Comparing and interpolating distributions on manifold

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Abstract

We are interested in comparing probability distributions defined on Riemannian manifold. The traditional approach to study a distribution relies on locating its mean point and finding the dispersion about that point. On a general manifold however, even if two distributions are sufficiently concentrated and have unique means, a comparison of their covariances is not possible due to the difference in local parametrizations. To circumvent the problem we associate a covariance field with each distribution and compare them at common points by applying a similarity invariant function on their representing matrices. In this way we are able to define distances between distributions. We also propose new approach for interpolating discrete distributions and derive some criteria that assure consistent results. Finally, we illustrate with some experimental results on the unit 2-sphere.

1 Introduction

The problem of comparing distributions defined on a non-Euclidean space or to be more specific, a Riemannian manifold, becomes increasingly important. A typical example of non-trivial manifold is the unit 2-sphere $S^2$, which is the domain of our experiments in this work. In this sense, our study has as

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main application problems from directional statistics, a branch of statistics dealing with directions and rotations in \( \mathbb{R}^3 \).

Pioneers in the field are Fisher, R.A. (1953) and von Mises. In recent years directional statistics proved to be useful in variety of disciplines like shape analysis [26], geology, crystallography [24], bio-informatics [28] and data mining [4]. Most of the practitioners in these fields use parametric distributions to model directional data, like von Mises-Fisher distribution and Fisher-Bingham-Kent (FBK) distributions.

There are application areas however, where parametric models are insufficient. A recent example is provided by medical imaging community. In a new technique based on MRI and called High Angular Resolution Diffusion Imaging (HARDI), the data is represented by Orientation Distribution Functions (ODFs) which are nothing but discrete distributions on the unit 2-sphere. These distributions by their nature are multi-modal - they are not concentrated about a particular direction. They do not follow a parametric model and even if they do the eventual model would be too complicated to be efficient. Consequently, a non-parametric approach is more natural in processing ODFs.

In analysis of HARDI data researchers first have to solve the problem of registration between different volumes of ODFs, corresponding to the images of different subjects. For this purpose they need models and algorithms for interpolation between ODFs. Second, researchers are interested in comparing different groups of subjects using HARDI imaging. Usually, a statistical procedure is employed and hypotheses are tested. However, comparison between volumes requires comparison between corresponding ODFs and no standard method for this is available. A third problem in processing HARDI data is building connectivity paths for a given volume. Once again we need a consistent way to interpolate between ODFs in order to follow an optimal propagating direction.

There are no many choices for interpolation procedure beyond the simplest linear one. A recent alternative, using the square root representation of probability mass functions, was proposed by Srivastava (2007) and implemented in [9]. No existing solution though respects the geometry of the underlying domain.

In conclusion, we need more models and non-parametric procedures for comparing and interpolating distributions on the sphere and on Riemannian manifolds in general. Approaches that address the non-Euclidean nature of the random variables and provide adequate solutions. It is the main subject
What we propose basically is a generalization of the classical concept of covariance of distribution. We allow covariance to be defined with respect to any point of distribution domain and by doing so we try to workaround the problem of finding the mean point, which might not exist or be ambiguous. Also, since compact manifolds like $S^2$ do not admit global parametrizations, we pay special attention to use the correct mathematical tool for describing the covariance. We not only point out to the well known fact that covariance can be viewed as a bi-linear operator and thus defined as a tensor, but specify the exact variance of this tensor. It is important to make a distinction between covariance tensor and metric tensor on manifold. A central observation in our approach is that at any point of the domain, the product of the metric and covariance tensors is a linear operator on the respected tangent space. We call it covariance operator. Collectively they form a field of operators. Then we introduce instruments, the so called similarity invariant functions, that can be used to study properties of these fields and to manipulate them.

After a formal introduction to the concept of covariance operators in section 2, we continue in section 3 with motivating examples showing the advantages of the new approach. We consider a two-sample location problem of the sphere and apply several classical non-parametric tests to solve it. Test statistics are based on projections defined by covariance operator fields.

In section 4 we consider the problem of interpolation between distributions on the sphere, and discuss and compare several alternatives. We also show some examples of interpolation between ODFs. The results are encouraging in the possibility of developing new applications for processing HARDI.

Although in all our experiments we stay on the unit sphere, the theoretical framework still holds on a general Riemannian manifold and this is one of its main strengths.

2 Covariance fields

2.1 Random variables on manifold

Let $M$ be a Riemannian $n$-manifold, $q \in M$ and let $Exp_q$ be the exponential map at $q$, $Exp_q : M_q \to M$. If $M$ is complete, then the exponential map $Exp_q$ is defined on the whole tangent space $M_q$. Throughout this paper for convenience we will assume that $M$ is a complete Riemannian $n$-manifold,
although often that is not necessary.

There is a maximal open set $U(q)$ in $M_p$ containing the origin, where $\text{Exp}_q$ is a diffeomorphism. Then the set $\mathcal{U}(q) = \text{Exp}_q(U(q))$ is called maximal normal neighborhood of $q$. On this normal neighborhood the exponential map is invertible and let

$$\text{Log}_q = \text{Exp}_q^{-1} : \mathcal{U}(q) \rightarrow M_p$$

be its inverse, the so called log-map. $\text{Log}_q$ is diffeomorphism on $\mathcal{U}(q)$. We adopt the notation $\overrightarrow{qp} = \text{Log}_q p$ in analogy to the Euclidean case, $M = \mathbb{R}^n$, where $\text{Log}_q p = p - q = \overrightarrow{qp}$.

In particular, for $M = \mathbb{S}^n$ the log-map has a closed-form expression

$$\overrightarrow{qp} = \frac{\cos^{-1} < p, q >}{(1 - < p, q >^2)^{1/2}}(p - < p, q > q),$$

which greatly simplifies metric related operations on the unit sphere.

The Borel sets on $M$ generated by the open sets on $M$ form a $\sigma$-algebra $\mathcal{A}(M)$ on $M$. Any Riemannian manifold has a natural measure $\mathcal{V}$ on $\mathcal{A}(M)$, called volume measure. In local coordinates $x$ it is given by

$$d\mathcal{V}(x) = \sqrt{|G_x|} dx,$$

where $G_x$ is the matrix representation of the metric tensor, $|G_x|$ is its determinant and $dx$ is the Lebesgue measure in $\mathbb{R}^n$.

**Example 1** Consider the two sphere, $\mathbb{S}^2$, parametrized in geographical coordinates $(\theta, \phi)$. Then the metric tensor is represented by

$$G_{(\theta, \phi)} = \begin{pmatrix} 1 & 0 \\ 0 & \cos^2(\theta) \end{pmatrix}$$

and the volume form is $V(\theta, \phi) = \cos(\theta) d\theta d\phi$.

A random variable $X$ on $M$ is any measurable function from a probability space $(\Omega, \mathcal{B}, P)$ to $(M, \mathcal{A}(M), \mathcal{V})$. The distribution function $F$ of $X$ is defined as

$$F(A) = \mathcal{P}(X^{-1}(A)), A \in \mathcal{A}(M).$$

If $F$ satisfies

$$F(A) = \int_A f(p) d\mathcal{V}(p), \forall A \in \mathcal{A}(M),$$

for almost everywhere continuous (w.r.t. $\mathcal{V}$) function $f$, then $F$ is said to be absolute continuous (w.r.t. $\mathcal{V}$) and $f$ is its density (pdf).
2.2 Intrinsic and Extrinsic mean and covariance

Let $(M, \rho)$ be a metric space. The Fréchet mean set of a distribution $F$ is the set of minimizers of $Q(q) = \int \rho^2(q, p) dF(p)$. It was introduced by Frechet (1948). If $M$ is a Riemannian manifold $M$ with metric structure $g$, then the intrinsic mean of $F$, is the Frechet mean of $(M, d_g)$, where $d_g$ is the geodesic distance. Karcher (1977) considered the intrinsic mean on $M$ and gave conditions for its existence and uniqueness. An alternative to intrinsic mean is the extrinsic one, which is obtained by embedding $M$ into a higher dimensional Euclidean space. We point to the influential paper of Bhattacharya R. and Patrangenaru, V. (2005) where the properties of extrinsic and intrinsic means and their relation and asymptotic properties are considered in details.

Once a mean point (intrinsic or extrinsic) is specified, the covariance can be defined as usual after fixing a coordinate system about that point.

To compare two distributions one may first look at their intrinsic means. If they differ, the distributions differ, otherwise one may compare further their covariances at the common mean point. This approach however suffers from at least two drawbacks. First, if the population mean set is large, then the finite sample intrinsic mean will have substantial variance. That will diminish the power of any test for equality of means and more importantly, will inevitably require comparing covariances at different points. Second, the intrinsic mean, provided it exists and it is unique, and the covariance alone do not specify completely a distribution.

Thus, if we want to answer the problem of comparing distributions, we need a more informative structure that completely represents distributions and that is defined in coordinates free manner for seamless manipulation and comparison.

2.3 Covariance operators

Many parametric families of distributions can be defined as functions on linear operators. Consider for example the standard normal distribution in $\mathbb{R}^n$ with density

\[ f(x) \propto \exp\left(-\frac{1}{2} \|x - \mu\|^2\right), \]

where $\mu \in \mathbb{R}^n$ is its mean. Since $\|x - \mu\|^2 = tr((x - \mu)(x - \mu)')$ and the matrix $L(x) = (x - \mu)(x - \mu)'$ defines a linear operator

\[ L(x)(u, v) = u' L(x)v = [u'(x - \mu)][(x - \mu)']v, \quad u, v \in \mathbb{R}^n, \]

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we can express the density by \( f(x) \propto h(L(x)), \) \( h(T) := \exp\left(-\frac{1}{2}tr(T)\right) \).

The von Mises-Fisher and FBK distributions \[22\] on the unit 2-sphere give us other such examples. For example, the latter is given by density

\[
f(x) = \frac{1}{c(\kappa, \beta)} \exp\{\kappa \gamma_1 \cdot x + \beta[(\gamma_2 \cdot x)^2 - (\gamma_3 \cdot x)^2]\},
\]

where \( \gamma_1, \gamma_2 \) and \( \gamma_3 \) are three points on \( S^2 \) representing orthonormal directions in \( \mathbb{R}^3 \). We have \( f(x) \propto h(L_1(x), L_2(x), L_3(x)) \), where

\[
L_i(x) = G(x)(\overrightarrow{x\gamma_i})(\overrightarrow{x\gamma_i})',
\]

are linear operators at the tangent space at \( x \in S^2 \) and

\[
h(T_1, T_2, T_3) = \exp(\kappa \cos(tr(T_1)) + \beta[\cos^2(tr(T_2)) - \cos^2(tr(T_3)))].
\]

In fact, any \( L : x \mapsto L(x) \) in the presented examples is a field of linear operators on tangential spaces. The concept we are going to introduce generalizes the above observations.

We return to a general Riemannain manifold \( M \) with metric \( G \). Fix a point \( q \in M \). Recall that the metric \( G(q) \) is a co-variant 2-tensor at \( M_q \), while the quantity \( (\overrightarrow{qp})(\overrightarrow{qp})' \) is a contra-variant 2-tensor at \( M_q \). The contraction of their tensor product, \( G(q)(\overrightarrow{qp})(\overrightarrow{qp})' \), is a \((1,1)\)-tensor, which is nothing but a linear operator at \( M_q \).

Now the idea becomes clear. For a distribution \( F \) on \( M \), a linear operator at \( M_q \) can be obtained by taking the expectation of \( G(q)(\overrightarrow{qp})(\overrightarrow{qp})', p \sim F \).

From now on we will use the standard notation \( T^2(M_q) \) for co-variant 2-tensors on \( M_q \), \( T_2(M_q) \) for contra-variant 2-tensors on \( M_q \) and \( T^1_1(M_q) \) for bi-linear operators on \( M_q \).

**Definition 1** Let \( r : \mathbb{R}^+ \rightarrow \mathbb{R}^+ \) be a continuous function. Covariance of distribution \( F \) on \( M \) at point \( q \in M \) is defined by

\[
\Sigma(q) = \int_{U(q)} (\overrightarrow{qp})(\overrightarrow{qp})'r(||\overrightarrow{qp}||)dF(p) \tag{2}
\]

and \( \Sigma : q \mapsto \Sigma(q) \in T^2(M_q) \) is called covariance field of \( F \).

With \( r = 1 \) we obtain the generic covariance field associated with \( F \) and this is the default choice.

As noted above, \( G(q)\Sigma(q) \) is a linear operator on \( M_q \), which we call covariance operator. Hence, \( G\Sigma \) is a field of linear operators on \( M \). With respect to
a coordinate system \( x \) at \( q \), \( G(q)\Sigma(q) \) is represented by a symmetric and positive definite matrix \( G_x\Sigma_x \), where \( G_x \) and \( \Sigma_x \) are the representations of \( G(q) \) and \( \Sigma(q) \). In other words, \( G\Sigma \) is a field of symmetric and positive definite operators on \( M \).

If \( v \in M_q \) has components \( v_x \) with respect to \( x \), we define

\[
(G(q)\Sigma(q))v := \Sigma_xG_xv_x
\]

and

\[
<v, (G(q)\Sigma(q))v> := v'_xG_x\Sigma_xG_xv_x.
\]

One can check that indeed the last quantity is invariant to coordinate change at \( q \).

It is worth to mention that for a covariance field \( \Sigma \) on \( M \), \( \Sigma^{-1} \) is also symmetric and positive definite and when it is differentiable, \( \Sigma^{-1} \) introduce a new Riemannian metric on \( M \).

If \( \Sigma_1 \) and \( \Sigma_2 \) are two covariance fields on \( M \), then \( \Sigma_1\Sigma_2^{-1} \) is a field of linear operators, i.e. for any \( q \in M \), \( \Sigma_1(q)\Sigma_2^{-1}(q) \in T^1_q(M_q) \).

On a complete Riemannian manifold, the problem of minimizing the trace of the default covariance field is equivalent to the problem of finding the intrinsic mean of \( F \), i.e.

\[
\mu = \arg\min_{q \in M} \{ \int_{d(q)} tr(G(q)(\overline{qP})(\overline{qP})')dF(p) = \int_M d^2_g(q,p)dF(p) \}.
\]

### 2.4 Similarity invariants

Let \( Sym^+_n \) denote the space of symmetric and positive definite matrices. Since this is the representation domain for covariance operators it is of obvious importance for us. \( Sym^+_n \) attracted the attention of many researchers in the recent years due to its non-Euclidean nature and consequently, the variety of research opportunities it provides. For the purposes of Diffusion Tensor Imaging, Fletcher, P. T., Joshi, S., (2007) and Pennec. X., Fillard, P., Ayache, N (2006) proposed the use of affine invariant distance, while Arsigny,V., Fillard, P., Pennec X., and Ayache, N. (2007) proposed the so called log-Euclidean distance. A good survey of the available distances and estimators in \( Sym^+_n \) along with new ones is provided by Dryden, I., Koloydenko, A., and Zhou, D., (2008). We aim a more general treatment of \( Sym^+_n \)
and instead of dealing with specific matrix functions we define a class of in-
variants. What particular member of this class should be used is application-
problem specific choice.

Two matrices $A, B \in Sym_{n}^{+}$ are said to be similar if

$$A = X^{-1}BX, \text{ for } X \in GL_n.$$  

Matrix representations of linear operators are similar and thus, this fact holds
for the representations of $G\Sigma$ and $\Sigma_1\Sigma_2^{-1}$. Next we define an important class
of functions that respect similarity.

**Definition 2** A similarity invariant function on $Sym_{n}^{+}$ is any continuous
bi-variate $h$ that satisfies

(i) $h(AXA', AYA') = h(X, Y), \forall X, Y \in Sym_{n}^{+}$ and $A \in GL_n$.

It is a non-negative with a unique root if

(ii) $h(X, Y) \geq 0, \forall X, Y \in Sym_{n}^{+}$ and $h(X, Y) = 0 \iff X = Y$.

Moreover, $h$ is called similarity invariant distance, if in addition to (i) and
(ii) also satisfies

(iii) $h(X, Y) + h(Y, Z) \geq h(X, Z), \forall X, Y, Z \in Sym_{n}^{+}$.

Below we list several examples of similarity invariant function we use in our
experiments.

1. For a fixed $Z \in Sym_{n}^{+}$, the similarity invariant

$$h_{\text{trdif}}(X, Y; Z) = ||tr(Z^{-1}X - Z^{-1}Y)||,$$

satisfies (iii) but not (ii). Default choice will be $Z = G^{-1}$, the inverse
of the metric tensor representation.

2. The second one is sometimes referred as affine-invariant distance in
$Sym_{2}^{+}$, see for example [29], [13], [5], [13] and [30], and it is defined by

$$h_{\text{trln2}}(X, Y) = \{tr(ln^2(XY^{-1}))\}^{1/2}, X, Y \in Sym_{2}^{+}.$$  

Actually, $h_{\text{trln2}}$ is not a unique choice for a distance in $Sym_{2}^{+}$.  

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3. Log-likelihood function gives us another choice for $h$,

$$h_{\text{lik}}(X, Y) = \text{tr}(XY^{-1}) - \ln|XY^{-1}| - n.$$  

It satisfies (i) and (ii) but it fails to satisfy the triangular inequality.

4. Another interesting choice for $h$ is

$$h_{\text{lnpr}}(X, Y) = \left\{ \ln(\text{tr}(XY^{-1})\text{tr}(YX^{-1})) \right\}^{1/2},$$

that satisfies (iii) and 'almost' satisfies (ii): $h_{\text{lnpr}}(X, Y) = 0 \iff X = cY$, for $c > 0$.

The concept of covariance fields can be used for measuring the difference between distributions on $M$. Let $f$ and $g$ be two densities on $M$ and $\Sigma[f]$ and $\Sigma[g]$ be their respected covariance fields.

For a non-negative $h \in \mathcal{SI}(n)$ we define

$$d_h(f, g) := \int_M h(\Sigma[f](p), \Sigma[g](p))dV(p). \quad (3)$$

When $M$ is a compact, the above integral is well defined and finite. Moreover, if $h(X, Y)$ is a distance function on $\text{Sym}^+_n$, then $d_h$ will be a distance in the space of densities on $M$.

Equation (3) gives a very general but impractical way to compare distributions due to the fact that the integration domain is the whole manifold. For application purposes however, one may restrict to a smaller domain or perform the comparison on discrete set of points which are of particular interest.

3 Two-sample location problem on $S^2$

In this section we make an application of covariance operators to non-parametric distribution comparison. It will serve more illustration purposes rather than strong application ones. The goal is to provide motivating examples showing the new opportunities provided by the proposed covariance structure. We choose to apply simple procedures, as Wilcoxon signed rank and rank sum tests, in order to have a good look and intuition of what happens.
Let \( \{p_{i,1}\}_{i=1}^m \) and \( \{p_{i,2}\}_{i=1}^m \), be random samples from distributions \( F_1 \) and \( F_2 \) on \( S^2 \), respectively, and the two samples be independent of each other.

Fix a point \( q \in M \) and define
\[
\eta^1_i = G(q)\left(\overrightarrow{qp_{i,1}}\right)\left(\overrightarrow{qp_{i,1}}\right)' \quad \text{and} \quad \eta^2_i = G(q)\left(\overrightarrow{qp_{i,2}}\right)\left(\overrightarrow{qp_{i,2}}\right)',
\]
Using tensor notation we can write \( \eta^l_i \in T^1_1(S^2_q) \). The respective sample covariance operators at \( q \) are
\[
\hat{L}^1(q) = \frac{1}{m} \sum_{i=1}^m \eta^1_i \quad \text{and} \quad \hat{L}^2(q) = \frac{1}{m} \sum_{i=1}^m \eta^2_i.
\]
We call \( q \) observation point and basically, what we are going to show is how its choice influences the inference about \( F_1 \) and \( F_2 \).

Fix a tangent vector \( v \in S^2_q \) and consider following (ordinary) random variables
\[
\xi^l_i(v) = \langle v, \eta^l_i(v) \rangle_q \quad \text{and} \quad \xi^2_i(v) = \langle v, \eta^2_i(v) \rangle_q,
\]
where \( \langle \ldots \rangle_q \) is the dot product in the tangent space \( S^2_q \).

**Definition 3** We say that \( F_1 \) and \( F_2 \) have the same location w.r.t. \( q \in S^2 \) and write \( F_1 \overset{\sim}{=} q F_2 \) if for any \( v \in S^2_q \cong \mathbb{R}^2 \), random variables
\[
\xi^l_i(v) = \langle v, (G(q)(\overrightarrow{qX_l})(\overrightarrow{qX_l})') \rangle_q, \quad X_l \sim F_l, \quad l = 1, 2
\]
have the same median.

Under the hypothesis \( H_0 : F_1 \overset{\sim}{=} q F_2 \), for any \( v \), \( \xi^1_i(v) \) and \( \xi^2_i(v) \) are random samples from distributions with equal median.

To test \( H_0 \) we propose two procedures based on the Wilcoxon signed rank test, [17], page 36. Let \( T_{xi}(v) \) be the signed rank statistics based on \( \xi_i(v) \)'s and \( T_{xi} = \max\{T_{xi}(v), v \in \mathbb{R}^2\} \). Then we reject \( H_0 \) when \( T_{xi} \) is sufficiently large.

The second test is based on \( T_d \), the Wilcoxon signed rank statistics for the distances
\[
d^1_l = tr(\eta^1_l(v)) = d^2(q, p_{i,1}) \quad \text{and} \quad d^2_l = tr(\eta^2_l(v)) = d^2(q, p_{i,1}),
\]
where \( d^2 \) stands for the spherical distance, \( d^2(q, p) = \cos^{-1}(\langle q, p \rangle) \).

\(^1T_{xi} = \sum r_is_i, \) where for \( z_i = \xi^1_i - \xi^2_i, s_i = 1\{z_i > 0\} \) and \( r_i \) are the ranks of \( |z_i| \).
If we choose an orthonormal basis \( \{ v_s \}_{s=1}^2 \) of \( S_q^2 \cong \mathbb{R}^2 \) and define
\[
\xi_{i,s}^1 = \langle v_s, \eta_i^1 v_s \rangle_q \quad \text{and} \quad \xi_{i,s}^2 = \langle v_s, \eta_i^2 v_s \rangle_q,
\]
then the following holds: for any \( i = 1, \ldots, m \) and \( l = 1, 2 \)
\[
\sum_{s=1}^2 \xi_{i,s}^l = \sum_{s=1}^2 \langle v_s, \overrightarrow{q p_i} \rangle^2 = ||\overrightarrow{q p_i}||^2 = tr(\eta_i^l(v)) = d_l^i. \tag{4}
\]

It is clear that if \( \xi^1(v_1) \) and \( \xi^2(v_1) \) have the same median and \( \xi^1(v_2) \) and \( \xi^2(v_2) \) also have the same median, then \( \xi^1(v) \) and \( \xi^2(v) \) will have the same median for every \( v \).

\( \{d_{1,i}\} \) and \( \{d_{2,i}\} \) are samples from marginals of \( F_1 \) and \( F_2 \), which under the null hypothesis have the same location. As distances, they are invariant to rotation of the samples \( p_{i,l} \) on the sphere. On the other hand, for any \( l \), \( \{\xi_{i,1}^l\}_i \) and \( \{\xi_{i,2}^l\}_i \) follow two marginal distributions that can be considered projections of \( F_l \) onto two orthogonal axes. As such they form more discriminating set of variables than \( \{d_{i}^l\}_i \).

These observations motivate the following procedure for testing \( H_0 \).

**Test Procedure 1** Let \( \{p_{i,l}\}_{i=1}^m, l=1,2 \) be two random samples, independent of each other.

1. Find the operators \( \eta_i^1 \) and \( \eta_i^2 \) and set
\[
\hat{L}(q) = \hat{L}_1(q) - \hat{L}_2(q) = \frac{1}{m} \sum_{i=1}^m \eta_i^1 - \frac{1}{m} \sum_{i=1}^m \eta_i^2.
\]

2. Let \( \lambda_s \) and \( v_s \) be the eigenvalues and eigenvectors of \( \hat{L}(q) \). Set \( \xi_{i,s} = \langle v_s, \eta_i v_s \rangle_q \).

3. Calculate statistics \( T_{xi,s} \) based on \( \xi_{i,s} \) and set
\[
T_{xi} = \max\{T_{xi,1}, T_{xi,2}\}.
\]

4. Choose a significance level \( \alpha \). If \( pval(T_{xi}) < \alpha/2 \), reject \( H_0 \).

\( ^2 \)We apply Bonferroni correction for the p-value.
Figure 1: Testing $H_0 : F_1 \cong_q F_2$ when $H_0$ is false. Sample examples from $F_1$ (red) and $F_2$ (blue) are given in the left. Observation point $q$, shown in green, is fixed and equals distribution parameter $\mu$. Top right plot shows $T_{xi}$ and $T_d$ statistics along with 1 and 5 percentile lines, while the bottom right plot shows $W_{xi}$ and $W_d$ by their p-values. Test procedure 1 is run 100 times with sample size of 50. $T_{xi}$ clearly outperforms $T_d$ statistics by rejecting the null hypothesis most of the time and the same is true for $W_{xi}$ versus $W_d$.

We also employ the rank sum test (Wilcoxon, Mann and Whitney), [17], page 106, to compare the performance of $\xi_i^l$ and $d_{i,l}$ random variables. For the statistics $W_{xi}$ and $W_d$, we calculate corresponding p-values using large sample approximation. The second test procedure is the same as the first one but uses $W$ instead of $T$ statistics.

Note that if $F_2$ distribution is a rotation of $F_1$ about $q$, then the type II error of $T_d$ statistics will be 1, i.e. the power will be 0.

The way of choosing the basic vectors $v_s$ of $S_q^2$ resembles the Principal Component Analysis (PCA) of the operator $\hat{L}(q)$ and its derivatives like Principal Geodesic Analysis (PGA), introduced by Fletcher, 2004. In the standard setup, PCA is applied on the covariance defined at the (extrinsic or intrinsic) mean point. However, not only the existence of a mean is not guaranteed, but its properties may not be optimal in the context of the test statistic. In contrast, in our approach we allow freedom of choosing the observation point $q$ according to a criteria favoring that statistic.

Figures 1 and 2 show some experimental results using the proposed pro-

\[ W_{xi} = \sum_i r_i, \] where for $r_i$ are the ranks of $\xi_i^1$ in the joint sample $\{\xi_i^1, \xi_i^2\}$.
Figure 2: Performance of $T$ and $W$ statistics when the observation point $q$ varies. In the left plot $q$ is chosen uniformly on the sphere. The experiment confirms a clear advantage for $T_{xi}$. In the right plot preference is given to those observation points for which $tr^2(\hat{L})$ is large. Now $T_d$ is on a par to $T_{xi}$ with both being very high. Corresponding $W_d$ and $W_{xi}$ also have very significant p-values.

For testing $H_0 : F_1 \cong_q F_2$. We consider a family of distributions given by density

$$f(p; a, \mu) \propto \exp(-tr(G(\mu)(\mu\mu^T))^2 - a)^2)$$

(5)

where $\mu$ is a fixed point (not to be mistaken as a mean) and $a$ is a parameter. Top plots show Wilcoxon sign rank statistics $T$, while bottom plots show rank sum statistics $W$. As we see in figure 2 left, where the observation point $q$ varies uniformly on $S^2$, for the majority of positions, $T_{xi}$ and $W_{xi}$ achieve higher p-values than $T_d$ and $W_d$. This result is not isolated and can be repeated for a great variety of distributions besides (5).

How the choice of observation point $q$ affects the relative performance of $T$ and $W$ statistics? We have that

$$d_i^1 - d_i^2 = \sum_{s=1}^{2} (\xi_{i,s}^1 - \xi_{i,s}^2) \text{ and } \frac{1}{m} \sum_{i=1}^{m} (\xi_{i,s}^1 - \xi_{i,s}^2) = \lambda_s,$$

thus

$$\frac{1}{m} \sum_{i=1}^{m} (d_i^1 - d_i^2) = \sum_s \lambda_s.$$
Figure 3: Comparing the performances of $T_{xi}$ and $T_d$ statistics (top) for a fixed pair of samples by varying the observation point. Samples are drawn from $(5)$. Observation points are ordered decreasingly in $\text{det} (\hat{L}(q))$ in the left plot and decreasingly in $\text{tr}^2 (\hat{L}(q))$ in the right. The bottom plot shows the eigenvalues of $\hat{L}(q)$. We note that $T_d$ is the larger statistics and thus, has lower p-values, only when both eigenvalues are strictly positive.

Therefore, if all $\lambda_s$ are of equal sign, the absolute value of the sample expectation of $(d^1_i - d^2_i)$ will be higher than that of $(\xi^1_{i,s} - \xi^2_{i,s})$, for all $s$. In case when the eigenvalues are of different signs the reverse is expected, the absolute value of the sample expectation of $(\xi^1_{i,s} - \xi^2_{i,s})$ for the maximal $|\lambda_s|$ will be higher than that of $(d^1_i - d^2_i)$, which means that $T_{xi}$ is expected to be higher than $T_d$. Of course these considerations are only approximate because the tests for $T$ and $W$ statistics are based on assumptions on the medians not on the means. Nevertheless, we may take the above as a general observation that can be made more formal and rigorous using other appropriate statistical tests.

We provide some experimental evidence confirming the above expectations. For comparison the performance of $T_{xi}$ and $T_d$ we use $\text{det}(\hat{L}(q))$. We expect for $T_d$ to benefit from positive values of $\text{det}(\hat{L}(q))$ and indeed this is the case as seen in figure 3 left. There, for a fixed pair of samples, we calculate and compare $T_{xi}$ and $T_d$ statistics at 50 observation points on the sphere. Then we sort the results such that $\text{det}(\hat{L}(q))$ decreases. In the far left, both $\lambda_1$ and $\lambda_2$ are positive, which leads to a clear advantage for $T_d$. Once the sign of $\text{det}(\hat{L}(q))$ goes negative, the situation reverses.

We also expect that at observation points with high values of $\text{tr}^2(\hat{L})$, all
statistics to be strong in rejecting a false null hypothesis. Some evidence confirming this is shown in figures 2 right and 3 right. \( tr^2(\hat{L}) \) is probably the simplest statistics that measures the difference between the two samples and it is in fact, an application of the similarity invariant function \( h_{trdif} \) as defined in section 2.2.

One can show that \( \hat{L} \) is a continuous field of linear operators on \( S^2 \) (the proof is beyond the scope of the paper). Therefore, if there exists a point \( q \) with \( det(\hat{L}(q)) < 0 \), then that sign is negative on non-vanishing area. Only when samples \( p_{i,l} \) collectively are highly concentrated, the area \( S_+ \) where \( det(\hat{L}(q)) > 0 \) will dominate over \( S_- \), the area where \( det(\hat{L}(q)) < 0 \). In case when \( H_0 \) is false, we expect that \( S_+ < S_- \).

Figure 4 gives another useful way to visualize the sample operator \( \hat{L} \) at different observation points. By choosing a point \( q \), one can draw the projections \( < v, \eta^l_i(v) >_q \) for a set of directions \( v \) spanning a circle to obtain the so called sample profile.

In conclusion, choosing an observation point for comparing locations of two distributions is an important issue since not all positions provide same test performance. Position optimality depends on the statistic applied on the covariance operator. For the projection based statistics we used as examples, optimal observation points can be chosen by maximizing the squared trace of the difference of the covariance operators.

We also showed that distance based statistics have limited performance and in general, employing the whole covariance structure is beneficial.

We also note that most of the presented results do not depend on the specific geometry of the unit sphere and still hold on a general Riemannian manifold.

4 Interpolation of discrete distributions on \( S^2 \)

The second application of the covariance operators we are going to consider is interpolation between discrete distributions on the unit sphere. We suppose that the distributions are defined on a common domain - a fixed set of points on the sphere. The approach we propose is first, to generate an interpolated field based on the covariance fields of the initial distributions and second, to find a probability mass function which covariance field is close to the interpolated one. Closeness is measured using a suitable similarity invariant function. Covariance fields are also considered discrete ones - they are
Figure 4: Two samples of size 50 are drawn from \( f(p; 0.2) \) and \( f(p; 0.3) \) as given by (5). Points \( q_{\text{min}} \) and \( q_{\text{max}} \) are chosen to minimize and maximize \( tr^2(\hat{L}_1 - \hat{L}_2) \). Shown are sample profiles and their difference (right) at these points, defined by the projections \( \xi = \langle v, \eta(v) \rangle \) along 50 directions \( v \) spanning uniformly \([0, 2\pi]\). Profiles of \( \xi^1 \) and \( \xi^2 \) are concentrated and look similar at \( q_{\text{min}} \), but are diffused and very different at \( q_{\text{max}} \). These plots visualize clearly the difference between two extreme observation points.
defined on a finite set of observation points. With a fixed coordinate system at each observation point, not necessarily a global one, the covariance field is represented by a set of matrices. As always, we are going to use the tensor notation to guarantee a coordinate free approach.

Let \( \{ p_i \}_{i=1}^k \) and \( \{ q_i \}_{i=1}^k \) be two sets of \( k \) points on \( S^2 \). The first set is the distribution domain. The second one is the observation set. Hereafter, a discrete mass function (pmf) is any \( k \)-vector \( f \), such that \( f = \{ f_i = f(p_i) \geq 0 \}_{i=1}^k \) and \( \sum_{i=1}^k f_i = 1 \). We write \( f \in P_k^+ \), where \( P_k^+ \) denotes the compact \( k \)-simplex.

The number of observation points may be in fact less than \( k \), the size of the pmfs. However, with a smaller observation set one may lose the uniqueness and the continuity of an estimation. Particular geometric configurations also lead to the same result and one has to check carefully the consistency conditions corresponding to the problem.

The covariance field of \( f \in P_k^+ \) at \( q_j \) is defined as

\[
\Sigma[f]_j := \Sigma[f](q_j) = \sum_{i=1}^k (q_j p_i)(q_j p_i)' r(||q_j p_i||) f(p_i),
\]

where

\[
q_j p_i = \frac{\cos^{-1} < p_i, q_j >}{(1 - < p_i, q_j >^2)^{1/2}} (p_i - < p_i, q_j > q_j).
\]

We use either \( r = 1 \) or

\[
r(t) = \left(1 - \frac{\pi}{2t}\right)^2.
\]

The second choice is known to be optimal on \( S^2 \) in the class of functions \( r_a(t) = (1 - \frac{\pi}{2t})^2 \) because it minimizes the maximum of \( tr(G\Sigma(q)) \).

Let \( f^s, s=1,...,m \), be a collection of pmfs and 

\[
\{ C_j^s = \Sigma[f^s]_j \}_{j=1}^k, s = 1, ..., m,
\]

be their covariance fields.

For a non-negative similarity invariant function \( h \), we define

\[
d_h(f, f^s) := \sum_{j=1}^k h(\Sigma[f]_j, C_j^s), s = 1, ..., m.
\]
For $\alpha \in P^+_m$, i.e. $\alpha = \{\alpha_s\}_{s=1}^m$, such that $\alpha_s \geq 0$ and $\sum_s \alpha_s = 1$, we define the functional

$$H(f; \alpha) := \sum_{s=1}^m \alpha_s d_h(f, f^s).$$  \hspace{1cm} (8)$$

Then we formulate the following optimization problem: find a probability mass function $\hat{f}$ such that

$$\hat{f}(\alpha) = \arg\min_f H(f; \alpha).$$  \hspace{1cm} (9)$$

Below we show some results regarding the consistency of the estimators.

**Lemma 1** Let $h \in \text{SIM}(n)$, $\alpha_s \in P^+_M$ and $f^s \in P^+_k$. If $\alpha_s \to \alpha_0$ and $f^s \to f^0$ (in $L_2$ norm), then

$$H(f^s, \alpha_s) \to H(f^0, \alpha_0).$$

**Proof.** Observe that

$$|H(f^s; \alpha_s) - H(f^0; \alpha_0)| \leq |H(f^s; \alpha_s) - H(f^*; \alpha_0)| + |H(f^*; \alpha_0) - H(f^0; \alpha_0)|.$$

Since $H(f; \alpha_0)$ is continuous in $f$, the second term above goes to zero. The first term is bounded by

$$|H(f^s; \alpha_s) - H(f^*; \alpha_0)| \leq ||\alpha_s - \alpha_0||_{L_2} \max_{j,m} h(\Sigma[f^j], C^s_j).$$

The sets $\{\Sigma[f^j]| f \in P^+_k\}$ are compact in $\text{Sym}^+_n$ and $h$ is continuous, therefore $\max_{j,m} h(\Sigma[f^j], C^s_j) = C < \infty$ and

$$H(f^s; \alpha_s) \to H(f^*; \alpha_0).$$

□

For a sequence $\alpha_s$, define $\hat{f}^s = \arg\min_f H(f; \alpha_s)$. We have the following

**Lemma 2** If $h \in \text{SIM}(n)$ and $\alpha_s \to \alpha_0$, then

$$H(\hat{f}^s, \alpha_s) \to H(\hat{f}^0, \alpha_0).$$  \hspace{1cm} (10)
Proof. Since $P_k^+$ is a compact any sub sequence of $f^s$ has a point of convergence in $P_k^+$. Without loss of generality we may assume that $\hat{f}^s \to g \in P_k^+$. Accounting for the minimizing properties of $\hat{f}$ and applying lemma [1] we can write

$$H(\hat{f}^0, \alpha_s) \geq H(f^s, \alpha_s) \to H(g, \alpha_0) \geq H(\hat{f}^0, \alpha_0).$$

Because of $H(\hat{f}^0, \alpha_s) \to H(\hat{f}^0, \alpha_0)$ we have (10). □

Unfortunately, (10) is not enough to claim that $\hat{f}^s \to \hat{f}^0$. However, if $H(f; \alpha_0)$ has a well separated minimum at $\hat{f}^0$ we indeed have the wanted consistency.

**Corollary 1** $\hat{f}(\alpha)$ is continuous at all $\alpha$ for which $H(f, \alpha)$ has a well separated (global) minimum.

Another problem is how to find the global minimum $\hat{f}$ of $H(f; \alpha)$, provided it is unique. We know that the minimum is easily found in case of convex function $H$, by gradient descent algorithm for example. Moreover, the convexity of $H(f; \alpha_0)$ in $P_k^+$ guarantees the well separability of its minimum and that gives us the desired consistency.

**Proposition 1** If $\alpha_s \to \alpha_0$ and $h \in STM(n)$ is such that $H(f; \alpha_0)$ is convex in $P_k^+$, then

$$\hat{f}^s \to \hat{f}^0.$$  \hspace{1cm} (11)

Proof. Suppose the contrary of (11), that there exists $g \in P_k^+$, and sub sequence $\hat{f}^s \to g$, such that $||\hat{f}^0 - g|| > 0$. Then $H(g; \alpha_0) > H(\hat{f}^0; \alpha_0)$ by the separability of the minimum. But $H(\hat{f}^s; \alpha_s) \to H(g; \alpha_0)$ by lemma [1] and $H(\hat{f}^s; \alpha_s) \to H(\hat{f}^0; \alpha_0)$ by lemma [2] which imply $H(g; \alpha_0) = H(\hat{f}^0; \alpha_0)$. The contradiction proves the claim. □

### 4.1 Linear Interpolation

Consider first one of the simplest similarity invariant functions $h^2_{trdif}(\cdot, \cdot; G^{-1})$. The corresponding optimization functional is

$$H_{trdif}(f, \alpha) = \sum_{s=1}^m \alpha_s \sum_{j=1}^k tr^2(G(q_j)\Sigma[f]_{j} - G(q_j)C^s_{j}).$$
Denote $a_{ij} = \text{tr}(G(q_j)(\overrightarrow{q_jp_i})'(\overrightarrow{q_jp_i})) = d^2(q_j, p_i)$ and $c^s_j = \text{tr}(G(q_j)C^s_j)$, then

$$H_{tr dif}(f, \alpha) = \sum_{s=1}^{m} \alpha_s \sum_{j=1}^{k} (\sum_{i} a_{ij} f_i - c^s_j)^2.$$ We have

$$\frac{\partial H_{tr dif}}{\partial f_i} = 2 \sum_{s=1}^{m} \alpha_s \sum_{j=1}^{k} a_{ij} (\sum_{l} a_{lj} f_l - c^s_j).$$

The second partial derivatives are

$$\frac{\partial^2 H_{tr dif}}{\partial f_i \partial f_l} = 2 \sum_{s=1}^{m} \alpha_s \sum_{j=1}^{k} a_{ij} a_{lj}$$

Let $w = \{w_i\} \in \mathbb{R}^k$, then

$$\sum_{i,l} w_i w_l \frac{\partial^2 H_{tr dif}}{\partial f_i \partial f_l} = 2 \sum_{s=1}^{m} \alpha_s \sum_{j=1}^{k} (\sum_{i=1}^{k} w_i a_{ij})^2 \geq 0.$$ Therefore, if the matrix $A = \{a_{ij}\}_{i=1,j=1}^{k,k}$ is of full rank $k$, then $H_{tr dif}$ is convex in $P^+_k$. Moreover, the optimal solution of (9) satisfies

$$\sum_{i} a_{ij} f_i = \sum_{s=1}^{m} \alpha_s c^s_j, j = 1, ..., k,$$

with a unique solution

$$\hat{f} = \sum_{s=1}^{m} \alpha_s f^s,$$

since for every $s$ and $j$, $\sum_{i} a_{ij} f^s_i = c^s_j$.

Thus, we showed the following

**Proposition 2** If the matrix $A$ has full rank, $\text{rank}(A) = k$, then the linear interpolation is the unique solution of the optimization problem (9) for $H_{tr dif}$.

### 4.2 Non-Linear Interpolations

Consider similarity invariant function $h_{tr ln}$ and corresponding optimization functional $H_{tr ln}$

$$H_{tr ln}(f; \alpha) = \sum_{s=1}^{m} \alpha_s \sum_{j=1}^{k} \text{tr}(\ln^2(\Sigma[f]_j(C^s_j)^{-1})).$$
The value of $H_{trln2}(f)$ is small when $G(q_j)\Sigma[f]_j$ is close to covariance operators $G(q_j)C_j^s$ for all $j$ and $s$. This is a much stronger condition than the requirement for their traces to be close as in the problem of minimizing $H_{trdif}$. Consequently the minimum of $H_{trln2}(f)$, in general, will be strictly positive and the optimal pmf will be different from the linear interpolation.

Experiments show great improvement in convergence of gradient descent algorithm for problem (9), when instead of the generic covariance one uses the second choice (6).

Define the operators

$$Z_{ij}^s = (q_j p_i)(q_j p_i)'(1 - \frac{\pi^2}{2||q_j p_i||})^2(C_j^s)^{-1}$$

and set $Y_j^s = \sum_i f_i Z_{ij}^s$. The gradient of $H_{trln2}$ is

$$\nabla H_{trln2}(f, \alpha) = \{ f_i \sum_{s=1}^m \alpha_s \sum_{j=1}^k \frac{tr(ln(Y_j^s)Z_{ij}^s)}{tr(Z_{ij}^s)} \}_{i=1}^k.$$ 

The optimization problem (9) is solved by gradient descent algorithm, which shows relatively fast convergence, unfortunately not always to the global minimum, because $H_{trln2}(f, \alpha)$ is not convex in $f \in P_k^+$. Log-likelihood function gives us another choice for $H$,

$$H_{lik}(f; \alpha) = \sum_{s=1}^m \alpha_s \sum_{j=1}^k \{ tr(\Sigma[f]_j(C_j^s)^{-1}) - ln|\Sigma[f]_j(C_j^s)^{-1}| - n \} =$$

$$\sum_{s=1}^m \alpha_s \sum_{j=1}^k \{ tr(Y_j^s) - ln|Y_j^s| - n \}.$$ 

The gradient of $H_{lik}$ is

$$\nabla H_{lik}(f; \alpha) = \{ f_i \sum_{s=1}^m \alpha_s \sum_{j=1}^k \frac{tr((Y_j^s - I_n)Z_{ij}^s)}{tr(Z_{ij}^s)} \}_{i=1}^k.$$ 

Note that $h_{lik}$ is neither symmetric nor satisfies the triangular inequality, but its importance is determined by the relation to normal distributions and its analytical properties. Define the matrix

$$B = \{ b_{ij} = (d(q_j, p_i) - \frac{\pi}{2})^2 \}_{i=1,j=1}^{k,k}.$$ 

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Proposition 3 If $B$ has full rank, $\text{rank}(B) = k$, then for all $\alpha$, $H_{lik}(f; \alpha)$ is a convex function in $P_k^+$.

Proof. We have

$$\frac{\partial H_{lik}}{\partial f_i} = \sum_{s=1}^{m} \alpha_s \sum_{j=1}^{k} \text{tr}(Z_{ij}^s - Z_{ij}^s(Y_j^s)^{-1}).$$

and

$$\frac{\partial^2 H_{lik}}{\partial f_i \partial f_l} = \sum_{s=1}^{m} \alpha_s \sum_{j=1}^{k} \text{tr}(Z_{ij}^s(Y_j^s)^{-1}Z_{lj}^s(Y_j^s)^{-1}).$$

We want to show that the matrix of second partial derivatives is positive definite. Let $w = \{w_i\} \in \mathbb{R}^k$ and $w \neq 0$, then

$$\sum_{i,l} w_i w_l \frac{\partial^2 H_{lik}}{\partial f_i \partial f_l} = \sum_{s=1}^{m} \alpha_s \sum_{j=1}^{k} \text{tr}(\sum_{i=1}^{k} w_i Z_{ij}^s(Y_j^s)^{-1})^2 > 0,$$

since by the assumption for $B$, for at least one $j$, $\sum_{i=1}^{k} w_i Z_{ij}^s \neq 0$. □

The rank of $B$ can be calculated using the pairwise distances between $q$ and $p$ points and only in very special circumstances this rank will be less than $k$. More formally, if a random process chooses the points, then

$$P(\text{rank}(B) < k) = 0.$$

4.3 Examples and conclusions

Figure 5 shows interpolation between two pmfs of size 6 ($m = 2, k = 6$) applying $h_{\text{trln2}}$. We compare it to the linear and the square root interpolations. Square root interpolation, as suggested by the name, relies on the observation that for a pmf $f \in P_k^+$, $\sqrt{f} = (\sqrt{f_1}, ..., \sqrt{f_k}) \in S^k$. Then one finds

$$\hat{p} = \arg\min_{p \in S^k} \sum_s \alpha_s d^2(p, \sqrt{f}^s)$$

and sets $\hat{f}_{\text{sqrt}} = \hat{p}^2$. (12)

It is also informative to compare the Mean-Squared Error (MSE) between different interpolations. It is defined by

$$\text{MSE}(\hat{f}) = \sum_{s=1}^{2} \alpha_s \sum_{i=1}^{k} (\hat{f}_i - f_i^s)^2.$$
Figure 5: Two examples of interpolation of pmfs on $S^2$ using $h_{trln2}$. The linear and square root (see (12)) interpolations are also given for reference. Top plots show $H_{trln2}$ and $H_{lik}$ for the three interpolations. Bottom plots show corresponding MSEs (see (13)) in the left and FAs (see (14)) in the right.

Linear and square root interpolations, by their nature, are very close in MSE, but very different from $\hat{f}_{trln2}(\alpha)$, which manifests the non-linear origin of the latter.

Another performance criteria relevant to the study of spherical data is the Fractional Anisotropy (FA). Let $\{\lambda_i\}_{i=1}^n$ be the eigenvalues of $\sum_{i=1}^k \overrightarrow{p}_i \overrightarrow{p}_i' f_i$, where $\overrightarrow{p}_i$ are considered vectors in $\mathbb{R}^3$ (thus $FA$ is defined only for distributions on $S^2$). Then we define

$$FA(f) = \left\{ \frac{n}{n-1} \sum_{i=1}^n (\lambda_i - \bar{\lambda})^2 / \sum_{i=1}^n \lambda_i^2 \right\}^{1/2}. \quad (14)$$

Fractional Anisotropy measures a distribution concentration. The higher FA the more concentrated it is about particular axes. A uniform distribution has $FA = 0$. As we may expect the linear interpolation substantially reduces the FA index, $h_{trln2}$-based one however, is more conservative and manage to sustain higher FA. Preserving the concentration factor is of importance for processing ODFs in HARDI, and the empirical evidence for the good FA performance of $h_{trln2}$ is encouraging.

A second set of examples in figure 6 illustrates interpolation based on the likelihood function, $h_{lik}$. As we showed, this choice guarantees the convexity
of $H_{lik}$ and thus the continuity of the optimal solution $\hat{f}_{lik}(\alpha)$.

The likelihood based interpolation $\hat{f}_{lik}$ exhibits behaviour similar to that of $\hat{f}_{trln2}$. Again, it is very distinguished from the linear and the square-root one and tends to preserve the anisotropy.

5 Summary

The main goal of this article is to introduce covariance operator fields and provide some arguments showing their potential and usefulness.

There is a covariance field associated with any distribution on a Riemannian manifold. It defines a linear operator on the tangent space of each point on the manifold. By applying a similarity invariant to that operator field one can obtain a scalar field that represents the distribution. It reveals important spatial characteristics of the distribution. Similarity invariants can also be used for comparing and interpolating distributions.

We demonstrated several non-parametric procedures for solving a two-sample location problem on the sphere and showed how covariance operator fields can be used for locating observation points that maximize test performance.

We also implemented two non-linear procedures for interpolating distributions on the sphere and compared them to the linear and square-root
interpolations. The proposed approach is general enough to allow a great variety of choices and promises a good application potential.

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