Measures of goodness of fit obtained by canonical transformations on Riemannian manifolds

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Abstract

The standard method of transforming a continuous distribution on the line to the uniform distribution on [0, 1] is the probability integral transform. Analogous transforms exist on compact Riemannian manifolds, \( X \), in that for each distribution with continuous positive density on \( X \), there is a continuous mapping of \( X \) to itself that transforms the distribution into the uniform distribution. In general, this mapping is far from unique. This paper introduces the construction of a version of such a probability integral that (under mild conditions) is canonical. The construction is extended to shape spaces, simply-connected spaces of non-positive curvature, and simplices.

The probability integral transform is used to derive tests of goodness of fit from tests of uniformity. Illustrative examples of these tests of goodness of fit are given involving (i) Fisher distributions on \( S^2 \), (ii) isotropic Mardia–Dryden distributions on the shape space \( \Sigma^2 \). Their behaviour is investigated by simulation.

Keywords: Cartan–Hadamard manifold, Compositional data, Directional statistics, Exponential map, Probability integral transform, Shape space, Simplex.

1 Introduction

Directional statistics, shape analysis and compositional data analysis are concerned with probability distributions on Riemannian manifolds, shape spaces and simplices, respectively. The aim of this paper is to introduce and explore a canonical method of constructing transformations from such
manifolds, \( \mathcal{X} \), to certain associated manifolds, \( \mathcal{Y} \), that send arbitrary continuous distributions on \( \mathcal{X} \) into standard distributions on \( \mathcal{Y} \). More precisely, \( \mathcal{Y} \) is \( \mathcal{X} \) itself, or a tangent space to \( \mathcal{X} \), or a star-shaped open subset of a tangent space. Given a basepoint \( x \) in \( \mathcal{X} \) and a standard continuous distribution, \( \nu \), on \( \mathcal{Y} \), for any continuous distribution, \( \mu \), on \( \mathcal{X} \), we construct a function \( \phi: \mathcal{X} \to \mathcal{Y} \) that is an almost-diffeomorphism (a diffeomorphism on the complement of some null set) that sends \( \mu \) to \( \nu \). Under mild conditions on uniqueness of medians of \( \mu \) and of some distributions derived from it, \( \phi \) as constructed here is canonical (in that any two versions differ only on a null set). These almost-diffeomorphisms, \( \phi \), are used to obtain tests of goodness of fit to \( \mu \) from tests of goodness of fit to \( \nu \). If \( \mathcal{X} \) is a compact Riemannian manifold then we can take \( \mathcal{Y} = \mathcal{X} \), \( \nu \) as the uniform distribution, and \( \phi \) can be regarded as a form of probability integral transformation. On compact manifolds our tests of goodness of fit complement the general Wald-type tests of Beran [1], the score tests of Boulerice and Ducharme [3] and the Sobolev tests of Jupp [12], as well as the more specific tests in [18, 24, 5, 2] (see [23, Section 12.3]) and in [10, Section 4.2], [26] and [13, Section 4.4] in the case of copulae.

One important class of models on compact Riemannian manifolds \( \mathcal{X} \) for which there is a canonical function \( \phi: \mathcal{X} \to \mathcal{X} \) that takes any given distribution to the uniform distribution consists of those transformation models that are obtained from the uniform distribution by the action of some group \( G \) on \( \mathcal{X} \), i.e., the distribution of \( x \) in \( \mathcal{X} \) under parameter \( g \) in \( G \) is that of \( gx \), where \( x \) is uniformly distributed and \( gx \) denotes the image of \( x \) under \( g \). Then \( \phi(x) = g^{-1}x \). An example is the angular central Gaussian distributions on the real projective space \( \mathbb{R}^{p-1} \) with probability density functions

\[
f(\pm x; A) = |A|^{-1/2}(x^T A^{-1}x)^{-p/2}, x \in \mathbb{R}^p,
\]

where \( A \) is a non-singular symmetric \( p \times p \) matrix and we may suppose that \( |A| = 1 \); see [23, Section 9.4.4]. Then \( \phi(\pm x) = \pm\|A^{-1/2}x\|^{-1}A^{-1/2}x \). For general \( A \), this transformation is different from that constructed in Section 2.2. If \( A \) has only 2 distinct eigenvalues then the two transformations are the same; see (b) after Remark 1.

The canonical transformations, \( \phi \), are introduced in Section 2, first for spheres and then for compact Riemannian manifolds, shape spaces, Cartan–Hadamard manifolds and simplices. Section 3 shows how these transformations send general tests of uniformity (or of goodness of fit to some standard distribution) into general tests of goodness of fit. The behaviour of these goodness-of-fit tests is illustrated in Section 4 by some simulation studies on
the sphere, $S^2$, and on the shape space, $\Sigma^5_2$.

2 Canonical transformations

2.1 Spheres

Let $X$ be a random variable on the unit circle and suppose that an orientation and an initial direction on the circle have been chosen. Then the probability integral transformation of the distribution is the transformation of the circle which sends $\theta$ to $U$, where $U = 2\pi \Pr(0 < X \leq \theta)$. If the distribution of $X$ is continuous then $U$ is distributed uniformly on the circle. Thus the probability integral transformation can be used to transform any test of uniformity into a corresponding test of goodness of fit (see [23, Section 6.4]). For continuous distributions (with positive density) $\mu$, on $S^{p-1}$, the unit sphere in $\mathbb{R}^p$, with $p > 2$, there are analogues $\phi : S^{p-1} \to S^{p-1}$ of the probability integral transformation that transform $\mu$ into the uniform distribution, $\nu$. Such $\phi$ are far from unique, since if $\psi : S^{p-1} \to S^{p-1}$ preserves $\nu$ then the composite function $\psi \circ \phi : S^{p-1} \to S^{p-1}$ also transforms $\mu$ into $\nu$.

Homeomorphisms $\psi$ that preserve $\nu$ can be constructed from embeddings $\gamma : D^{p-1} \to S^{p-1}$ that map the uniform distribution on the disc, $D^{p-1}$, to the uniform distribution on $\gamma(D^{p-1})$, together with functions $t \mapsto U_t$ from $[0, 1]$ to the rotation group $SO(p - 1)$ with $U_t = I_3$ for $t$ near 0 or 1. Then $\psi$ is the identity outside $\gamma(D^{p-1})$ and is given by $\psi\{\gamma(r, \theta)\} = \gamma(r, U_r(\theta))$ on $\gamma(D^{p-1})$, where $(r, \theta)$ are polar coordinates on $\gamma(D^{p-1})$.

Our construction of canonical versions of the probability integral transformation $\phi$ on $S^{p-1}$ is based on a set $S^{p-1} \supset S^{p-2} \supset \ldots \supset S^s$ of nested spheres for which

$$S^{k-1}$$

constitutes the great sphere in $S^k$ normal to $m_k$ in $S^k$, for $k = p - 1, \ldots, s + 1$, (2)

where $m_k$ is some point in $S^k$. The tangent-normal decomposition [23, (9.1.20)] expresses each $x$ in $S^k$ as

$$x = t m_k + \sqrt{1 - t^2} u$$

(3)

$$= \cos(r) m_k + \sin(r) u,$$

(4)

where $t = x^\top m$, $u \in S^{k-1}$, the sphere normal to $m_k$, and $r = \arccos t$ is the colatitude of $x$. The function $p_k : x \mapsto u$ sends $S^k \setminus \{\pm m_k\}$ into $S^{k-1}$, so that, given a distribution $\mu$ on $S^{p-1}$, we can define distributions $\mu_{p-1}, \ldots, \mu_s$ on $S^{p-1}, S^{p-2}, \ldots, S^s$ recursively by $\mu_{p-1} = \mu$ and $\mu_{k-1}$ as the marginal
distribution of \( u \) on \( S^{k-1} \) for \( k = p - 1, \ldots, s + 1 \). We shall assume that

\[
\mu \text{ is either uniform or has a unique (Fréchet) median } \mathbf{m}_{p-1}, \tag{5}
\]

for \( k = p - 2, \ldots, s + 1, \mu_k \text{ has a unique median } \mathbf{m}_k, \tag{6} \]

\( \mu_s \) is the uniform distribution on \( S^s \). \( \tag{7} \)

If \( \mu_1 \) has a unique median \( \mathbf{m}_1 \) then \( \mu_0 \) is automatically the uniform distribution on \( S^0 \). The nested spheres in (2) are reminiscent of the principal nested spheres of [11] but, whereas principal nested spheres may be small spheres and are chosen to give closest fit to the data, the spheres in (2) are great spheres and are chosen to be orthogonal to \( \mathbf{m}_{p-1}, \ldots, \mathbf{m}_{s+1} \). In cases in which (5)–(7) hold, Proposition 1 provides a canonical version of the probability integral transformation on \( S^{p-1} \).

**Proposition 1**

Let \( \mu \) be a probability distribution on \( S^{p-1} \) such that the density of \( \mu \) with respect to the uniform distribution, \( \nu \), is continuous and positive. Suppose that \( \mu \) satisfies conditions (5)–(7). Then homeomorphic almost-diffeomorphisms \( \phi_k : S^k \rightarrow S^k \) for \( k = s, \ldots, p - 1 \) can be defined inductively by (a) \( \phi_s \) is the identity, (b) for \( k = s + 1, \ldots, p - 1 \),

\[
\phi_k(r, u) = \psi_k|\phi_{k-1}(u)(r) \phi_{k-1}(u), \tag{8}
\]

where

\[
\psi_k|u = \tilde{F}_u^{-1} \circ F_u
\]

with

\[
F_u(v) = \Pr(0 < R \leq v | U = u) \text{ under } \mu_k \tag{9}
\]

\[
\tilde{F}_u(v) = \Pr(0 < R \leq v | U = u) \text{ under } \nu_k \tag{10}
\]

for \( 0 < v \leq \pi \), points \( x \) in \( S^{k+1} \) are identified with their coordinates \((r, u)\) as in (4). \((R, U)\) denotes a random element of \( S^{k+1} \), and \( \nu_k \) is the uniform distribution on \( S^k \). Then \( \phi_{p-1} \) is a homeomorphic almost-diffeomorphism that transforms \( \mu \) into \( \nu \).

**Proof**

From (20) and continuity of the density, \( \phi_k \) is a homeomorphism of \( S^k \) and its restriction to \( S^k \setminus \{\pm \mathbf{m}_k\} \) is a diffeomorphism. It is straightforward to show that \( \phi_{p-1} \) transforms \( \mu \) into \( \nu \). \( \square \)
2.2 Compact Riemannian manifolds

We now show how the probability integral transformation can be extended to arbitrary compact Riemannian manifolds in a canonical way.

Let $\mathcal{X}$ be a compact Riemannian manifold. The Riemannian metric determines the volumes of infinitesimal cubes, and so equips $\mathcal{X}$ with a unique uniform probability measure, $\nu_\mathcal{X}$. Let $\mu$ be a probability distribution on $\mathcal{X}$ having continuous positive density with respect to $\nu_\mathcal{X}$. If $\mathcal{X}$ is connected then there are homeomorphisms of $\mathcal{X}$ that transform $\mu$ into $\nu_\mathcal{X}$; see [13, Proposition 1]. One way of constructing such homeomorphisms, $\phi$, is by using the multivariate probability integral transformation (alias Rosenblatt transformation, [27]) in coordinate neighbourhoods, as in the first proof in [25]. In the case in which the density is smooth, there is also a slick differential-geometric proof [25, Theorem 2]. This proof can be used to provide a canonical choice of $\phi$ but this involves solving a differential equation and does not give $\phi$ explicitly. If $\mathcal{X} = S^1$ or $\dim \mathcal{X} > 1$ then, as in the spherical case, the homeomorphism $\phi$ is far from unique and it is not obvious how to make a canonical choice of $\phi$. To obtain a canonical choice of $\phi$ by extending the construction in Proposition 1 to compact Riemannian manifolds, we exploit the fact that, if $\mathcal{X}$ is a Riemannian manifold and $m$ is any point in $\mathcal{X}$ then the exponential map (see e.g., [8, Section 1.6]) from the tangent space, $T\mathcal{X}_m$, at $m$ into $\mathcal{X}$ defines a system of Riemannian normal coordinates around $m$ as follows. The inverse of this coordinate system maps the open set $\{(r, u) : 0 \leq r < r_u, u \in T_1\mathcal{X}_m\}$ diffeomorphically onto an open set $B$ of $\mathcal{X}$ by

$$ (r, u) \mapsto \exp(ru), \quad (11) $$

where $T_1\mathcal{X}_m$ denotes the set of unit tangent vectors at $m$ and $r_u = \sup\{r : \text{there is a unique minimising geodesic from } m \text{ to } \exp(ru)\}$.

For $\mathcal{X} = S^{p-1}$, the tangent-normal decomposition [3] is related to the normal coordinates by $t = \cos r$. If $\mathcal{X}$ is compact then $\mathcal{X}\setminus B$ has measure zero. See, e.g., [6, Proposition 2.113, Corollary 3.77, Lemma 3.96]. Thus absolutely continuous probability distributions on $\mathcal{X}$ can be identified with absolutely continuous probability distributions on $\{(r, u) : 0 \leq r < r_u, u \in T_1\mathcal{X}_m\}$. In particular, such a distribution induces a marginal distribution on $T_1\mathcal{X}_m$.

**Proposition 2**

Let $\mu$ be a probability distribution on a compact Riemannian manifold $\mathcal{X}$ of dimension $d$ such that the density of $\mu$ with respect to the uniform distribution, $\nu$, is continuous and positive. Suppose that $\mu$ is
either uniform or has a unique median, \( m \). If \( \mu \) is the uniform distribution then define \( \phi : \mathcal{X} \to \mathcal{X} \) as the identity. If \( \mu \) is non-uniform then let \( \{(r, u) : 0 \leq r < r_u, u \in T_1\mathcal{X}_m\} \) be (maximal) Riemannian normal coordinates on \( B \) with \( m \) corresponding to the origin. Assume that the marginal distributions on \( T_1\mathcal{X}_m \) obtained from \( \mu \) and \( \nu \) by using (11) satisfy conditions (5)–(7).

Define the function \( \phi : \mathcal{X} \to \mathcal{X} \) by

\[
\phi \{\exp(ru)\} = \exp\left[\tilde{F}^{-1}_{\psi_{d-1}(u)} \{F_u(r)\} \psi_{d-1}(u)\right] \quad ru \in \exp^{-1}(B) \tag{12}
\]

and arbitrarily on \( \mathcal{X} \setminus B \), where \( F_u \) and \( \tilde{F}_u \) are defined by (21) and (10), \( \psi_{d-1} = \tilde{\phi}_{d-1} \circ \phi_{d-1} \) with \( \phi_{d-1}, \tilde{\phi}_{d-1} : T_1\mathcal{X}_m \to T_1\mathcal{X}_m \) being the canonical uniformising almost-diffeomorphisms corresponding to \( \mu \) and \( \nu \), respectively, given by Proposition 1 and identification of \( T_1\mathcal{X}_m \) with \( S^{d-1} \). Then \( \phi \) is a diffeomorphism almost everywhere and transforms \( \mu \) into \( \nu \).

**Proof**

This is a straightforward calculation. \( \square \)

**Example**

The torus, \( S^1 \times S^1 \), can be written as \([-\pi, \pi] \times [-\pi, \pi] \), where \(-\pi\) and \(\pi\) are identified. Then \( B \) can be taken as \((-\pi, \pi) \times (-\pi, \pi)\) and

\[
r_u = \pi / \max\{|\cos(u)|, |\sin(u)|\} \quad u \in [0, 2\pi].
\]

We call the almost-diffeomorphism \( \phi \) of Propositions 1 or 2 the **probability integral transformation**. It is canonical, since it is determined (except on null sets) by unique medians at each stage.

**Remark 1**

The appropriate general mathematical setting for the constructions in Propositions 1 and 2 is that of orthonormal frames in a tangent space. An orthonormal frame at a point \( m \) in a \( d \)-dimensional manifold \( \mathcal{X} \) is an ordered set of orthonormal vectors in the tangent space \( T\mathcal{X}_m \). Let \( \mu \) be a probability distribution on \( \mathcal{X} \) such that the density of \( \mu \) with respect to the uniform distribution, \( \nu \), is continuous and positive. Let \( (m_{d-1}, \ldots, m_{s+1}) \) be an orthonormal frame at \( m \) and suppose that the distribution on the \( u \)-sphere normal to \( m_{d-1}, \ldots, m_{s+1} \) is uniform. Then replacing the successive medians in Propositions 1 and 2 by \( m, m_{d-1}, \ldots, m_{s+1} \) defines an almost-diffeomorphism \( \phi \) of \( \mathcal{X} \) that takes \( \mu \) to \( \nu \). \( \square \)
A class of distributions for which the probability integral transformation takes a particularly simple form consists of those with unique median \( m \) on \( X \) and for which the corresponding marginal distribution on \( T_{1 \cdot X_m} \) (obtained using (11)) is uniform. If \( X \) is the sphere \( \mathbb{S}^{p-1} \), the projective space \( \mathbb{R}P^{p-1} \), the rotation group \( SO(3) \) or the complex projective space \( \mathbb{C}P^{k-2} \), then these include the distributions that have rotational symmetry about the unique median. Some examples are:

(a) For a distribution \( \mu \) on \( \mathbb{S}^{p-1} \) that is rotationally symmetric about a unit vector \( \mu \), the transformation \( \phi \) given by (12) that sends \( \mu \) into the uniform distribution has the form

\[
\phi(x) = u\mu + \sqrt{(1-u^2)/(1-t^2)} \left( I_p - \mu\mu^\top \right) x, \quad (13)
\]

where \( t = x^\top \mu \), \( I_p \) denotes the \( p \times p \) identity matrix and

\[
u = G_0^{-1}(G_\mu(t)), \quad (14)
\]

\( G_\mu \) and \( G_0 \) denoting the cumulative distribution functions of \( x^\top \mu \) when \( x \) has distribution \( \mu \) and the uniform distribution, respectively. In particular, for the Fisher distribution, \( F(\mu, \kappa) \), on \( S^2 \) with mean direction \( \mu \) and concentration \( \kappa \),

\[
u = \left( 2e^{\kappa t} - e^\kappa - e^{-\kappa} \right) / \left( e^\kappa - e^{-\kappa} \right), \quad \kappa > 0 \quad (15)
\]

and \( u = t \) for \( \kappa = 0 \) (see [13, Example 1]).

(b) Among the angular central Gaussian distributions on the real projective space \( \mathbb{R}P^{p-1} \) with probability density functions (1), those that are symmetrical about the modal axis \( \pm \mu \) have \( A = a \mu\mu^\top + b (I_p - \mu\mu^\top) \) with \( a > b > 0 \). Then \( \phi \) is given by

\[
\phi(\pm x) = \pm \left\{ u\mu + \sqrt{(1-u^2)/(1-t^2)} \left( I_p - \mu\mu^\top \right) x \right\},
\]

where \( t = x^\top \mu \) and

\[
u = t/\sqrt{a/b + (1-a/b)t^2}.
\]

The transformation \( \phi \) coincides with the standard transformation \( \pm x \mapsto \pm \| A^{-1/2}x \|^{-1} A^{-1/2}x \) to uniformity on \( \mathbb{R}P^{p-1} \) [23, Section 9.4.4].
(c) For the matrix Fisher distribution on $SO(3)$ with density proportional to $\exp \left\{ \text{tr} \left( \kappa X^\top M \right) \right\}$ for $\kappa \geq 0$ and $M$ in $SO(3)$, Example 2 shows that $M^\top X$ and $M^\top \phi(X)$ have the same rotation axis, and that the rotation angle, $u$, of $M^\top \phi(X)$ is related to the rotation angle, $t$, of $M^\top X$ by

$$
\tilde{F}_0(u)/\tilde{F}_0(\pi) = \tilde{F}_\kappa(t)/\tilde{F}_\kappa(\pi),
$$

where $\tilde{F}_\kappa(\theta) = \int_0^\theta e^{4\kappa \cos^2(\omega/2)} \sin^2(\omega/2) d\omega$.

(d) On the shape space $\Sigma^k_2$ of $k$ non-identical labelled landmarks in $\mathbb{R}^2$, the isotropic Mardia–Dryden distributions, alias isotropic offset normal distributions, $MD([\mu], \kappa)$ [4, Section 11.1.2] of shapes $[X]$ obtained by isotropic Gaussian perturbation of the landmarks of shapes $[\mu]$ have densities

$$
f([X]; [\mu], \kappa) = e^{-\kappa(1-\cos^2(\rho([X],[\mu])))} \mathcal{L}_{k-2}(-\kappa \cos^2(\rho([X],[\mu]))) \tag{16}
$$

where $\mathcal{L}_{k-2}$ is the Laguerre polynomial of order $k-2$, $\rho$ is the Riemannian shape distance and $\kappa$ is a concentration parameter [4, equations (11.11), (11.15)]. Identification of $2 \times (k-1)$ real matrices $Z$ satisfying $\text{trace}(ZZ^\top) = 1$ with unit vectors $z$ in $\mathbb{C}^{k-1}$ leads to identification of the space $\Sigma^k_2$ with the complex projective space $\mathbb{C}P^{k-2}$. Calculation shows that for the distribution with density (16), the homeomorphism $\phi$ is

$$
\phi([z]) = [u\mu + \sqrt{(1-u^2)/(1-t^2)} \left\{ z - (z^\top \mu)\mu \right\}],
$$

where $t = \cos(\rho([X],[\mu]))$, $u^2 = F_{[X],0}^{-1} \left\{ F_{[X],\kappa}(t^2) \right\}$ with $F_{[X],\kappa}$ defined by

$$
F_{[X],\kappa}(x) = (k-2)e^{k-2} \sum_{i=0}^{k-3} \sum_{r=0}^{k-3} \binom{k-3}{i} \binom{k-3}{r} (-1)^r \kappa^i \int_0^x e^{-\kappa s^2 + i s} ds.
$$

For $\kappa = 0$ (corresponding to the uniform distribution) $F_{[X],\kappa}$ takes the simple form

$$
F_{[X],0}(x) = 1 - (1-x)^{k-2}.
$$

### 2.3 Shape spaces

The probability integral transformation can be defined also for the shape spaces, $\Sigma^k_m$, of shapes of $k$ non-identical labelled landmarks in $\mathbb{R}^m$. As indicated after (16), the space $\Sigma^k_2$ can be identified with the complex projective
space $\mathbb{C}P^{k-2}$, and so is a compact Riemannian manifold. For $m > 2$, $\Sigma^k_m$ is not a manifold but for our purposes, it is enough to work on the non-singular part of $\Sigma^k_m$, which is the open set consisting of the shapes of $k$ non-identical labelled landmarks in $\mathbb{R}^m$ that do not lie in any $(m-2)$-dimensional affine subspace.

It follows from [17, Section 6.3 and Theorem 6.5] that, for $x$ in the non-singular part of $\Sigma^k_m$ there is a system of Riemannian normal coordinates with inverse that maps an open set $\{(r, u) : 0 \leq r < r_u, u \in T_1X_x\}$ diffeomorphically onto an open set $B$ of $\Sigma^k_m \setminus B$ has measure zero. If the distribution on $T_1 \mathcal{X}$ satisfies conditions (5)–(7) then the probability integral transform can be defined as in Proposition 2.

### 2.4 Cartan–Hadamard manifolds

The Cartan–Hadamard manifolds are the complete simply-connected manifolds with non-positive curvature. It follows from the Cartan–Hadamard theorem [8, Theorem I 13.3], [19] that on a Cartan–Hadamard manifold, $\mathcal{X}$, the inverse of the exponential map at any basepoint $x$ identifies $\mathcal{X}$ with $T_1 \mathcal{X}_x$. Then the choice of some ‘basepoint’ distribution $\nu$ on $\mathcal{X}$ enables an extension of the approach used in Section 3. Important instances of such manifolds are the simplicial shape spaces of shapes of $(m+1)$-simplices in $\mathbb{R}^m$ with positive volume, equipped with a Riemannian metric derived from a natural metric on $SL(m)$ [28, Section 3.6.2], [21, Section 3]. The case $m = 2$ gives the space of shapes of non-degenerate triangles in the plane, which can be identified with the Poincaré half-plane, $\mathbb{H}^2 = \{(x_1, x_2) \in \mathbb{R}^2 : x_2 > 0\}$, with Riemannian metric $g_{ij} = \delta_{ij} x_2^{-2}$. This space was used in [22] as a sample space for electrical impedances.

**Proposition 3**

Let $\mu$ and $\nu$ be probability distributions on a Cartan–Hadamard manifold, $\mathcal{X}$. Let $m$ be a point of $\mathcal{X}$ and $\{(r, u) : 0 \leq r, u \in T_1 \mathcal{X}_m\}$ be Riemannian normal coordinates on $\mathcal{X}$ with $m$ corresponding to the origin. Define the function $\phi : \mathcal{X} \to \mathcal{X}$ by

$$\phi \{\exp(ru)\} = \exp \left[ \tilde{F}_{\psi_{d-1}}(u)^{-1}\{F_u(r)\}\psi_{d-1}(u) \right],$$

where $F_u$ and $\tilde{F}_u$ are defined by (21) and (10), and $\psi_{d-1} = \tilde{\phi}_{d-1}^{-1} \circ \phi_{d-1}$ with $\phi_{d-1}, \tilde{\phi}_{d-1} : T_1 \mathcal{X}_m \to T_1 \mathcal{X}_m$ being the canonical uniformising almost-diffeomorphisms corresponding to $\mu$ and $\nu$, respectively.
Then $\phi$ is an almost-diffeomorphism that maps geodesics through $m$ into geodesics through $m$ and transforms $\mu$ into $\nu$.

2.5 Simplices

The open $(p-1)$-simplex is

$$\Delta_{p-1} = \left\{ (y_1, \ldots, y_p) : y_j > 0, \sum_{j=1}^{p} y_j = 1 \right\}.$$

There is a canonical base point, the centroid, $c = (p^{-1}, \ldots, p^{-1})$ and a canonical Riemannian metric obtained by regarding $\Delta_{p-1}$ as an affine subspace of $\mathbb{R}^p$. The unit tangent sphere at $c$ is

$$T_{1,\Delta_{p-1},c} = \left\{ u = (v_1, \ldots, v_p) : \sum_{j=1}^{p} v_j = 0, \sum_{j=1}^{p} v_j^2 = 1 \right\}$$

and the exponential map is

$$\exp(ru) = c + ru$$

for $r \in [0, 1/(p \max_{1 \leq j \leq p} |v_j|)]$. The uniform distribution is a scaled version of Lebesgue measure on $\Delta_{p-1}$ and the corresponding marginal distribution on the unit tangent sphere is the uniform distribution on $T_{1,\Delta_{p-1},c}$.

2.5.1 Using the exponential map

The manifold $\Delta_{p-1}$ is simply connected and has curvature 0 but it is not complete. The exponential map (17) is a diffeomorphism between a star-shaped portion of $T_{1,\Delta_{p-1},c}$ and $\Delta_{p-1}$. Let $\mu$ be a distribution on $\Delta_{p-1}$ with continuous positive density with respect to the uniform distribution, $\nu$. Then a minor variant of Proposition 3 produces a canonical almost-diffeomorphism $\phi : \Delta_{p-1} \rightarrow \Delta_{p-1}$ that transforms $\mu$ into $\nu$.

**Proposition 4**

Let $\mu$ be a probability distribution on $\Delta_{p-1}$ having continuous positive density with respect to Lebesgue measure. Let $c$ be the barycentre of $\Delta_{p-1}$ and $\{(r, u) : 0 \leq r, u \in T_{1,\Delta_{p-1},c}\}$ be Riemannian normal coordinates on $\Delta_{p-1}$ with $c$ corresponding to the origin. Let $(R, U)$ be the normal coordinates of a random element of $\Delta_{p-1}$. Define the function $\phi : \Delta_{p-1} \rightarrow \Delta_{p-1}$ by

$$\phi \{\exp(ru)\} = \exp \left[ \tilde{F}^{-1}_{\psi(u)} \{F_u(r)\} \psi(u) \right],$$
where \( F_u \) and \( \tilde{F}_u \) are defined by (21) and (10) and \( \psi : T_1 \Delta_{p-1,c} \to T_1 \Delta_{p-1,c} \) is the almost-canonical homeomorphism such that \( \psi(U) \) is uniformly distributed. Then \( \phi \) is a diffeomorphism almost everywhere, maps geodesics through \( c \) into geodesics through \( c \), and transforms \( \mu \) into \( \nu \).

2.5.2 Using radial projection

An alternative to using the exponential map (17) is to use ‘radial projection’ of \( \Delta_{p-1}\{c\} \) onto its boundary \( \partial \Delta_{p-1} \). The coordinates \((r, z_1, \ldots, z_p)\) given by radial projection are defined by

\[
    r = \begin{cases} 
      0 & \text{if } x = c, \\
      1 - p y_{(1)} & \text{if } x \neq c 
    \end{cases} 
    \tag{18}
\]

\[
    z_j = r^{-1} (y_j - y_{(1)}) \quad j = 1, \ldots, p, \tag{19}
\]

where \( y_{(1)} \) denotes the smallest of \( y_1, \ldots, y_p \). Then \( r \in [0, 1) \). A simple calculation shows that the density of the uniform distribution with respect to \( dr \, dz_1 \ldots dz_{i-1} \, dz_{i+1} \ldots dz_p \) is proportional to \( r^{-(p-1)} \). It follows that, for \( i = 1, \ldots, p \), radial projection of \( \Delta_{p-1,i} = \{(y_1, \ldots, y_p) \in \Delta_{p-1} \setminus \{c\} : y_{(1)} = y_i\} \) onto the face \( \partial_1 \Delta_{p-1} = \{(z_1, \ldots, z_p) : z_i = 0\} \) sends the uniform distribution on \( \Delta_{p-1,i} \) to the uniform distribution on the \((p-2)\)-simplex \( \partial_1 \Delta_{p-1} \). The boundary, \( \partial \Delta_{p-1} \), of \( \Delta_{p-1} \) is the union of \( \partial_1 \Delta_{p-1}, \ldots, \partial_p \Delta_{p-1} \).

The next proposition shows that radial projection provides canonical uniformising homeomorphic almost-diffeomorphisms of simplices that are analogous to those for spheres that are described in Proposition 1. Unlike the construction in Proposition 1, the construction in Proposition 5 does not assume uniqueness of medians, as in (5)–(6).

**Proposition 5**

Let \( \mu \) be a probability distribution on \( \Delta_{p-1} \) having continuous positive density with respect to Lebesgue measure. For \( k = 0, \ldots, p-2 \), denote by \( \partial^{p-1-k} \Delta_{p-1} \), the union of the \( k \)-dimensional faces of \( \Delta_{p-1} \). Then repeated radial projection sends \( \mu \) to a probability distribution \( \mu_k \) on \( \partial^{p-1-k} \Delta_{p-1} \). Let \( s \) be the largest value of \( k \) for which \( \mu_k \) is uniform. For \( k = s + 1, \ldots, p-1 \), let \( r, z_1, \ldots, z_{i-1}, z_{i+1}, \ldots, z_k \) be coordinates (defined analogously to those in (18)–(19)) on the part of the \((p-1-k)\)-simplex in \( \partial^{p-1-k} \Delta_{p-1} \) on which \( z_i = 0 \). Define functions \( \phi_k : \partial^{p-k-1} \Delta_{p-1} \to \partial^{p-k-1} \Delta_{p-1} \) for \( k = s, \ldots, p-1 \) recursively by (a) \( \phi_s \) is the identity, (b) for \( k = s + 1, \ldots, p-1 \),

\[
    \phi_k(r, z) = F_z(r)^{1/(k+2-p)} \phi_{k-1}(z), \tag{20}
\]
where
\[ F_z(v) = \Pr(0 < R \leq v | Z = z) \quad \text{under } \mu_k \] under \( \mu_k \).

for \( 0 \leq v \leq 1 \) and \( z = (z_1, \ldots, z_{i-1}, z_{i+1}, \ldots, z_k) \), Then \( \phi_{p-1} \) is a homeomor-
phic almost-diffeomorphism that transforms \( \mu \) into \( \nu \).

Proof
This is a straightforward calculation using the fact that
\[ \Pr(0 < R \leq v | Z = z) = v^{k+2-p} \] under the uniform distribution on this
\((p-1-k)\)-simplex.

Remark 2
The almost-canonical homeomorphisms \( \phi \) introduced in this Section
can be used in the simulation of arbitrary continuous distributions on \( \mathcal{X} \).

Let \( \mu \) and \( \nu \) be probability distributions on \( \mathcal{X} \) and \( \phi \) any transformation
that takes \( \mu \) into \( \nu \). If \( x_1, \ldots, x_n \) in \( \mathcal{X} \) are a random sample from \( \nu \) then
\( \phi^{-1}(x_1), \ldots, \phi^{-1}(x_n) \) are a random sample from \( \mu \).

3 Goodness-of-fit tests via transformation

Let \( \mu \) and \( \nu \) be probability distributions on \( \mathcal{X} \). Then any transformation, \( \phi \),
that takes \( \mu \) into \( \nu \) can be used to transform any test, \( T \), of goodness of fit
to \( \nu \) into a test, \( \phi^*T \), of goodness of fit to \( \mu \). Given points \( x_1, \ldots, x_n \) in \( \mathcal{X} \),
\( \phi^*T \) is obtained by applying \( T \) to the transformed data, \( \phi(x_1), \ldots, \phi(x_n) \).
The null distribution of \( \phi^*T \) is the same as that of \( T \).

Often the null hypothesis about the distribution generating the data
is not that it is some specified distribution but that it is a distribution
in a given parametric model, \( \{\mu_\theta : \theta \in \Theta\} \). For each \( \theta \) in \( \Theta \), let \( \phi_\theta \) be a
transformation that takes \( \mu_\theta \) into \( \nu \). Let \( \hat{\theta} \) be an estimate of \( \theta \). Then
goodness of fit to \( \{\mu_\theta : \theta \in \Theta\} \) is tested by applying \( T \) to the transformed
data, \( \phi_\hat{\theta}(x_1), \ldots, \phi_\hat{\theta}(x_n) \). Significance can be assessed by simulation from
the fitted distribution. If a good approximation to the null distribution of
\( T \) is available then simulation can be avoided by using this approximation.

Provided that the estimator giving \( \hat{\theta} \) is consistent, the consistency prop-
erties of \( \phi^*T \) are inherited from those of \( T \). In particular, if \( \hat{\theta} \) is the maximum
likelihood estimate then \( \phi^*T \) is consistent against all alternatives if and only
if \( T \) is consistent against all alternatives.
3.1 Spheres

On a sphere the uniform distribution provides a canonical choice for \( \nu \). Then the transformation, \( \phi \), of Proposition 1 that takes \( \mu \) into \( \nu \) can be used to transform tests of uniformity into tests of goodness of fit to \( \mu \).

One nice characterisation of the uniform distributions on \( S^2 \) is that, for a uniformly distributed random vector with longitude \( \psi \) and colatitude \( \theta \), (a) \( \psi \) is uniformly distributed on \([0, 2\pi]\), (b) \( \cos \theta \) is uniformly distributed on \([-1, 1]\), (c) \( \psi \) and \( \theta \) are independent. Thus combining any tests of (a), (b) and (c) gives a test of uniformity on \( S^2 \). Using the general construction given in the previous paragraph with \( \phi : S^2 \rightarrow S^2 \) given by (12) but with (15) replaced by the approximation \( 2e^{\kappa(t-1)}-1 \) to (15) for \( \kappa \) not close to 0, taking the tests in (a), (b) and (c) to be Kuiper’s \( V_n \), the Kolmogorov–Smirnov test, and a rather special ‘2-variable’ test yields the standard method [23, Section 12.3.1] of investigating goodness of fit of Fisher distributions on \( S^2 \).

3.2 Compact Riemannian manifolds and shape spaces

On a compact Riemannian manifold or a shape space the uniform distribution provides a canonical choice for \( \nu \). Then the transformation, \( \phi \), of Proposition 2 that takes \( \mu \) into \( \nu \) can be used to transform tests of uniformity into tests of goodness of fit to \( \mu \).

3.3 Cartan–Hadamard manifolds

Let \( m \) be a point in a Cartan–Hadamard manifold, \( \mathcal{X} \), and let \( \mu \) and \( \nu \) be probability distributions on \( \mathcal{X} \) and \( T\mathcal{X}_m \), respectively, such that the density of \( \mu \) with respect to \( \nu \) is positive. By Proposition 3, there is a canonical almost-diffeomorphism \( \phi : \mathcal{X} \rightarrow T\mathcal{X}_m \) that transforms \( \mu \) into \( \nu \). Since \( T\mathcal{X}_m \) can be identified with \( \mathbb{R}^p \) (where \( p \) is the dimension of \( \mathcal{X} \)), standard goodness-of-fit tests on \( \mathbb{R}^p \) can be adapted to give goodness-of-fit tests on \( \mathcal{X} \).

3.4 Simplices

On the simplex \( \Delta_{p-1} \) the uniform distribution provides a canonical choice for \( \nu \). Then the transformation, \( \phi \), of Proposition 4 or Proposition 5 that takes \( \mu \) into \( \nu \) can be used to transform tests of uniformity into tests of goodness of fit to \( \mu \).

An appealing test of uniformity on \( \Delta_{p-1} \) is the score test of uniformity \( (\alpha_1 = \ldots = \alpha_p = 1) \) within the Dirichlet family with densities (with respect
to the uniform distribution)

\[ f(y_1, \ldots, y_p; \alpha) = \frac{\Gamma\left(\sum_{j=1}^{p} \alpha_j\right)}{\prod_{j=1}^{p} \Gamma(\alpha_j)} \prod_{j=1}^{p} y_j^{\alpha_j-1}, \]

where \( \alpha = (\alpha_1, \ldots, \alpha_p) \) with \( \alpha_i > 0 \) for \( i \in \{1, \ldots, p\} \). For independent observations \( y_1, \ldots, y_n \) on \( \Delta_{p-1} \) with \( y_i = (y_{i1}, \ldots, y_{ip}) \) (for \( i = 1, \ldots, n \)), this score test rejects uniformity for large values of

\[ S_n = n \frac{\psi'(p)}{\psi'(1)} \left\{ \frac{\psi'(p)}{p\psi'(p) - \psi'(1)} \sum_{j=1}^{p} \sum_{k=1}^{p} w_j w_k - \sum_{j=1}^{p} w_j^2 \right\}, \]

where \( w_j = n^{-1} \sum_{i=1}^{n} \ln y_{ij} \) and \( \psi \) denotes the digamma function. Under uniformity the large-sample asymptotic distribution of \( S_n \) is \( \chi^2_p \).

## 4 Simulation studies

In order to assess the performance of our tests, we consider three simulation studies. The first involves the goodness-of-fit test on \( S^2 \) based on the Rayleigh test of uniformity. First 10,000 random samples of size 50 were simulated from the Fisher distribution \( F(\mu, \kappa) \) with given mode \( \mu \) and concentration \( \kappa = 10 \). For each sample, goodness of fit to (a) the true \( F(\mu, 10) \) distribution, (b) the fitted \( F(\hat{\mu}, \hat{\kappa}) \) distribution, where \( \hat{\mu} \) and \( \hat{\kappa} \) are the maximum likelihood estimates of \( \mu \) and \( \kappa \), was assessed. Then 10,000 random samples of size 50 were simulated from the projected normal \( \mathcal{PN}_3(\mu, I_3) \) distribution (obtained by projecting the trivariate normal \( \mathcal{N}_3(\mu, I_3) \) distribution radially onto \( S^2 \)) and goodness of fit to the \( F(\mu, 10) \) distribution was assessed. The resulting \( p \)-values (based on the large-sample asymptotic \( \chi^2_3 \) distribution) are shown in the histograms on the left of Figure [1]. Corresponding histograms for 1,000 samples of size 500 are given on the right of Figure [1]. The fairly uniform distribution of \( p \)-values for fit to the true distribution indicates that the test detects good fit when it is present, whereas the clustering of \( p \)-values near 1 when assessing goodness of fit to the fitted distribution shows the anticipated excellent fit in this case. For samples generated from \( \mathcal{PN}_3(\mu, I_3) \), the \( p \)-values for fit to the \( F(\mu, 10) \) distribution also cluster near 1, meaning that this test does not detect that the data come from the wrong model.

One possible explanation for the inability of the above test to detect that the data come from the wrong model is that the Rayleigh test of uniformity
Figure 1: Behaviour of test of goodness of fit (a) to true $F(\mu, 10)$ distribution on $S^2$ (black), (b) to fitted $F(\hat{\mu}, \hat{\kappa})$ distribution (red), (c) to projected normal $PN_3(\mu, I_3)$ distribution (blue), using test based on Rayleigh’s test of uniformity. The histograms are of $p$-values (based on the large-sample asymptotic $\chi^2_3$ distribution). Each histogram summarizes 10,000 simulations, each of size 50 (left) or 500 (right).

is not consistent against all alternatives. Therefore a second simulation study was carried out, which was like the first but with the Rayleigh test replaced by Giné’s $F_n$ test [23, Section 10.4.1], which is consistent against all alternatives to uniformity on $S^2$. Histograms of the resulting values of $F_n$ are shown in Figure 2 for sample sizes, $n$, of 50 (left) and 500 (right). Significance was assessed using the asymptotic quantiles given in [16] [23, Section 10.4.1]. For assessing goodness of fit to the true distribution, the proportions of the values of the statistic that exceeded the asymptotic 10%, 5% and 1% upper quantiles were 0.10, 0.05 and 0.01 ($n = 50$) and 0.10, 0.04 and 0.01 ($n = 500$), respectively, indicating that the test detects good fit when it is present. For fit to the fitted distribution, none of the values of $F_n$ exceeded the asymptotic 10% quantile, indicating the anticipated excellent fit in this case. For samples generated from $PN_3(\mu, I_3)$, the proportions of the values of $F_n$ that exceeded the asymptotic 10%, 5% and 1% upper quantiles were 0.58, 0.34 and 0.05 for $n = 50$, while for $n = 500$, all the values of $F_n$ far exceeded the asymptotic 1% upper quantile. This indicates
clearly that the test can detect bad fit.

Figure 2: Behaviour of test of goodness of fit (a) to true $F(\mu, 10)$ distribution on $S^2$ (black), (b) to fitted $F(\hat{\mu}, \hat{\kappa})$ distribution (red), (c) to projected normal $PN_3(\mu, I_3)$ distribution (blue), using test based on Giné’s $F_n$ test of uniformity. The histograms are of values of $F_n$. Each histogram summarizes 10,000 simulations, each of size 50 (left) or 500 (right). Green arrows on horizontal axes are 10%, 5% and 1% upper quantiles of asymptotic distribution.

The third simulation study involves the goodness-of-fit test on $\Sigma^5_2$ based on Mardia’s test of uniformity. First, 10,000 random samples of size 50 were simulated from the isotropic Mardia–Dryden $MD([\mu], 0.125)$ distribution with given mode $[\mu]$. For each sample, goodness of fit to (a) the true $MD([\mu], 0.125)$ distribution, (b) the fitted $MD(\hat{\mu}, \hat{\kappa})$ distribution, where $[\mu]$ and $\kappa$ are the maximum likelihood estimates of $[\mu]$ and $\kappa$ (calculated by the EM method of [20]), was assessed using Mardia’s uniformity test on $\Sigma^5_2$. Then 10,000 random samples of size 50 were simulated from the non-isotropic Mardia–Dryden distribution obtained by Gaussian $N_2(0, \Sigma)$ perturbations of $\mu$, where $\Sigma = \text{diag}(1, 25)$, and goodness of fit to the $MD([\mu], 0.125)$ distribution was assessed. The resulting $p$-values based on the large-sample asymptotic $\chi^2_{15}$ distribution are shown in the histograms on the left of Figure 3. Corresponding histograms for 10,000 samples of size 500 are given on the right. The fairly uniform distribution of $p$-values for fit to the true distribution indicates that the test detects good fit when it
is present. The clustering of \(p\)-values near 1 for fit to the fitted distribution shows the anticipated excellent fit in this case. For samples generated from the non-isotropic distribution, the \(p\)-values cluster near 0, indicating that the test can detect bad fit.

![Graph showing behavior of test of goodness of fit](image)

Figure 3: Behaviour of test of goodness of fit (a) to true isotropic Mardia–Dryden \(MD([\mu], 0.125)\) distribution on \(\Sigma_2^5\) (black), (b) to fitted isotropic \(MD([\hat{\mu}], \hat{\kappa})\) distribution (red), (c) to non-isotropic Mardia–Dryden distribution obtained by Gaussian \(N_2(0, \text{diag}(1, 25))\) perturbations of \(\mu\) (blue), using test based on Mardia’s test of uniformity. The histograms are of \(p\)-values (based on the large-sample asymptotic \(\chi^2_{15}\) distribution). Each histogram summarizes 10,000 simulations, each of size 50 (left) or 500 (right).

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