negative provided that $|b_k| \leq 1$. We have for all $k$
\[
\frac{\langle T^* T f_k, f_k \rangle}{\langle f_k, f_k \rangle} = \frac{\mu_k + b_k^2 \lambda_k}{\mu_k} \geq b_k^2 5^k \to \infty
\]if $b_k = 2^{-k}$, say. Therefore $\Sigma - c(T^* T)$ is not non-negative for any $c > 0$.

Also, $\|T - \mathcal{I}\|_\infty = 1/2$ so $T$ has a bounded inverse and $2\mathcal{I} - T$ is also
non-negative. To complete the proof it suffices to see that $\Sigma$ is the Fréchet
mean of $\Sigma_1 = T^* T$ and $\Sigma_2 = (2\mathcal{I} - T) \Sigma (2\mathcal{I} - T)$. Indeed, the bounded
operator $(2\mathcal{I} - T) \circ T^{-1} = 2T^{-1} - \mathcal{I}$ is positive (as a composition of two
positive operators that commute), and thus the optimal map $t_1^{\mathcal{H}}$ from $\Sigma_1$
to $\Sigma_2$. The Fréchet mean is then the midpoint in McCann’s interpolant,
\[
[(t_1^\mathcal{H} + \mathcal{I})/2] \# \Sigma_1 = T^{-1} \# \Sigma_1 = \Sigma.\]
(The Fréchet mean is unique here even if $\Sigma_i$ are not injective, since they have the same kernel and we can replace $\mathcal{H}$
by the orthogonal complement of this kernel to make them injective.)

Note that $T$ (and $2\mathcal{I} - T$) can be very close to the identity in any Schatten
norm, since we can multiply all the $b_k$’s by an arbitrary small constant. It
is therefore unlikely that Hajek–Feldman type conditions on the operators
be relevant.

An alternative line of proof is by a variational argument. Suppose that
$\Sigma v = 0$ for $\|v\| = 1$ and define $\Sigma' = \Sigma + \epsilon v \otimes v$. The quantity $\text{tr} \Sigma'$ in the
Fréchet functional increases by $\epsilon$, and we believe that $\text{tr}(\Sigma_i \Sigma' \Sigma_i)^{1/2}$ behaves
like $\sqrt{\epsilon}$ for $\epsilon$ small, and consequently $\Sigma'$ has a better Fréchet value.
Another important line of enquiry is the consistency of the (empirical) Fréchet mean of $\Sigma_1, \ldots, \Sigma_n$ towards its population counterpart, as the sample size grows to infinity. Under mild conditions on the law of $\Sigma$, this population mean is guaranteed to be unique (see Proposition 10 in Section 6). However, it is not known to exist in general; the existence results of Le Gouic and Loubes (2017) do not apply to $\mathcal{H}$ because the latter is not locally compact. In view of Ziezold’s (Ziezold, 1977) results, if a population mean exists and the sequence of empirical means converge, then the limit must be the population mean (under uniqueness). These questions appear to be more subtle and we leave them for further work.

Finally, a last interesting question would be to establish the stability of the Procrustes algorithm to increasing projection dimension. In other words: if we had access to the fully infinite-dimensional covariances, it would still make sense to apply the Procrustes algorithm to obtain the Fréchet mean. Would this still converge? The methods of proof of Álvarez-Esteban et al. (2016) & Zemel and Panaretos (2017) are intrinsically finite dimensional, and cannot be lifted to infinite dimensions. Extending this convergence to the infinite dimensional case would precisely establish the stability of the Procrustes algorithm to increasingly finer discretisations, and this is likely to require new tools. Preliminary simulation results indicate that the convergence is indeed quite stable to increasing the projection dimension, so we conjecture that the convergence result should be true. In fact, this very issue may also lead to a resolution of Conjecture 17.

13 Auxiliary Results

This section contains some auxiliary results made use of at various parts of the paper that are certainly known, but for which we could not find a convenient reference for our purposes, and thus state/prove them here for completeness.

**Lemma 19.** An operator $A \in \mathcal{L}_2(N(0, \Sigma))$, possibly unbounded, is optimal from $N(0, \Sigma)$ to $A^#N(0, \Sigma)$ if and only if $A$ is non-negative, and then $A^#N(0, \Sigma) = N(0, A\Sigma A)$.

**Proof.** Optimality is equivalent to cyclical monotonicity (Ambrosio et al., 2008, Theorem 6.1.4), which is in turn equivalent to being a subgradient of a convex function (Villani, 2003, Theorem 2.27). If $A$ is optimal, then $Ax$ is a subgradient of a convex function $\varphi$ for all $x$ in $D$, the domain of definition of $A$. At every such $x$, $\varphi(x)$ is finite and by definition, since $D$ is linear,

$$\varphi(tx) - \varphi(sx) \geq \langle Asx, tx - sx \rangle = s(t - s) \langle Ax, x \rangle, \quad x \in D, \quad s, t \in \mathbb{R}.$$
Fix an integer $n$ and $x \in D$ and observe that the above inequality gives

$$\varphi(x) - \varphi(0) = \sum_{k=0}^{n-1} \varphi\left(\frac{k+1}{n}x\right) - \varphi\left(\frac{k}{n}x\right) \geq \sum_{k=0}^{n-1} \frac{k+1}{n} \langle Ax, x \rangle = \frac{n-1}{2n} \langle Ax, x \rangle,$$

and similarly

$$\varphi(0) - \varphi(x) = \sum_{k=0}^{n-1} \varphi\left(\frac{k}{n}x\right) - \varphi\left(\frac{k+1}{n}x\right) \geq \sum_{k=0}^{n-1} \frac{k+1}{n} - \frac{1}{n} \langle Ax, x \rangle = -\frac{n}{2n} \langle Ax, x \rangle.$$

By letting $n \to \infty$ we conclude that $\varphi(x) - \varphi(0) = \langle Ax, x \rangle / 2$ for all $x \in D$. The subgradient inequality with $s = 0$, $t = 1$ shows that $\langle Ax, x \rangle \geq 0$. To see that $A$ is self-adjoint we fix $x, y \in D$ and notice that

$$\langle Ax, y \rangle \leq \lim_{t \searrow 0} \varphi(x + ty) - \varphi(x) = \langle Ax, y \rangle / 2 + \langle Ay, x \rangle / 2.$$

Interchanging $x$ and $y$ shows that $\langle Ax, y \rangle = \langle Ay, x \rangle$ for all $x \in D$.

Conversely, if $A$ is non-negative, then one can verify directly that

$$\int_{H} \|Ax - x\|^2 dN(0, \Sigma)(x) = \text{tr}[(A - I)\Sigma(A - I)] = \text{tr}[\Sigma + A\Sigma A - 2A\Sigma] = W_2^2(N(0, \Sigma), N(0, A\Sigma A)),$$

because $(\Sigma^{1/2}A\Sigma A\Sigma^{1/2})^{1/2} = \Sigma^{1/2}A\Sigma^{1/2}$ has trace $\text{tr}A\Sigma$.

Lastly, as $A$ is self-adjoint, $A\#N(0, \Sigma) = N(0, A\Sigma A)$.

**Lemma 20** (trace of tensors). For all $f, g \in H$ we have $\|f \otimes g\|_1 = \|f\|\|g\|$.

**Proof.** This is clear if $f = 0$ or $g = 0$. Otherwise, since $f \otimes g$ is rank one, its trace norm equals its operator norm, which is

$$\sup_{\|h\| = 1} \|f \otimes gh\| = \sup_{\|h\| = 1} \|f\|\|\langle g, h \rangle\| = \|f\|\|g\|.$$

**Lemma 21** (compact convex hulls). Let $K$ be a compact subset of a Banach space. Then its closed convex hull $\text{conv}K$ is compact.

**Proof.** We need to show that Conv$K$ is totally bounded. For any $\delta > 0$ there exists a $\delta$-cover $x_1, \ldots, x_n \in K$. The simplex

$$S = \text{Conv}(x_1, \ldots, x_n) = \left\{ \sum_{i=1}^{n} a_i x_i : a_i \geq 0, \sum_{i=1}^{n} a_i = 1 \right\}$$
(a subset of Conv$K$) is compact as a continuous image of the unit simplex in $\mathbb{R}^n$. Indeed, if $v_i$ is the $i$-th column of the $n \times n$ identity matrix, then

$$\omega \left( \sum_{i=1}^{n} a_i v_i \right) = \sum_{i=1}^{n} a_i x_i$$

does the job. Let $y_1, \ldots, y_m$ be a $\delta$-cover of $S$ and let $y \in \text{Conv}K$. Then $y = \sum a_j z_j$ for $z_j \in K$ and $a_j \geq 0$ that sum up to one. For each $j$ there exists $i(j)$ such that $\|z_j - x_{i(j)}\| < \delta$. Then $x = \sum a_j x_{i(j)}$ is in $S$ and $\|x - y\| < \delta$. Thus, there exists $y_j$ such that $\|x - y_j\| < \delta$ and therefore $\|y - y_j\| < 2\delta$ and total boundedness is established.

**Lemma 22 (Gaussian fourth moment).** Let $X$ centred Gaussian with covariance $\Sigma$. Then

$$\mathbb{E}\|X\|^4 \leq 3(\mathbb{E}\|X\|^2)^2 = 3(\text{tr}\Sigma)^2.$$  

**Proof.** Let $(e_k)$ be a basis of eigenvectors of $\Sigma$ with eigenvalues $\lambda_k$. Then $X_k = \langle X, e_k \rangle \sim N(0, \lambda_k)$ are independent and $\|X\|^2 = \sum X_k^2$ has expectation $\sum \lambda_k = \text{tr}\Sigma$. Squaring gives

$$\mathbb{E}\|X\|^4 = \sum_{k,j} \mathbb{E}X_k^2 X_j^2 = \sum_k 3\lambda_k^2 + \sum_{k \neq j} \lambda_k \lambda_j = (\sum \lambda_k)^2 + 2 \sum \lambda_k^2 = (\text{tr}\Sigma)^2 + 2\|\Sigma\|_2^2 \leq 3(\text{tr}\Sigma)^2.$$ 

Interestingly, equality holds if and only if all but one eigenvalues are zero, i.e. $\Sigma$ has rank of at most one.

**Corollary 23.** Let $\mathcal{B} \subset \mathcal{W}(\mathcal{H})$ be a collection of centred Gaussian measures. If $\mathcal{B}$ is tight and $\int_{\mathcal{H}} \|x\|^2 d\mu(x) \leq R$ for all $\mu \in \mathcal{B}$, then $\mathcal{B}$ is precompact in the Wasserstein space.

**Proof.** By Lemma 22 the fourth moment of all measures in $\mathcal{B}$ is bounded by $3R^2$. Therefore

$$\sup_{\mu \in \mathcal{B}} \int_{\|x\| > M} \|x\|^2 d\mu(x) \leq \frac{1}{M^2} \sup_{\mu \in \mathcal{B}} \int_{\|x\| > M} \|x\|^4 d\mu(x) \leq 3R^2 \frac{1}{M^2} \to 0, \quad M \to \infty.$$ 

Any sequence $(\mu_n) \subseteq \mathcal{B}$ is tight and has a limit $\mu$ in distribution, and by Theorem 7.12 in Villani (2003), $\mu$ is also a limit in $\mathcal{W}(\mathcal{H})$.

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