Nonparametric Bayesian density estimation on manifolds with applications to planar shapes

BY ABHISHEK BHATTACHARYA AND DAVID B. DUNSON

Department of Statistical Science, Box 90251, Duke University, Durham, North Carolina 27708-0251, U.S.A.

ab216@stat.duke.edu dunson@duke.edu

SUMMARY

Statistical analysis on landmark-based shape spaces has diverse applications in morphometrics, medical diagnostics, machine vision and other areas. These shape spaces are non-Euclidean quotient manifolds. To conduct nonparametric inferences, one may define notions of centre and spread on this manifold and work with their estimates. However, it is useful to consider full likelihood-based methods, which allow nonparametric estimation of the probability density. This article proposes a broad class of mixture models constructed using suitable kernels on a general compact metric space and then on the planar shape space in particular. Following a Bayesian approach with a nonparametric prior on the mixing distribution, conditions are obtained under which the Kullback–Leibler property holds, implying large support and weak posterior consistency. Gibbs sampling methods are developed for posterior computation, and the methods are applied to problems in density estimation and classification with shape-based predictors. Simulation studies show improved estimation performance relative to existing approaches.

Some key words: Dirichlet process mixture; Discriminant analysis; Kullback–Leibler property; Metric space; Non-parametric Bayes; Planar shape space; Posterior consistency; Riemannian manifold.

1. INTRODUCTION

In recent years, there has been considerable interest in the statistics literature in the analysis of data having support on a non-Euclidean manifold M. Our focus is on nonparametric approaches, which avoid modelling assumptions about the distribution of the data over M. Although we are particularly motivated by landmark-based analyses of planar shapes, we develop nonparametric Bayes theory and methods also for general compact metric spaces and manifolds.

There is a rich literature on frequentist methods of inference on manifolds, which avoid a complete likelihood specification in conducting nonparametric estimation and testing based on manifold data. See, for example, Bhattacharya & Bhattacharya (2008) and the references cited therein. Such methods are based on estimates of centre and spread, which are appropriate for manifolds. However, aspects of the distribution other than centre and spread may also be important. Pelletier (2005) develops frequentist methods for density estimation on compact Riemannian manifolds using a kernel that generalizes location-scale kernels used in Euclidean spaces. The sample points are used as the kernel locations while assuming a fixed bandwidth, and the estimator is shown to be L^2 consistent for a sufficiently small bandwidth.

Bayesian nonparametric methods have the advantage of providing a full probabilistic characterization of uncertainty, which is valid even in small samples. Nonparametric Bayes density estimation in Euclidean spaces commonly relies on kernel mixture models, with a Dirichlet process prior (Ferguson, 1973, 1974) placed on the unknown mixture distribution and a Gaussian kernel assumed (Lo, 1984; Escobar & West, 1995). Our focus is on developing Bayesian kernel mixture models for nonparametric density estimation on compact metric spaces, with manifolds arising as a special case. The manifold of special interest is the planar shape space Σ_2^k corresponding to similarity shapes of configurations of k landmarks in two-dimensions (Kendall, 1984).

The kernel should be carefully chosen, so that the induced prior will have large support, meaning that the prior assigns positive probability to arbitrarily small neighbourhoods around any density f_0 . Such a support condition is important in allowing the posterior to concentrate increasingly around the true density as the sample size n grows. From Schwartz (1965), prior positivity of Kullback–Leibler neighbourhoods around the true density f_0 implies that the posterior probability of any weak neighbourhood of f_0 converges to unity as $n \to \infty$. Showing that a proposed prior has Kullback–Leibler support is important in providing a proof of the concept that the prior is sufficiently flexible, but is difficult for new priors even in Euclidean spaces. We extend the sufficient conditions of Wu & Ghosal (2008) to arbitrary compact metric spaces, and apply this theory to general manifolds and planar shape spaces.

For landmark-based shape data, current Bayesian analyses focus on parametric models. For example, Kume & Walker (2006) recently proposed a method for posterior computation in complex Watson models (Watson, 1965, 1983), with Dryden & Mardia (1998) proposing the complex Watson as a convenient parametric distribution for planar shape data. Lennox et al. (2009) proposed a Dirichlet process mixture of bivariate von Mises–Fisher distributions for protein configuration angles, modifying the finite mixture model of Mardia et al. (2007). Their model arises as a special case of the framework we propose, and is not applicable to shape data. The von Mises–Fisher kernel is quite restrictive, and it is not clear whether mixtures of such kernels induce priors with large support. Lennox et al. (2009) do not present any theoretical results. However, our theory can be used to show that such a prior has full support, and weak posterior consistency follows, providing conditions for strong consistency. Computation in Lennox et al. (2009) relies on the auxiliary Gibbs sampler of Neal (2000). In this paper, for applications to landmark-based shape data, we focus on Dirichlet process mixtures of complex Watson distributions. We show that such priors have large support, while also developing efficient methods of posterior computation.

2. NONPARAMETRIC DENSITY ESTIMATION ON COMPACT METRIC SPACES

Let *M* be a compact metric space and let *X* be a random variable on *M*. We assume that the distribution of *X* has a density with respect to some fixed base measure λ on *M* and we are interested in modelling this density via a flexible model. Let $K(m; \mu, \sigma)$ be a probability kernel on *M* with location $\mu \in M$ and scale $\sigma \in \Re^+$, with $\int_M K(m; \mu, \sigma)\lambda(dm) = 1$. We can define a location mixture probability density model for *X* as

$$f(m; P, \sigma) = \int_{M} K(m; \mu, \sigma) P(d\mu)$$
(1)

or a location-scale mixture model

$$g(m;Q) = \int_{M \times \Re^+} K(m;\mu,\sigma) Q(d\mu d\sigma).$$
⁽²⁾

For a prespecified kernel K, a prior on $\mathcal{D}(M)$, the space of all probability densities on M with respect to the set base measure λ , is induced through a prior $(P, \sigma) \sim \Pi_1$ in (1) and a prior $Q \sim \Pi_2$ in (2). In order to evaluate whether a particular kernel K and prior Π_1 or Π_2 induces a prior for the unknown density on M that is sufficiently flexible, it would be appealing to have simple sufficient conditions to check.

We make the following assumptions about the kernel K.

Assumption 1. The kernel K is continuous on $M \times M \times (0, \sigma_0)$ for some $\sigma_0 > 0$.

Assumption 2. For any $\phi \in C(M)$, with C(M) the space of continuous functions on M,

$$\lim_{\sigma \to 0} \sup_{m \in M} \left| \phi(m) - \int_M K(m; \mu, \sigma) \phi(\mu) \lambda(d\mu) \right| = 0$$

These assumptions place minor regularity conditions on the kernel. If K is symmetric in m and μ , Assumption 2 implies that K converges weakly to the degenerate point mass at μ uniformly in μ as $\sigma \rightarrow 0$.

In addition, we make the following assumptions about f_0 , the true density of X, and the support of the prior Π_1 .

Assumption 3. For any $\sigma > 0$, there exists $\tilde{\sigma} \leq \sigma$ such that $(F_0, \tilde{\sigma}) \in \text{supp}(\Pi_1)$, with F_0 the probability distribution corresponding to f_0 and $\text{supp}(\Pi_1)$ denoting the weak support of Π_1 .

Assumption 4. The true density is continuous, so that $f_0 \in C(M)$.

THEOREM 1. Define f as in (1). Under Assumptions 1–4, for any $\epsilon > 0$,

$$\Pi_1\Big\{(P,\sigma): \sup_{m\in M} |f_0(m) - f(m;P,\sigma)| < \epsilon\Big\} > 0.$$

Theorem 1 shows that the density prior induced through the location mixture model (1) assigns positive probability to arbitrarily small L^{∞} neighbourhoods of the true density under mild assumptions. For a proposed prior chosen for a particular M, one can simply verify that the assumed kernel K and prior Π_1 satisfy the assumptions to show large support. We will illustrate how these assumptions are met using a complex Watson kernel on a planar shape space in § 3.

To show full Kullback–Leibler support for the prior, we require an additional assumption, as follows.

Assumption 5. The true density is everywhere positive so that $f_0(m) > 0$ for all $m \in M$.

COROLLARY 1. Under Assumptions 1–5, the prior on $\mathcal{D}(M)$ induced by Π_1 through (1) assigns positive probability to any Kullback–Leibler neighbourhood around f_0 .

Assumption 6. For any $\sigma > 0$, there exists $\tilde{\sigma} \in (0, \sigma]$ such that $F_0 \times \delta_{\tilde{\sigma}} \in \text{supp}(\Pi_2)$.

THEOREM 2. Let g be a density as in (2). Under Assumptions 1–2 and 4–6, the prior on $\mathcal{D}(M)$ induced by Π_2 assigns positive probability to any Kullback–Leibler neighbourhood around f_0 .

The assumptions on the priors in Theorems 1 and 2 are trivially satisfied by standard nonparametric priors. For example, for model (1) we can choose Π_1 to be $\Pi_{11} \times \pi_1$, with Π_{11} a Dirichlet process prior $DP(\omega_0 P_0)$ with $supp(P_0) = M$ and π_1 having a density that is strictly positive in some neighbourhood of zero. For model (2), we can instead choose the prior Π_2 for the mixing measure Q to correspond to a Dirichlet process with base $P_0 \times \pi_1$. Under these priors, models (1) and (2) are Dirichlet process mixture models and standard algorithms can be applied for posterior computation.

A special case of a compact metric space is a compact Riemannian manifold with the distance metric being the geodesic distance induced by the Riemannian metric tensor. The natural choice of base measure for modelling densities is then the Riemannian volume form. For background in differential geometry, the reader is referred to Willmore (1993). Pelletier (2005) introduced a geodesic distance based kernel and performed frequentist density estimation on compact Riemannian manifolds. Under mild restrictions on the form of this kernel, it can be shown that it satisfies the assumptions of Theorem 1. The details and proofs are omitted since we have found alternative kernels to also satisfy these assumptions for manifolds corresponding to the unit hypersphere and the planar shape space, while having computational advantages over the Pelletier (2005) class of kernels. For the unit hypersphere, von Mises–Fisher kernels can be used, but here we focus on the landmark-based planar shape space $M = \sum_{n=1}^{k} \frac{1}{2}$.

3. The planar shape space Σ_2^k

3.1. Geometry

Consider a set of k points, k > 2, on the two-dimensional plane, not all points being the same. We refer to such a set as a k-ad or a set of k landmarks. The similarity shape of this k-ad is what remains after we remove the effects of the Euclidean rigid body motions of translation, rotation and scaling. For convenience we denote a k-ad by a complex k-vector $z = (z_1, \ldots, z_k)^T$ in c^k . To remove the effect of translation from z, let $z_c = z - \overline{z}$, with $\overline{z} = (\sum_{j=1}^k z_j)/k$ being the centroid. The centred k-ad z_c lies in a (k - 1)-dimensional complex subspace, and hence we can use k - 1 complex coordinates. The effect of scaling is removed by normalizing the coordinates of z_c to obtain a point w on the complex unit sphere cs^{k-2} in c^{k-1} . Since w contains the shape information of z along with rotation, it is called the preshape of z.

The similarity shape of z is the orbit of w under all two-dimensional rotations. Since a rotation by an angle θ of a landmark (x, y) can be achieved by multiplying its complex version x + iy by $\exp(i\theta)$, the shape of z is the set or orbit $[w] = \{\exp(i\theta)w : \theta \in (-\pi, \pi]\}$. The space of all such orbits constitutes the planar shape space Σ_2^k . Any shape can be represented as the set of intersection points of a unique complex line passing through the origin with cs^{k-2} . With this identification proposed by Kendall (1984), Σ_2^k is a compact Riemannian manifold of dimension 2k - 4. It can be embedded into the space of all complex Hermitian matrices via the embedding J([w]) = ww^* , with * denoting the complex conjugate transpose. The extrinsic distance between the two shapes [u] and [v] is the one induced from this embedding, namely, $d_E([u], [v]) = ||J([u]) - J([v])|| = \{2(1 - |u^*v|^2)\}^{1/2}$. This distance is equivalent to the geodesic distance $d_g([u], [v]) =$ $\operatorname{arccos}(|u^*v|)$.

Let Q be a probability distribution on Σ_2^k . The extrinsic mean of Q is defined as the minimizer of the loss function $F(p) = \int_{\Sigma_2^k} d_E^2(m, p)Q(dm)$, $p \in \Sigma_2^k$, provided F has a unique minimizer. The minimum value of F is called the extrinsic variation of Q. Let $\tilde{\mu} = \int_{\Sigma_2^k} J(m)Q(dm)$, λ be its largest eigenvalue and U be a corresponding unit norm eigenvector. Then it can be shown that the extrinsic variation equals $2(1 - \lambda)$ and the extrinsic mean is given by [U] provided λ has multiplicity 1. Given a random sample from Q, one can define the sample extrinsic mean and variation analogously. For more details, see Bhattacharya & Patrangenaru (2003) and Bhattacharya & Bhattacharya (2008).

3.2. Uniform distribution

Let V(dm) and $V_1(dz)$ denote the volume forms on the shape space Σ_2^k and the preshape sphere cs^{k-2} , respectively. The uniform distribution on Σ_2^k has constant density $1/\int_{\Sigma_2^k} V(dm)$. Kent (1994) constructs a useful coordinate chart on Σ_2^k as follows. For $z = (z_1, \ldots, z_{k-1})^T \in cs^{k-2}$, write $z_j = r_j^{1/2} \exp(i\theta_j)$ $(j = 1, \ldots, k-1)$ with $r = (r_1, \ldots, r_{k-2})^T$ lying on the (k-1)-unit simplex S_{k-2} , and $\theta_j \in (-\pi, \pi)$ $(j = 1, \ldots, k-1)$. Then $(r_1, \ldots, r_{k-2}, \theta_1, \ldots, \theta_{k-1})$ form the

Kent preshape coordinates of z. Since the shape of z can be obtained by rotating it around a fixed axis, we may set $\theta_{k-1} = 0$ and use the Kent shape coordinates $(r_1, \ldots, r_{k-2}, \theta_1, \ldots, \theta_{k-2})^T$ for [z] as in Dryden & Mardia (1998). These Kent (1994) coordinate systems have the advantage of leading to simple expressions for the volume forms,

$$V_1(dz) = 2^{2-k} dr_1 \cdots dr_{k-2} d\theta_1 \cdots d\theta_{k-1}, \quad V(d[z]) = 2^{2-k} dr_1 \cdots dr_{k-2} d\theta_1 \cdots d\theta_{k-2}.$$

This implies that, in terms of these shape coordinates, the uniform distribution on Σ_2^k remains uniform on $S_{k-2} \times (-\pi, \pi)^{k-2}$. This property simplifies simulations and proofs.

3.3. Complex Bingham distribution

The complex Bingham distribution on Σ_2^k (Kent, 1994) has the following density with respect to the volume form

$$f(m; A) = c^{-1}(A) \exp(z^* A z), \quad m = [z] \in \Sigma_2^k$$

where A is a $(k - 1) \times (k - 1)$ complex Hermitian matrix and c(A) is the normalizing constant. Denoting this density by CB(A), we find that $CB(A) = CB(A + \alpha I)$ for any $\alpha \in \Re$. Hence, without loss of generality, we may assume A to be positive semidefinite with the smallest eigenvalue equal to zero. Let $A = U\Lambda U^*$ be a singular value decomposition of A with $U = [U_1, \ldots, U_{k-1}] \in$ SU(k - 1), $\Lambda = diag(\lambda_1, \ldots, \lambda_{k-1})$, and $0 = \lambda_1 \leq \cdots \leq \lambda_{k-1}$, where SU(k - 1) is the space of all $(k - 1) \times (k - 1)$ special unitary matrices having $UU^* = I$ and det(U) = 1. Letting $z_1 = U^*z$ and using Kent's shape coordinates (r, θ) for $[z_1]$, the complex Bingham distribution can be written as

$$f(m;A)V(dm) = c^{-1}(A)2^{2-k} \exp\left(\sum_{j=1}^{k-1} \lambda_j r_j\right) dr_1 \cdots dr_{k-2} d\theta_1 \cdots d\theta_{k-2}$$
(3)

with $r_{k-1} = 1 - \sum_{j=1}^{k-2} r_j$. Expression (3) suggests that r has a density $g(r) \propto \exp(\sum_{j=1}^{k-1} \lambda_j r_j)$ on S_{k-2} while $\theta_1, \ldots, \theta_{k-2}$ are independent and identically distributed as $Un(-\pi, \pi)$ and r and θ are independent. This characterization is helpful in sampling from the complex Bingham distribution. Under high concentrations, that is when $\lambda_{k-1} \gg \lambda_{k-2}$, one may use an independent Metropolis–Hasting step with an independent exponential approximation to sample from g. That is, we draw $r_j, j = 1, \ldots, k-2$ independently from the density proportional to $\exp\{(\lambda_j - \lambda_{k-1})r_j\}$ on (0, 1), accept the draw if $\sum_{i=1}^{k-2} r_i \leq 1$ and then set $r_{k-1} = 1 - \sum_{j=1}^{k-2} r_j$.

3.4. Complex Watson distribution

When A has complex rank equal to one, the complex Bingham distribution CB(A) corresponds to a complex Watson distribution (Dryden & Mardia, 1998) having density

$$f(m;\mu,\sigma) = c^{-1}(\sigma) \exp(|z^*\nu|^2/\sigma), \tag{4}$$

with z and v preshapes of m and $\mu \in \Sigma_2^k$, respectively. Here, μ is the extrinsic mean, $\sigma > 0$ is a scale parameter related to the extrinsic variation, and $c(\sigma)$ is the normalizing constant. Denoting this density by $CW(\mu, \sigma)$, $CW(\mu, \sigma)$ is equivalent to CB(A) with $A = \nu \nu^* / \sigma$. As A has eigenvalues $\lambda_1 = \cdots = \lambda_{k-2} = 0$, $\lambda_{k-1} = \sigma^{-1}$, the distribution of r defined in § 3.3 can be written as $g(r) \propto \exp(\sigma^{-1}r_{k-1})$ implying that r_{k-1} has the marginal density

$$h(r_{k-1}) = c_{k-1}^{-1}(\sigma) \exp(r_{k-1}\sigma^{-1})(1-r_{k-1})^{k-3}, \quad r_{k-1} \in (0, 1).$$

where $c_{k-1}(\sigma) = \sigma^{k-2} \exp(\sigma^{-1}) \Gamma(k-2; \sigma^{-1})$ with $\Gamma(m, a) = \int_0^a \exp(-t) t^{m-1} dt = (m-1)! \exp(-a) \{\exp(a) - \sum_{r=0}^{m-1} a^r / r!\}$ denoting the partial gamma function. Conditionally on r_{k-1} ,

 (r_1, \ldots, r_{k-2}) has a uniform distribution on the set $\{r_j \ge 0, j = 1, \ldots, k-2, \sum_{j=1}^{k-2} r_j = 1 - r_{k-1}\}$. Transforming by letting $s = \sigma^{-1}(1 - r_{k-1})$, s has a density proportional to $\exp(-s)s^{k-3}$ on $(0, \sigma^{-1})$, which is $\operatorname{Ga}(k-2, 1)$ restricted to $(0, \sigma^{-1})$. This characterization can be used to easily draw exact samples from a complex Watson distribution. The normalizing constant is $c(\sigma) = (\pi\sigma)^{(k-2)} \{\exp(\sigma^{-1}) - \sum_{r=0}^{k-3} \sigma^{-r}/r!\}$. In Dryden & Mardia (1998), $\operatorname{Cw}(\mu, \sigma)$ is viewed as a distribution on the preshape sphere and the normalizing constant is instead $2\pi c(\sigma)$.

4. DENSITY ESTIMATION ON THE PLANAR SHAPE SPACE

To model an unknown density on Σ_2^k , we use a mixture density as in (1) with K corresponding to the complex Watson density in expression (4).

PROPOSITION 1. For the complex Watson kernel, Assumptions 1 and 2 are satisfied.

Hence, if we choose a complex Watson kernel in (1) and choose Π_1 to satisfy Assumption 3 from Theorem 1, we induce a prior with L^{∞} support on the space of continuous densities over Σ_2^k and with Kullback–Leibler support on the space of continuous and everywhere positive densities over Σ_2^k . It follows from Schwartz (1965) that this specification leads to weak posterior consistency at any continuous, everywhere positive f_0 .

To specify a Π_1 that satisfies the assumptions and that leads to simplifications in implementing posterior computation, we follow the recommendation given at the end of § 2 and let $P \sim DP(\omega_0 P_0)$, with P_0 corresponding to $CW(\mu_0, \sigma_0)$, independently of $\sigma^{-1} \sim Ga(a, b)$. These priors lead to conditional conjugacy so that posterior computation can proceed via Gibbs sampling algorithms previously developed for Dirichlet process mixture models. For the location-scale mixture (2), the computations are similar and are left to the reader.

Here, we follow the exact block Gibbs sampler proposed in a yet unpublished paper by Yau, Papaspiliopoulos, Roberts and Holmes. Let $x_i \sim Cw(\mu_i, \sigma)$, independently for i = 1, ..., n, with $\mu_i \sim P$, and P, σ assigned the prior described above. We introduce uniformly distributed slice sampling latent variables, $u = \{u_i\}_{i=1}^n$ and let S_i denote the mixture component for subject i, with $\mu_i = \tilde{\mu}_{S_i}$. The complete data likelihood is then $\prod_{i=1}^n Cw(X_i; \tilde{\mu}_{S_i}, \sigma) 1(u_i < w_{S_i})$, and we sequentially sample through the following steps.

Step 1. Update S_i , for i = 1, ..., n, by sampling from the multinomial conditional posterior distribution with $\operatorname{pr}(S_i = j) \propto \operatorname{CW}(x_i; \tilde{\mu}_j, \sigma)$ for $j \in A_i$, where $A_i = \{j : j = 1, ..., l, w_j > u_i\}$ and l is the smallest index satisfying $1 - u_{(1)} < \sum_{j=1}^l w_j$ with $u_{(1)} = \min\{u_1, ..., u_n\}$. In implementing this step, draw $V_j \sim \operatorname{Be}(1, \omega_0)$ and $\tilde{\mu}_j \sim P_0$ for $j > S_{(n)}$, with $S_{(n)} = \max\{S_1, ..., S_n\}$.

Step 2. Update the kernel locations $\tilde{\mu}_j$ ($j = 1, ..., S_{(n)}$) by sampling from the conditional posterior

$$\tilde{\mu}_j \sim \operatorname{CB}\left(\frac{m_j}{\sigma} \bar{X}_j + A_0\right),$$

where $m_j = \sum_{i=1}^n \mathbb{1}(S_i = j)$, $\bar{X}_j = \sum_{i:S_i=j} z_i z_i^* / m_j$ $(x_i = [z_i])$, $A_0 = \sigma_0^{-1} v_0 v_0^*$ and $\mu_0 = [v_0]$. We use a Metropolis–Hastings step developed in § 3·3 to draw $\tilde{\mu}_j$.

Step 3. The full conditional posterior of σ is proportional to

$$(\sigma^{-1})^{n(k-2)+a+1} \exp\left\{-\frac{1}{\sigma}\left(n+b-\sum_{j=1}^{S_{(n)}} m_j \nu_j^* \bar{X}_j \nu_j\right)\right\} \left\{1-\exp(-\sigma^{-1})\sum_{r=0}^{k-3} (r!)^{-1} \sigma^{-r}\right\}^{-n},$$

where $\tilde{\mu}_j = [\nu_j]$. For σ small, this conditional density is approximately equivalent to

$$\sigma^{-1} \sim \operatorname{Ga}\left\{a + n(k-2), b + \sum_{j=1}^{S_{(n)}} m_j(1 - v_j^* \bar{X}_j v_j)\right\}.$$

Hence, we get approximate conjugacy for the conditional distribution of σ^{-1} under a gamma prior. Numerical studies show that this approximation is very accurate even for σ moderately small, so we recommend a Metropolis–Hastings independence step with candidates generated from the approximation.

Step 4. Update the stick-breaking random variables V_j ($j = 1, ..., S_{(n)}$), from their conditional posterior distributions given the cluster allocation but marginalizing out the slice sampling variables,

$$V_j \sim \text{Be}\left\{1 + m_j, \omega_0 + \sum_{i=1}^n 1(S_i > j)\right\}.$$

Step 5. Update the slice sampling latent variables from their conditional posterior by letting $u_i \sim \text{Un}(0, w_{S_i})$ (i = 1, ..., n).

We also incorporate label-switching moves as recommended in Papaspiliopoulos & Roberts (2008). In cases we have considered, the algorithm is efficient, with rapid convergence and no evidence of slow mixing. Due to label switching issues (Stephens, 2000), we recommend assessing convergence and mixing by examining trace plots and applying standard diagnostics for the density $f(m; P, \sigma)$ evaluated at a dense grid of *m* values. A draw from the posterior for *f* can be obtained using

$$f(m; P, \sigma) = \sum_{j=1}^{S_{(n)}} w_j \operatorname{CW}(m; \tilde{\mu}_j, \sigma) + \left(1 - \sum_{j=1}^{S_{(n)}} w_j\right) \int \operatorname{CW}(m; \tilde{\mu}, \sigma) \operatorname{CW}(\tilde{\mu}; \mu_0, \sigma_0) V(d\tilde{\mu}), \quad (5)$$

with σ and w_j , $\tilde{\mu}_j$ ($j = 1, ..., S_{(n)}$) a Markov chain Monte Carlo draw from the joint posterior of the bandwidth and the weights and atoms for each of the components up to the maximum occupied. A Bayes estimate of f can then be obtained by averaging these draws across many samples. Since it is difficult to evaluate the integral in (5) in closed form, we replace the integral by $CW(m; \mu_1, \sigma), \mu_1$ being a draw from $CW(\mu_0, \sigma_0)$.

5. Applications

5.1. Applications to simulated data

We draw $x_i \sim 0.5 \text{CW}(\mu_1, \sigma) + 0.5 \text{CW}(\mu_2, \sigma)$ independently for i = 1, ..., 200, with k = 4, $\sigma = 0.001, \mu_1 = (1, 0, 0)^T, \mu_2 = \{r, (1 - r^2)^{1/2}, 0\}^T$ and r = 0.9975 so that the extrinsic distance between μ_1 and μ_2 is 0.1. We compare our Bayesian nonparametric density estimate based on Dirichlet process mixtures of complex Watson kernels to a maximum likelihood estimate under a parametric complex Watson model (Dryden & Mardia, 1998) and to the frequentist kernel density estimate using a complex Watson kernel. We generated 20 simulated datasets, with the performance evaluated based on the L^1 distance and Kullback–Leibler divergence estimated by averaging over the data points. Our Bayesian nonparametric approach was implemented as described in § 4 with the Markov chain Monte Carlo algorithm run for 100 000 iterations with the first 15 000 discarded as a burn-in. The hyperparameters were chosen by setting μ_0 equal to the sample extrinsic mean and $\sigma_0 = 0.1$ in the complex Watson base measure P_0 for P, and

	Bayes		MLE		KDE	
	L^1	KL	L^1	KL	L^1	KL
min	0.27	0.02	0.60	0.33	0.56	0.14
25th	0.35	0.07	0.68	0.36	0.74	0.24
50th	0.42	0.08	0.73	0.43	0.87	0.26
75th	0.48	0.16	0.83	0.46	1.20	0.27
max	0.91	0.39	0.94	0.52	2.72	0.32
mean	0.44	0.13	0.75	0.41	1.03	0.25

Table 1. Summaries of estimated distances from the true density across the 20 simulations

Bayes, our proposed approach; MLE, maximum likelihood estimate; KDE, kernel density estimate; KL, Kullback-Leibler.

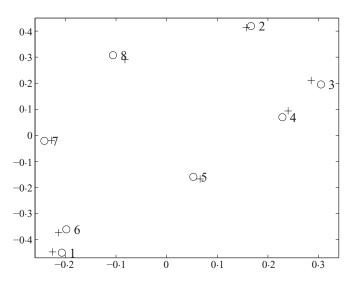


Fig. 1. Gorilla skull data. Landmarks from preshapes of $\hat{\mu}_1$ (female, \bigcirc) and $\hat{\mu}_2$ (males, +).

a = b = 0.1 in the gamma prior for σ^{-1} . By using the data to estimate the location of the base distribution, while choosing a moderate scale, we ensure that the prior introduces clusters close to the support of the data. The Dirichlet process precision parameter is fixed as $\omega_0 = 1$, which is a commonly used default in the literature favouring a sparse representation with few clusters.

Table 1 presents summaries of the results across the 20 simulated datasets. The proposed nonparametric Bayes estimator had consistently better performance across the datasets and for each choice of criterion. For the frequentist kernel density estimate, results are presented for a bandwidth of $\sigma = 0.001$. The performance was similar or worse for other choices of bandwidth, including setting σ equal to the maximum likelihood estimate under the parametric complex Watson model and the posterior mean of σ from the Bayes analysis.

5.2. Application to morphometrics: classification of gorilla skulls

The method is applied to data on the shape of 29 male and 30 female gorilla skulls, with eight landmarks chosen on the midline plane of two-dimensional images of each skull (Dryden & Mardia, 1998). The goal is to study how the shapes of the skulls vary between males and females, and build a classifier to predict gender. The shape samples lie on Σ_2^k , k = 8. We randomly pick 25 individuals of each gender as a training sample, with the remaining nine used as test data. Figure 1 shows the preshapes of the sample extrinsic means for the female and male

Gender	$\hat{p}([z])$	95% Confidence interval	$d_E([z_i], \hat{\mu}_1)$	$d_E([z_i], \hat{\mu}_2)$
F	1.000	(1.000, 1.000)	0.041	0.111
F	1.000	(0.999, 1.000)	0.036	0.093
F	0.023	(0.021, 0.678)	0.056	0.052
F	0.998	(0.987, 1.000)	0.050	0.095
F	1.000	(1.000, 1.000)	0.076	0.135
М	0.000	(0.000, 0.000)	0.167	0.103
М	0.001	(0.000, 0.004)	0.087	0.042
М	0.992	(0.934, 1.000)	0.091	0.121
М	0.000	(0.000, 0.000)	0.152	0.094

Table 2. Posterior probability of being female for each gorilla in the test sample

 $d_E([z_i], \hat{\mu}_i)$ = extrinsic distance from the mean shape in group *i*, with i = 1 for females and i = 2 for males.

training groups. The preshape of the male mean $\hat{\mu}_2$ has been rotated appropriately so as to bring it closest to the preshape of the female mean $\hat{\mu}_1$. Most of the landmarks corresponding to the preshapes of the sample means after rotation are close for females and males, but there is a larger difference in landmarks 3 and 8.

Applying nonparametric discriminant analysis, we assume that the probability of being female is 0.5 and use a separate Dirichlet process mixture of complex Watson kernels for the shape density in the male and female groups. Letting $f_1(m)$ and $f_2(m)$ denote the female and male shape densities, the conditional probability of being female given shape data [z] is simply $p([z]) = 1/\{1 + f_2([z])/f_1([z])\}\)$. To estimate the posterior probability, we average p([z]) across Markov chain Monte Carlo iterations to obtain $\hat{p}([z])$. The analysis was implemented as in the simulation examples, but with hyperparameters $\sigma_0 = 0.001$, a = 1.01 and b = 0.001 elicited based on our prior expectation for the gorilla example.

Table 2 presents the estimated posterior probabilities of being female for each of the gorillas in the test sample along with a 95% credible interval for p([z]). For most of the gorillas, there is a high posterior probability of assigning the correct gender. There is misclassification only in the third female and third male. For the third female, the credible interval includes 0.5, suggesting that there is insufficient information to be confident in the classification. However, for the third male, the credible interval suggests a high degree of confidence that this individual is female. Perhaps this individual is an outlier and there is something unusual about the shape of his skull, with such characteristics not represented in the training data, or perhaps alternatively it was labelled incorrectly.

In addition, we display the extrinsic distance between the shape for each gorilla and the female and male sample extrinsic means. Potentially we could define a distance-based classifier, which allocates a test subject to the group having mean shape closest to that subjects' shape. The table suggests that such a classifier will yield consistent results with our nonparametric Bayes approach. However, this distance-based classifier may be suboptimal in not taking into account the variability within each group. In addition, the approach is deterministic and there is no measure of uncertainty in classification. Figure 2 shows the male and female training sample preshape clouds, along with the two misclassified test samples. There seems to be a substantial deviation in the coordinates of these misclassified subjects from their respective gender training groups, especially for the male gorilla, even after having rotated each training preshape separately so as to bring each closest to the plotted test sample preshapes.

It is possible that classification performance could be improved in this application also by taking skull size into account. The proposed method can be easily extended to this case by using a Dirichlet process mixture density with the kernel being the product of a complex Watson kernel

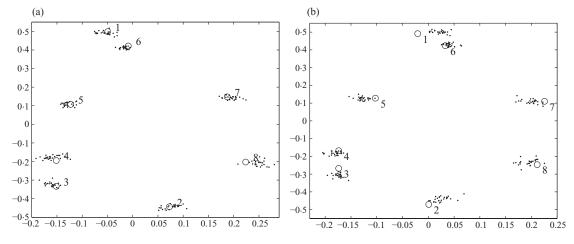


Fig. 2. Gorilla skull data. Landmarks from preshapes of training (dot) and misclassified test samples (circle) for females (a) and males (b).

for the shape component and a log-Gaussian kernel for the size. Such a model induces a prior with support on the space of densities on the manifold $\Sigma_2^k \times \Re^+$.

ACKNOWLEDGEMENT

This research was partially supported by a grant from the National Institute of Environmental Health Sciences (NIEHS) of the National Institutes of Health, U.S.A.

APPENDIX

Lemma A1

To prove Theorems 1 and 2, we will need the following lemma. Let $\mathcal{M}(M)$ denote the space of all probability distributions on M.

LEMMA A1. Given $\epsilon > 0$, if there exists (i) a $\sigma_{\epsilon} > 0$ and $P_{\epsilon} \in \mathcal{M}(M)$ such that

$$\sup_{m\in M} |f_0(m) - f(m; P_{\epsilon}, \sigma_{\epsilon})| < \frac{\epsilon}{3},$$

(ii) a set $W \subseteq \Re^+$ containing σ_{ϵ} such that

$$\sup_{m \in M, \sigma \in W} |f(m; P_{\epsilon}, \sigma_{\epsilon}) - f(m; P_{\epsilon}, \sigma)| < \frac{\epsilon}{3},$$

and (iii) a set $W \subseteq \mathcal{M}(M)$ containing P_{ϵ} such that

$$\sup_{m \in M, P \in \mathcal{W}, \sigma \in W} |f(m; P_{\epsilon}, \sigma) - f(m; P, \sigma)| < \frac{\epsilon}{3},$$

then

$$\sup_{m \in M} |f_0(m) - f(m; P, \sigma)| < \epsilon$$

for all $(P, \sigma) \in \mathcal{W} \times W$.

Proof. Follows from a direct application of the triangular inequality.

Proof of Theorem 1. The result follows from Lemma A1 if we can find a $W \subseteq \Re^+$ and $W \subseteq \mathcal{M}(M)$ satisfying the conditions and $\Pi_1(W \times W) > 0$.

Condition (i) is satisfied with $P_{\epsilon} = F_0$ from Assumptions 2 and 4 by taking $\phi = f_0$. From Assumption 3, it follows that by taking σ_{ϵ} sufficiently small, we can ensure that $\sigma_{\epsilon} < \sigma_0$ and $(F_0, \sigma_{\epsilon}) \in \text{supp}(\Pi_1)$.

Next we need to find a W for which condition (ii) is satisfied. From Assumption 1, it follows that the mapping from σ to K is uniformly equicontinuous on some compact neighbourhood of σ_{ϵ} . Hence we can get a compact set W containing σ_{ϵ} in its interior such that

$$\sup_{(m,\mu,\sigma)\in M\times M\times W} |K(m;\mu,\sigma)-K(m;\mu,\sigma_{\epsilon})| < \frac{\epsilon}{3}.$$

^

Then

$$\sup_{m \in M, \sigma \in W} |f(m; F_0, \sigma) - f(m; F_0, \sigma_{\epsilon})| \leq \int_M \sup_{m \in M, \sigma \in W} |K(m; \mu, \sigma) - K(m; \mu, \sigma_{\epsilon})| f_0(\mu) \lambda(d\mu)$$
$$\leq \sup_{m, \mu \in M, \sigma \in W} |K(m; \mu, \sigma) - K(m; \mu, \sigma_{\epsilon})| < \frac{\epsilon}{3}.$$

This verifies condition (ii).

Lastly, we need to find a \mathcal{W} for which condition (iii) is satisfied and $\Pi_1(W \times \mathcal{W}) > 0$. We claim that

$$\mathcal{W} = \left\{ P \in \mathcal{M}(M) : \sup_{m \in \mathcal{M}, \sigma \in \mathcal{W}} |f(m; P, \sigma) - f(m; F_0, \sigma)| < \frac{\epsilon}{3} \right\}$$

contains a weakly open neighbourhood of F_0 . For any $m \in M$, $\sigma \in W$, the mapping from μ to $K(m; \mu, \sigma)$ defines a continuous function on M. Hence

$$\mathcal{W}_{m,\sigma} = \left\{ P : |f(m; P, \sigma) - f(m; F_0, \sigma)| < \frac{\epsilon}{9} \right\}$$

defines a weakly open neighbourhood of F_0 for any (m, σ) in $M \times W$. The mapping from (m, σ) to $f(m; P, \sigma)$ is a uniformly equicontinuous family of functions on $M \times W$, labelled by $P \in \mathcal{M}(M)$, because, for $m_1, m_2 \in M$; $\sigma, \tau \in W$,

$$|f(m_1; P, \sigma) - f(m_2; P, \tau)| \leq \int_M |K(m_1; \mu, \sigma) - K(m_2; \mu, \tau)| P(d\mu)$$

and K is uniformly continuous on $M \times M \times W$. Therefore, there exists a $\delta > 0$ such that $\rho(m_1, m_2) + |\sigma - \tau| < \delta$ implies that

$$\sup_{P\in\mathcal{M}(M)}|f(m_1;P,\sigma)-f(m_2;P,\tau)|<\frac{\epsilon}{9}.$$

Cover $M \times W$ by finitely many balls of radius $\delta: M \times W = \bigcup_{i=1}^{N} B\{(m_i, \sigma_i), \delta\}$. Let $\mathcal{W}_1 = \bigcap_{i=1}^{N} \mathcal{W}_{m_i,\sigma_i}$ which is an open neighbourhood of F_0 . Let $P \in \mathcal{W}_1$ and $(m, \sigma) \in M \times W$. Then there exists a (m_i, σ_i) such that $(m, \sigma) \in B\{(m_i, \sigma_i), \delta\}$. Then $|f(m; P, \sigma) - f(m; F_0, \sigma)|$

$$\leq |f(m; P, \sigma) - f(m_i; P, \sigma_i)| + |f(m_i; P, \sigma_i) - f(m_i; F_0, \sigma_i)| + |f(m_i; F_0, \sigma_i) - f(m; F_0, \sigma)|$$

$$< \frac{\epsilon}{9} + \frac{\epsilon}{9} + \frac{\epsilon}{9} = \frac{\epsilon}{3}.$$

This proves that W contains W_1 and hence the claim is proved. Clearly, this W satisfies condition (iii). Since (F_0, σ_{ϵ}) is in supp (Π_1) and in the interior of $W \times W$, therefore $\Pi_1(W \times W) > 0$. This completes the proof.

Proof of Corollary 1. Since *M* is compact, Assumption 5 implies that $c_0 = \inf_{m \in M} f_0(m) > 0$. For $\delta > 0$ define

$$\mathcal{W}_{\delta} = \left\{ (P, \sigma) : \sup_{m \in M} |f_0(m) - f(m; P, \sigma)| < \delta \right\}.$$

Then if $(P, \sigma) \in \mathcal{W}_{\delta}$,

$$\inf_{m \in M} f(m; P, \sigma) \ge \inf_{m \in M} f_0(m) - \delta \ge \frac{c_0}{2}$$

if we choose $\delta \leq c_0/2$. Then for any given $\epsilon > 0$,

$$\int_{M} f_{0}(m) \log \left\{ \frac{f_{0}(m)}{f(m; P, \sigma)} \right\} \lambda(dm) \leq \sup_{m \in M} \left| \frac{f_{0}(m)}{f(m; P, \sigma)} - 1 \right| \leq \frac{2\delta}{c_{0}} < \epsilon$$

if we choose $\delta < c_0 \epsilon/2$. Hence for δ sufficiently small, $f(\cdot; P, \sigma) \in \text{KL}(f_0, \epsilon)$ whenever $(P, \sigma) \in \mathcal{W}_{\delta}$, with $\text{KL}(f_0, \epsilon)$ denoting an ϵ -sized Kullback–Leibler neighbourhood around f_0 . From Theorem 1 it follows that $\Pi_1(\mathcal{W}_{\delta}) > 0$ for any $\delta > 0$ and therefore

$$\Pi_1\{(P,\sigma): f(\cdot; P,\sigma) \in \mathrm{KL}(f_0,\epsilon)\} > 0.$$

Proof of Theorem 2. From the proof of Corollary 1, it follows that given any $\delta_1 > 0$, we can find a $\sigma_1 > 0$ such that with $Q_1 = F_0 \times \delta_{\sigma_1}$,

$$\sup_{m \in M} |f_0(m) - g(m; Q_1)| < \delta_1, \quad \int_M f_0(m) \log\left\{\frac{f_0(m)}{g(m; Q_1)}\right\} \lambda(dm) < \delta_1.$$
(A1)

Hence, if we choose $\delta_1 \leq c_0/2$ where $c_0 = \inf_{m \in M} f_0(m) > 0$ then $\inf_{m \in M} g(m; Q_1) \geq c_0/2$. From Assumption 6 it follows that we can choose σ_1 sufficiently small such that $\sigma_1 < \sigma_0$ and $Q_1 \in \text{supp}(\Pi_2)$. Let *E* denote a compact subset of $(0, \sigma_0)$ containing σ_1 in its interior. Then, being continuous in its arguments, *K* is uniformly continuous on $M \times M \times E$. For *Q* in $\mathcal{M}(M \times \Re^+)$, define

$$g(m; Q_E) = \int_{M \times E} K(m; \mu, \sigma) Q(d\mu d\sigma).$$

For fixed $m \in M$, the integral mapping from Q to $g(m; Q_E)$ is continuous at Q_1 because

$$Q_1\{\partial(M \times E)\} = Q_1\{M \times \partial(E)\} = 0,$$

 $\partial(A)$ denoting the boundary of a set A. Therefore, for $\delta_2 > 0$ and $m \in M$,

$$\mathcal{W}_m(\delta_2) = \{ Q : |g(m; Q_E) - g(m; Q_1)| < \delta_2 \}$$

defines a weakly open neighbourhood of Q_1 . We also claim that

$$\mathcal{W} = \left\{ \mathcal{Q} : \sup_{m \in M} |g(m; \mathcal{Q}_E) - g(m; \mathcal{Q}_1)| < \delta_2 \right\},\$$

contains an open neighbourhood of Q_1 . To see this, choose a $\delta_3 > 0$ such that $\rho(m_1, m_2) < \delta_3$ implies that

$$\sup_{(\mu,\sigma)\in M\times E}|K(m_1;\mu,\sigma)-K(m_2;\mu,\sigma)|<\frac{\delta_2}{3}$$

which in turn implies

$$|g(m_1; Q_E) - g(m_2; Q_E)| < \frac{\delta_2}{3}$$
 (A2)

for all $Q \in \mathcal{M}(M \times \mathfrak{R}^+)$. Next cover M by finitely many balls of radius δ_3 : $M = \bigcup_{i=1}^N B(m_i, \delta_3)$. Then we show that $\mathcal{W} \supseteq \bigcap_{i=1}^N \mathcal{W}_{m_i}(\delta_2/3)$. To prove that, pick Q in $\bigcap_{i=1}^N \mathcal{W}_{m_i}(\delta_2/3)$. Then for i = 1, ..., N,

$$|g(m_i; Q_E) - g(m_i; Q_1)| < \delta_2.$$
(A3)

Choosing $m \in B(m_i, \delta_3)$, (A2) implies that

$$|g(m; Q_E) - g(m_i; Q_E)| < \frac{\delta_2}{3}$$
(A4)

for all $Q \in \mathcal{M}(M \times \mathfrak{R}^+)$. From (A3) and (A4) it follows that $|g(m; Q_E) - g(m; Q_1)|$

$$\leq |g(m; Q_E) - g(m_i; Q_E)| + |g(m_i; Q_E) - g(m_i; Q_1)| + |g(m_i; Q_1) - g(m; Q_1)| < \delta_2/3 + \delta_2/3 + \delta_2/3 = \delta_2$$

for any $m \in M$ and $Q \in \bigcap_{i=1}^{N} \mathcal{W}_{m_i}(\delta_2/3)$. Hence $\mathcal{W} \supseteq \bigcap_{i=1}^{N} \mathcal{W}_{m_i}(\delta_2/3)$, which is an open neighbourhood of Q_1 . Therefore, $\Pi_2(\mathcal{W}) > 0$. For $Q \in \mathcal{W}$,

$$\inf_{m\in M} g(m; Q_E) \ge \inf_{m\in M} g(m; Q_1) - \delta_2 \ge \frac{c_0}{4}$$

if $\delta_2 < \frac{c_0}{4}$. Then

$$\int_{M} f_{0}(m) \log\left\{\frac{g(m;Q_{1})}{g(m;Q)}\right\} \lambda(dm) \leqslant \int_{M} f_{0}(m) \log\left\{\frac{g(m;Q_{1})}{g(m;Q_{E})}\right\} \lambda(dm)$$
$$\leqslant \sup_{m \in M} \left|\frac{g(m;Q_{1})}{g(m;Q_{E})} - 1\right| \leqslant \frac{\delta_{2}}{c_{0}/4} < \delta_{1},$$
(A5)

provided δ_2 is sufficiently small. From (A1) and (A5) we deduce that, for $Q \in W$,

$$\int_{M} f_{0}(m) \log\left\{\frac{f_{0}(m)}{g(m;Q)}\right\} \lambda(dm)$$

$$= \int_{M} f_{0}(m) \log\left\{\frac{f_{0}(m)}{g(m;Q_{1})}\right\} \lambda(dm) + \int_{M} f_{0}(m) \log\left\{\frac{g(m;Q_{1})}{g(m;Q)}\right\} \lambda(dm) < \delta_{1} + \delta_{1} = \epsilon$$

if $\delta_1 = \epsilon/2$. Hence

$$\{g(\cdot; Q): Q \in \mathcal{W}\} \subseteq \mathrm{KL}(f_0, \epsilon)$$

and since $\Pi_2(\mathcal{W}) > 0$, therefore

$$\Pi_2\{Q: g(\cdot; Q) \in \mathrm{KL}(f_0, \epsilon)\} > 0$$

Since ϵ was arbitrary, the proof is completed.

Proof of Proposition 1. Express *K* as

$$K(m;\mu,\sigma) = c^{-1}(\sigma) \exp\left\{\frac{2 - d_E^2(m,\mu)}{2\sigma}\right\}$$

where $c(\sigma) = (\pi \sigma)^{(k-2)} \{ \exp(\sigma^{-1}) - \sum_{r=0}^{k-3} \sigma^{-r} / r! \}$ and Assumption 1 is satisfied. As the kernel is symmetric in *m* and μ , for $\phi \in C(\Sigma_2^k)$,

$$I(m) \equiv \phi(m) - \int_{\Sigma_{2}^{k}} K(m;\mu,\sigma)\phi(\mu)V(d\mu) = \int_{\Sigma_{2}^{k}} \{\phi(m) - \phi(\mu)\}K(m;\mu,\sigma)V(d\mu).$$
(A6)

Choose preshapes z and ν for m and μ , respectively, in the complex sphere CS^{k-2} , so that m = [z] and $\mu = [\nu]$. Let V_1 denote the volume form on CS^{k-2} . Then for any integrable function $\phi : \Sigma_2^k \to \Re$,

$$\int_{\Sigma_2^k} \phi(\mu) V(d\mu) = \frac{1}{2\pi} \int_{CS^{k-2}} \phi([\nu]) V_1(d\nu)$$

Hence the integral in (A6) can be written as

$$I(m) = \frac{c^{-1}(\sigma)}{2\pi} \int_{CS^{k-2}} \{\phi([z]) - \phi([\nu])\} \exp(\sigma^{-1}\nu^* z z^* \nu) V_1(d\nu).$$
(A7)

Consider a singular value decomposition of zz^* as $zz^* = U\Lambda U^*$ where $\Lambda = \text{diag}(1, 0, \dots, 0)$ and $U = [U_1, \dots, U_{k-1}]$ with $U_1 = z$. Then $\nu^* zz^* \nu = x^* \Lambda x = |x_1|^2$ where $x = U^* \nu = (x_1, \dots, x_{k-1})^T$. Make a

change of variables from v to x in (A7). This is an orthogonal transformation, so does not change the volume form. Then (A7) becomes

$$I(m) = \frac{\exp(\sigma^{-1})}{2\pi c(\sigma)} \int_{CS^{k-2}} \{\phi([z]) - \phi([Ux])\} \exp\left(\frac{|x_1|^2 - 1}{\sigma}\right) V_1(dx).$$
(A8)

Write $x_j = r_j^{1/2} \exp(i\theta_j)$ (j = 1, ..., k - 1), with $r = (r_1, ..., r_{k-1})^{\mathsf{T}} \in S_{k-2}$ and $\theta = (\theta_1, ..., \theta_{k-1})^{\mathsf{T}} \in (-\pi, \pi)^{k-1}$, so that $V_1(dx) = 2^{2-k} dr_1 \cdots dr_{k-2} d\theta_1 \cdots d\theta_{k-1}$. Hence (A8) can be written as

$$I(m) = 2^{1-k} \pi^{-1} \exp(\sigma^{-1}) c^{-1}(\sigma) \int_{S_{k-2} \times [0, 2\pi)^{k-1}} \{\phi([z]) - \phi([v(r, \theta, z)])\} \exp\left(\frac{r_1 - 1}{\sigma}\right) dr d\theta,$$
(A9)

with $y \equiv y(r, \theta, z) = \sum_{j=1}^{k-1} r_j^{1/2} \exp(i\theta_j) U_j$. Then $d_E^2([y], [z]) = 2(1 - r_1)$. For $d \in \Re^+$, define

$$\psi(d) = \sup\{|\phi(m_1) - \phi(m_2)| : m_1, m_2 \in \Sigma_2^k, d_E^2(m_1, m_2) \leq d\}$$

Then the absolute value of $\phi([z]) - \phi([y(r, \theta, z)])$ in (A9) is at most ψ {2(1 - r_1)}, so that

$$\sup_{m \in \Sigma_{2}^{k}} |I(m)| \leq \pi^{k-2} \exp(\sigma^{-1}) c^{-1}(\sigma) \int_{S_{k-2}} \psi\{2(1-r_{1})\} \exp\left(\frac{r_{1}-1}{\sigma}\right) dr_{1} \dots dr_{k-2}$$
$$= \pi^{k-2} (k-3)!^{-1} \exp(\sigma^{-1}) c^{-1}(\sigma) \int_{0}^{1} \psi\{2(1-r_{1})\} \exp\left(\frac{r_{1}-1}{\sigma}\right) (1-r_{1})^{k-3} dr_{1}.$$
(A10)

Make a change of variable $s = \sigma^{-1}(1 - r_1)$ to rewrite (A10) as

$$\sup_{m \in \Sigma_{2}^{k}} |I(m)| \leq \pi^{k-2} (k-3)!^{-1} \sigma^{k-2} \exp(\sigma^{-1}) c^{-1}(\sigma) \int_{0}^{\sigma^{-1}} \psi(2\sigma s) \exp(-s) s^{k-3} ds$$

$$\leq C_{k} c_{1}^{-1}(\sigma) \int_{0}^{\infty} \psi(2\sigma s) \exp(-s) s^{k-3} ds, \qquad (A11)$$

where $c_1(\sigma) = 1 - \exp(-\sigma^{-1})\sum_{r=0}^{k-3} \sigma^{-r}/r!$ and C_k is some constant depending on k. Since ϕ is uniformly continuous on the compact metric space $(\Sigma_2^k, d_E), \psi$ is bounded and $\lim_{d\to 0} \psi(d) = 0$. Also, it is easy to check that $\lim_{\sigma\to 0} c_1(\sigma) = 1$. Since $\exp(-s)s^{k-3}$ is integrable on $(0, \infty)$, using the Lebesgue Dominated Convergence Theorem on the integral in (A11), we conclude that

$$\lim_{\sigma\to 0} \sup_{m\in\Sigma_2^k} |I(m)| = 0$$

Hence Assumption 2 is also satisfied.

REFERENCES

- BHATTACHARYA, A. & BHATTACHARYA, R. N. (2008). Nonparametric statistics on manifolds with applications to shape spaces. In *Pushing the Limits of Contemporary Statistics: Contributions in Honor of J. K. Ghosh*, 282–301. IMS Collections 3. Bethesda, MD: Institute of Mathematical Statistics.
- BHATTACHARYA, R. N. & PATRANGENARU, V. (2003). Large sample theory of intrinsic and extrinsic sample means on manifolds. Ann. Statist. 31, 1–29.
- DRYDEN, I. L. & MARDIA, K. V. (1998). Statistical Shape Analysis. New York: Wiley.
- ESCOBAR, M. D. & WEST, M. (1995). Bayesian density-estimation and inference using mixtures. J. Am. Statist. Assoc. 90, 577–88.
- FERGUSON, T. S. (1973). A Bayesian analysis of some nonparametric problems. Ann. Statist. 1, 209-30.
- FERGUSON, T. S. (1974). Prior distributions on spaces of probability measures. Ann. Statist. 2, 615–29.
- KENDALL, D. G. (1984). Shape manifolds, procrustean metrics, and complex projective spaces. Bull. Lond. Math. Soc. 16, 81–121.
- KENT, J. (1994). The complex Bingham distribution and shape analysis. J. R. Statist. Soc. B 56, 285–99.
- KUME, A. & WALKER, S. G. (2006). Sampling from compositional and directional distributions. *Statist. Comp.* 16, 261–5.

864

LENNOX, K. P., DAHL, D. B. & VANNUCCI, M. A. (2009). Density estimation for protein conformation angles using a bivariate von Mises distribution and Bayesian nonparametrics. J. Am. Statist. Assoc. 104, 586–96.

Lo, A. Y. (1984). On a class of Bayesian nonparametric estimates. 1. Density estimates. Ann. Statist. 12, 351-57.

- MARDIA, K. V., TAYLOR, C. C. & SUBRAMANIAM, G. K. (2007). Protein bioinformatics and mixtures of bivariate von Mises distributions for angular data. *Biometrics* **63**, 505–12.
- NEAL, R. M. (2000). Markov chain sampling methods for Dirichlet process mixture models. J. Comp. Graph. Statist. 9, 249–65.
- PAPASPILIOPOULOS, O. & ROBERTS, G. O. (2008). Retrospective Markov chain Monte Carlo methods for Dirichlet process hierarchical models. *Biometrika* 95, 169–86.
- PELLETIER, B. (2005). Kernel density estimation on Riemannian manifolds. Statist. Prob. Lett. 73, 297–304.

SCHWARTZ, L. (1965). On Bayes procedures. Z. Wahr. verw. Geb. 4, 10-26.

STEPHENS, M. (2000). Dealing with label switching in mixture models. J. R. Statist. Soc. B 62, 795-809.

WATSON, G. (1965). Equatorial distributions on a sphere. Biometrika 52, 193-201.

- WATSON, G. S. (1983). *Statistics on Spheres*. University of Arkansas Lecture Notes in the Mathematical Sciences 6. New York: Wiley.
- WILLMORE, T. (1993). Riemannian Geometry. Oxford: Oxford University Press.
- WU, Y. & GHOSAL, S. (2008). Kullback–Leibler property of kernel mixture priors in Bayesian density estimation. *Electron. J. Statist.* 2, 298–331.

[Received October 2009. Revised April 2010]