Score matching estimators for directional distributions

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Abstract

One of the major problems for maximum likelihood estimation in the well-established directional models is that the normalising constants can be difficult to evaluate. A new general method of “score matching estimation” is presented here on a compact oriented Riemannian manifold. Important applications include von Mises-Fisher, Bingham and joint models on the sphere and related spaces. The estimator is consistent and asymptotically normally distributed under mild regularity conditions. Further, it is easy to compute as a solution of a linear set of equations and requires no knowledge of the normalizing constant. Several examples are given, both analytic and numerical, to demonstrate its good performance.

Some key words: Exponential family, Fisher-Bingham distribution, Riemannian manifold, sphere, torus, von Mises distribution.

1 Introduction

A novel “score matching estimator” was proposed in Hyvärinen (2005, 2007) as an alternative to the maximum likelihood estimator. For exponential family models, a key advantage of this new estimator is that it avoids the need to work with awkward normalizing constants. A minor limitation is that it requires the underlying distributions to have sufficiently smooth probability densities.

The score matching estimator was originally developed for densities on Euclidean space. The extension to Riemannian manifolds was sketched in Dawid and Lauritzen (2005) and Parry et al. (2012), but without a detailed analysis. Here we give a systematic investigation on a compact oriented Riemannian manifold $M$. The main focus is on exponential family models. Key applications include the Fisher-Bingham and multivariate von Mises distributions, which lie on spheres and related spaces.
2 Background on Riemannian manifolds

A $p$-dimensional Riemannian manifold $M$, say, is characterized by a metric tensor $G = G(x) = (g_{ij}(x))$, where $G(x)$ is a $p \times p$ symmetric positive definite matrix. Here $x$ is a $p$-dimensional vector representing a typical element of $M$ in local coordinates. Let $G^{-1}(x) = (g^{-1}_{ij}(x))$ denote the inverse matrix. A uniform measure on $M$ can be defined in local coordinates by

$$\mu(dx) = \left\{ \text{det}(G(x)) \right\}^{1/2} dx.$$  

See, e.g., Jost (2005); Rosenberg (1997); Stein and Weiss (1971) for a background on Riemannian manifolds.

Next, let $u = u(x), \ v = v(x), \ x \in M$, be two real-valued functions on $M$. Let $\nabla u = (\partial u/\partial x_j, \ j = 1, \ldots, p)^T$ denote the gradient in local coordinates, i.e. the column vector of partial derivatives. An inner product on gradient vectors can be defined by

$$\langle u, v \rangle = \langle u, v \rangle(x) = (\nabla u)^T G^{-1} (\nabla v),$$  

treated as a function of the local coordinate vector $x$.

The Laplace-Beltrami operator, acting on $u$, is defined in local coordinates by

$$\Delta_M u = \sum_{i,j=1}^{p} \left\{ \text{det}(G(x)) \right\}^{-1/2} \partial/\partial x_i \left[ \left\{ \text{det}(G(x)) \right\}^{1/2} g^{ij}(x) \partial u/\partial x_j \right].$$  

treated as a function of the local coordinate vector $x$. Although the gradient vector $\nabla u$ depends on the choice of local coordinates, the uniform measure $\mu(dx)$, the gradient inner product (1) and the Laplace-Beltrami operator (2) are invariant under a change of local coordinates.

Stokes’ Theorem, also known as the divergence theorem, connects the gradient inner product and the Laplace-Beltrami operator. Further, if $M$ is assumed compact and oriented, there is no need for boundary conditions.

**Theorem 1** (Stokes’ Theorem). If $M$ is a compact oriented Riemannian manifold and $u(x), \ v(x)$ are twice continuously differentiable functions on $M$, then

$$\int_M \langle u, v \rangle(x) \mu(dx) = - \int_M (\Delta_M u) v \mu(dx).$$  

If $M$ is isometrically embedded as a $p$-dimensional surface in a Euclidean space, $M \subset \mathbb{R}^q$, then a point in $M$ can be represented either as a $p$-dimensional vector $x$ in local coordinates or as a $q$-dimensional vector $z = (z_1, \ldots, z_q)^T$, say, in Euclidean coordinates. In this setting it is possible to give simpler representations of the gradient inner product and the Laplace-Beltrami operators.

Given a point $z$ in $M$, the tangent plane to $M$ at $z$ is a $p$-dimensional hyperplane. Let $P(z) = P = (p_{ij})$ denote the $q \times q$ orthogonal projection matrix onto this hyperplane. Then $P = P^T$, $P = P^2$ and $P$ has rank $p$. Suppose the functions $u$ and $v$ have been extended to a neighbourhood $N$ of $M$ as functions $\tilde{u}(z), \ \tilde{v}(z)$ of $z \in N \subset \mathbb{R}^q$, and define the usual Euclidean gradient

$$\nabla_E \tilde{u} = (\partial \tilde{u}/\partial z_j, \ j = 1, \ldots, q)^T.$$
The gradient inner product and the Laplace-Beltrami operator were given by (1) and (2) in local coordinates. They can also be written in Euclidean coordinates as
\[
\langle u, v \rangle = (\nabla_E \tilde{u})^T P (\nabla_E \tilde{v}) = (P \nabla E \tilde{u})^T (P \nabla E \tilde{v})
\]
and
\[
\Delta_M u = \text{tr} \left\{ P \nabla^T E (P \nabla E \tilde{u}) \right\} = \sum_{i,j,k=1}^q p_{ij} \partial / \partial z_i (p_{jk} \partial \tilde{u} / \partial z_k).
\]
Note the derivatives in (4) are \( q \)-dimensional whereas the derivatives in (1) are \( p \)-dimensional; however, the inner product is the same.

The simplest example is the sphere \( S_2 = \{ z \in \mathbb{R}^3 : z^T z = 1 \} \). In polar coordinates, \( x = (\theta, \phi)^T \) with \( \theta \) colatitude and \( \phi \) longitude, the metric tensor becomes
\[
G = \begin{bmatrix}
1 & 0 \\
0 & \sin^2 \theta
\end{bmatrix},
\]
and the uniform measure becomes \( \sin \theta d\theta d\phi \). The Laplace-Beltrami operator becomes
\[
\Delta_M u = \partial^2 u / \partial \theta^2 + \cot \theta \partial u / \partial \theta + (\sin \theta)^{-2} \partial^2 u / \partial \phi^2.
\]
The Euclidean embedding takes the form \( z_1 = \cos \theta, \ z_2 = \sin \theta \cos \phi, \ z_3 = \sin \theta \sin \phi \), and the projection matrix is \( P = I_3 - zz^T \). It is straightforward to check that gradient inner products in (1) and (4) are two ways of writing the same function.

3 The score matching criterion on a compact oriented Riemannian manifold

One way to motivate a statistical estimator is through the minimization of a divergence between two probability distributions. The most common example is the Kullback-Liebler divergence, which leads to the maximum likelihood estimator. In this paper we use a divergence due to Hyvärinen, which leads to the score matching estimator.

Let \( f \) and \( f^* \) be two probability densities on a Riemannian manifold \( M \), defined with respect to the uniform measure \( \mu \), where \( f \) and \( f^* \) are assumed to be everywhere nonzero and twice continuously differentiable. Define the Hyvärinen divergence (Hyvärinen, 2005, 2007) between the two densities in terms of an integrated gradient inner product for the log ratio,
\[
\Phi(f; f^*) = \frac{1}{2} \int_M \langle \log(f / f^*), \log(f / f^*) \rangle f^*(x) \mu(dx)
\]
\[
= \frac{1}{2} \int_M \{ \langle \log f, \log f \rangle - 2\langle \log f, \log f^* \rangle + \langle \log f^*, \log f^* \rangle \} f^*(x) \mu(dx).
\]
Hyvärinen proposed this divergence in the setting where $M$ is a Euclidean space. In this setting the metric tensor $G = I$ is hardly needed, and the gradient inner product simplifies to $\langle u, v \rangle = \sum_{j=1}^{p} (\partial u / \partial x_j)(\partial v / \partial x_j)$.

For the rest of the paper we limit attention to the setting where $M$ is compact and oriented. In some ways this setting is more complicated than the Euclidean case. The gradient inner product $\langle \cdot \rangle$ is now given by (1); it can also be written as (4) when the manifold $M$ can be embedded in a Euclidean space. However, in other ways this setting is simpler. Stokes’ Theorem (3) holds automatically without the need for boundary conditions and all continuous functions on $M$ are automatically bounded and integrable.

Two simple properties ensure that minimizing (5) over $f$ is an identifiable approach to finding $f^*$.

**Property 1.** If $f = f^*$, then $\Phi(f; f^*) = 0$.

**Property 2.** If $f \neq f^*$, then $\Phi(f; f^*) > 0$.

To prove these properties note by inspection in (5) that $\Phi(f; f^*) \geq 0$ for all choices of densities and that $\Phi(f^*; f^*) = 0$. Conversely, if $f \neq f^*$, then we claim there must be at least one point $x$ in some set of local coordinates such that $\nabla f(x) \neq \nabla f^*(x)$; hence the integral must be strictly positive. For if there were no such $x$, a contradiction would arise: the gradients would be everywhere equal and so the densities would be the same up to a proportionality constant; further, since both densities integrate to 1, the proportionality constant would have to equal 1.

For fitting purposes, let $f^*(x)$ be regarded as the “true” distribution of the data and let $f(x) = f(x; \pi)$ denote a parametric model, where $\pi$ is an $m$-dimensional vector of parameters. Then a “best-fitting” model can be defined by minimizing $\Phi(f; f^*)$ over the parameters $\pi$.

Since the final term in (5) does not depend on $f$, it can be dropped from the minimization criterion. Further, by Stokes’ Theorem and the simple result, $\partial \log f^*(x)/\partial x_j = \{f^*(x)\}^{-1}\partial f^*(x)/\partial x_j$, the middle term becomes

$$- \int_M \langle \log f, \log f^* \rangle f^*(x) \mu(dx) = - \int_M \langle \log f, f^* \rangle (f^*)^{-1} f^*(x) \mu(dx)$$

$$= - \int_M \langle \log f, f^* \rangle \mu(dx)$$

$$= \int_M (\Delta_M \log f) f^*(x) \mu(dx).$$

The final term in (5) does not depend on $f$. Hence minimizing $\Phi(f; f^*)$ over the parameters $\pi$ in $f$ is equivalent to minimizing

$$\Psi(f; f^*) = \frac{1}{2} \int_M \{\langle \log f, \log f \rangle + 2(\Delta_M \log f)\} f^*(x) \mu(dx)$$

$$= \frac{1}{2} E \{\langle \log f, \log f \rangle + 2(\Delta_M \log f)\},$$

(6)
where $E$ denotes expectation under the measure $f^*(x)\mu(dx)$. At this stage it is no longer necessary to impose any regularity conditions on $f^*$; indeed it can be replaced by any probability measure $F^*$, say, in which case we write $\Psi(f, F^*)$.

For the rest of the paper we specialize to the case where $f(x; \pi)$ forms a canonical exponential family on a compact oriented Riemannian manifold $M$ with density

$$f(x) = f(x; \pi) \propto \exp\{\pi^T t(x)\}$$

(7)

with respect to the uniform measure $\mu(dx)$, where $\pi$ is an $m$-vector of natural parameters and $t(x) = (t_1(x), \ldots, t_m(x))$ is a vector of sufficient statistics. The sufficient statistics are assumed to satisfy the following regularity conditions.

A1 The constant function 1 and the functions $t_\ell(x)$ ($\ell = 1, \ldots, m$) are linearly independent on $M$.

A2 The functions $t_\ell(x)$ ($\ell = 1, \ldots, m$) are twice continuously differentiable with respect to $x$.

The first assumption ensures the identifiability of $\pi$; different values of $\pi$ correspond to different distributions. The second assumption justifies the use of Stokes’ Theorem.

In this exponential family setting (6) simplifies to

$$\Psi(f; F^*) = \frac{1}{2} \pi^TW\pi - \pi^Td,$$

(8)

where $W = (w_{\ell_1\ell_2})$ and $d = (d_\ell)$ have elements

$$w_{\ell_1\ell_2} = E\{(t_{\ell_1}, t_{\ell_2})(x)\}, \quad d_\ell = -E\{\Delta_M t_\ell(x)\} \quad (\ell, \ell_1, \ell_2 = 1, \ldots, m).$$

(9)

Minimizing (8) yields the moment equation $W\pi - d = 0$. In particular, if the “true” distribution $F^*(dx) = f(x; \pi_0)$ lies in the parametric family, it follows that $\pi_0$ can be recovered from the moments in $W$ and $d$ by

$$\pi_0 = W^{-1}d.$$

The identifiability property, Property 2 mentioned below [3], implies that $W$ must be nonsingular. In later sections we illustrate how to calculate $W$ and $d$ in particular cases.

In many examples the components of $t(x)$ are eigenfunctions of the Laplace-Beltrami operator, so that $\Delta_M t_\ell(x) = -\lambda_\ell t_\ell(x)$, for suitable constants $\lambda_\ell > 0$ ($\ell = 1, \ldots, m$) See, e.g., [Patrangenaru and Ellingson (2016, Ch 3.3)] for the eigenfunctions of various manifolds arising in Statistics; the specific example of the sphere is discussed below.

4 The score matching estimator and its properties

Let $F^* = F_n$ denote the empirical distribution for a set of data $\{x_h, h = 1, \ldots, n\}$. The value $\hat{\pi}$ minimizing $\Psi(f; F_n)$ is called the score matching estimator. More
explicitly,

\[ \hat{\pi}_{\text{SME}} = W_n^{-1} d_n, \]

where \( W_n \) and \( d_n \) are obtained from (9) after replacing the expectation under \( F^* \) by a sample average over the \( n \) data points.

To discuss the asymptotic sampling properties of the score matching estimator, suppose the data comprise a random sample from the exponential family model \( f(x; \pi) \) with \( \pi = \pi_0 \). Since \( W \) is nonsingular in the population case, it follows from the strong law of large numbers, that \( W_n \) must be positive definite with probability 1 for sufficiently large \( n \). This point has not generally been emphasized in the literature.

Further, in many models this nonsingularity statement about \( W_n \) can be strengthened to conclude that there is a fixed value \( n_0 \), depending on the model but not on the data, such that \( W_n \) must be positive definite with probability 1 for \( n \geq n_0 \). An analogous result for the \( p \)-dimensional multivariate normal distribution states that the sample covariance matrix is guaranteed to be positive definite with probability 1 for \( n \geq p + 1 \).

The limiting behaviour of \( \hat{\pi} \) is straightforward to describe. By the central limit theorem, \( d_n \) and \( W_n \) are asymptotically jointly normally distributed with population means \( d \) and \( W \). Hence by the delta method, it follows that

\[ n^{1/2}(\hat{\pi}_{\text{SME}} - \pi_0) \sim N_m(0, \Omega) \]

for some limiting covariance matrix \( \Omega \). Further, by the asymptotic optimality of maximum likelihood, \( \Omega \geq \mathcal{I}^{-1} \) under the usual ordering for positive semi-definite matrices, where \( \mathcal{I} \) denotes the Fisher information matrix.

The discussion here is limited to the exponential family case. Forbes and Lauritzen (2014) note that extra regularity conditions are needed for consistency and asymptotic normality when looking at score matching estimation for more general densities.

The term “score” has several distinct connotations in estimation. (a) Conventionally, the “score” refers to a derivative of the log likelihood with respect to the parameters; it has close connections to maximum likelihood estimation. (b) However, in the context of the score matching estimator, the “score” refers to the derivative of the log likelihood with respect to the state variable \( x \). (c) In addition, the term “scoring rule” (e.g., Forbes and Lauritzen, 2014; Parry et al., 2012) refers to a more general function of \( x \) and a distribution. Each scoring rule determines a divergence, and the minimization of the divergence leads to an estimator. A scoring rule is different from the scores in (a) and (b), though suitable choices for scoring rules lead to both the maximum likelihood and score matching estimators.

5 Details for the sphere

For this paper the most important choice for the manifold \( M \) is the unit sphere \( S_p = \{ z \in \mathbb{R}^q : \sum z_j^2 = 1 \} \), a \( p \)-dimensional manifold embedded in \( \mathbb{R}^q \), \( q = p + 1 \).
There are two natural coordinate systems: embedded Euclidean coordinates $z$ and local coordinates $x$, i.e. polar coordinates in this case.

First we set out the key steps for the derivative calculations. Let $\tilde{u}(z)$ denote a scalar-valued function in Euclidean coordinates. The projected Euclidean gradient vector becomes

$$P\nabla_E \tilde{u} = (I - zz^T)\nabla_E \tilde{u}, \quad P = I_q - zz^T.$$ 

The eigenfunctions of $\Delta_M$ on $S_p$, $p \geq 1$, are known as the spherical harmonics. A spherical harmonic of degree $k \geq 0$ has eigenvalue $-\lambda_k$ where $\lambda_k = k(k+p-1) = k(k+q-2)$; see, e.g., Chavel (1984, p. 35), Patrangenaru and Ellingson (2016, p. 125). The action of $\Delta_M$ on the linear and quadratic spherical harmonics, expressed in Euclidean coordinates, can be summarized as follows,

\begin{alignat}{2}
\Delta_M z_j &= -\lambda_1 z_j, \\
\Delta_M (z_i^2 - z_j^2) &= -\lambda_2 (z_i^2 - z_j^2), \\
\Delta_M (z_i z_j) &= -\lambda_2 (z_i z_j), 
\end{alignat} 

where $i \neq j \in \{1, \ldots, q\}$. A systematic construction of higher order spherical harmonics is given in Stein and Weiss (1971, pp. 137–152), but they will not be needed here. Statistical models involving spherical harmonics of degree greater than two are straightforward in principle (e.g. Beran, 1979), but in practice the components of $t(z)$ will usually consist of linear and quadratic functions of $z$.

To illustrate these calculations, consider the Fisher-Bingham density on $S_p$,

$$f(z) \propto \exp \left\{ b^T z + z^T A z \right\}, \quad (11)$$

where $b$ is a $q$-vector, and $A$ is a $q \times q$ symmetric matrix, $q = p + 1$. To ensure identifiability, the side condition $\sum_{j=1}^q a_{jj} = 0$ is imposed.

The density can be recast as

$$f(z) \propto \exp \left\{ b_1 z_1 + \cdots + b_q z_q + a_{11} (z_1^2 - z_q^2) + \cdots + a_{q-1,q-1} (z_{q-1}^2 - z_q^2) + a_{12} (2z_1 z_2) + \cdots + a_{1q} (2z_1 z_q) + \cdots + a_{q-1,q} (2z_{q-1} z_q) \right\}$$

$$= \exp \left\{ \sum_{\ell=1}^m \pi_{\ell} t_{\ell}(z) \right\}.$$ 

Here the vector $\pi$ denotes the $m = q + q - 1 + q(q-1)/2$ parameters in $b$ and $A$ in the order listed, and the vector $t = t(z)$ denotes the corresponding functions of $z$; that is, the linear terms, the diagonal quadratic terms, and the cross-product quadratic terms, respectively.

Next we gather the information needed to evaluate $W$ and $d$ in (9). For each sufficient statistic $t_\ell = t_\ell(z)$, create a vector-valued function $u_\ell = u_\ell(z) = \nabla_E t_\ell(z)$ by taking its Euclidean gradient, and create a scalar-valued function $v_\ell = v_\ell(z) = z^T u_\ell$. Then create an $m \times m$ matrix $W$ with entries

$$w_{\ell_1 \ell_2} = E \{ u_{\ell_1}^T u_{\ell_2} - v_{\ell_1} v_{\ell_2} \}. \quad (12)$$
Table 1: Gradient details for the Fisher-Bingham density \((11)\) on \(S_q\). Here \(t_\ell(z)\) and \(v_\ell(z)\) are scalars; \(u_\ell(z)\) is a \(q\)-dimensional vector. Also \(e_j\) represents a unit vector along the \(j\)th coordinate axis \((j = 1, \ldots, q)\).

\[
\begin{array}{ccc}
t_\ell(z) & u_\ell(z) & v_\ell(z) \\
z_j & e_j & z_j \\
z_j^2 - z_p^2 & 2(z_je_j - z_qe_q) & 2(z_j^2 - z_q^2) \\
2z_iz_j & 2(z_ie_j + z_je_i) & 4z_iz_j.
\end{array}
\]

Table 1 gives the entries for \(u_\ell\) and \(v_\ell\). Also create a vector \(d\) with entries

\[
d_\ell = -E\{\Delta_M t_\ell(z)\},
\]

using equation \((10)\) to evaluate the Laplace-Beltrami operator.

6 Hybrid estimators and reduced models

The parameters for directional distributions can typically be split into two parts: the concentration parameters and the orientation parameters, where the normalizing constant depends just on the concentration parameters. Further it is often possible to estimate the orientation parameters explicitly using sample moments. Often this orientation estimator can be viewed as an exact or an approximate maximum likelihood estimator, and it can be computed without needing estimates of the concentration parameters.

Further, if the orientation parameters are known, then the distribution of the data becomes a natural exponential family for the concentration parameters. We call this latter model reduced because the number of concentration parameters is smaller than the number of original parameters.

Hence, the following hybrid strategy provides a tractable estimation procedure:

(a) Split the parameters for the full model into orientation and concentration parameters.
(b) Estimate the orientation parameters for the original data and the transform the data to a standardized form.
(c) After standardization, the estimated orientation parameters take a simple canonical form. Treating them as known for the standardized data, the concentration parameters become natural parameters in a reduced exponential family.
(d) Use the score matching estimator to estimate the concentration parameters of the reduced model for the standardized data.
Table 2: Log densities for various standard directional distributions in full and reduced form. In full form, the models include both orientation and concentration parameters. In reduced form there are just concentration parameters. The models named in square brackets are too general to have a useful reduced form, but the submodels listed below them do have a useful reduced form. The first four models lie on the sphere $S_p$. The final two models are multivariate (MV) von Mises models lying on the torus $(S_1)^k$.

| Name                | Full                     | Reduced                  |
|---------------------|--------------------------|--------------------------|
| von Mises-Fisher    | $\mu^T z$               | $\kappa z_1$            |
| Bingham             | $z^T A z$                | $z^T \Lambda z = \sum_{j=1}^{q-1} \lambda_j (z_j^2 - z_p^2)$ |
| [Fisher-Bingham]    | $\mu^T z + z^T A z$     | $\kappa z_1 + \beta (z_2^2 - z_3^2)$ |
| Kent                | $A \mu = 0$; $\lambda_1 = 0$, $\lambda_2 = -\lambda_3 = \beta$ | $\kappa z_1 + \beta (z_2^2 - z_3^2)$ |
| [MV von Mises]      | $\sum_{r=1}^{k} \mu^{(r)} T z^{(r)} + \sum_{r<s} z^{(r)} T \Omega^{(r,s)} z^{(s)}$ | $\kappa z_1$ |
| MV von Mises sine   | $\left\{ \begin{array}{l} \sum_{r=1}^{k} \kappa^{(r)} c_r' + \sum_{r<s} \lambda^{(rs)} s_r s_s' \\ c_r' = \cos \theta^{(r)}; s_r' = \sin \theta^{(r)}; \\ \theta^{(r)} = \theta^{(r)} - \theta_0^{(r)} \end{array} \right.$ | Set $\theta_0^{(r)} = 0.$ |

The resulting estimator can be called the *hybrid score matching estimator* and denoted by $\hat{\pi}_{\text{SME,hybrid}}$.

The next section gives several examples from directional statistics to illustrate this estimation strategy. Table 2 summarizes the form of each density. See, e.g., [Jammalamadaka and Sengupta (2001); Mardia and Jupp (2000)] for background information on these distributions. The first three examples lie on the sphere $M = S_p$; the last example lies on the torus, a direct product of $k$ circles, $M = (S_1)^k$. In each case the details (a)–(d) are specified explicitly.

In all cases we assume a sample of size $n$ from the stated distribution. On the sphere the data are represented by an $n \times q$ matrix $Z$ whose rows $z_h^T$ $(h = 1, \ldots, n)$, say, are $q$-dimensional unit vectors in Euclidean coordinates. The models are special cases of the Fisher-Bingham density (11) and Table 1 gives the details needed for the gradient calculations. On the torus, it is more convenient to use polar coordinates to represent the data as an $n \times k$ matrix $\Theta$ of angles lying in $[0, 2\pi)$, with gradient calculations carried out directly. In each case the key step is to derive the formulas for the matrix $W_n$ and the vector $d_n$ in the reduced model.
7 Directional distributions

7.1 von Mises-Fisher distribution

(a) The density for the full von Mises-Fisher distribution takes the form in (7) with $t(z) = (z_1, \ldots, z_q)^T$ being the vector of linear functions in $z$. This model forms a canonical exponential family. The parameter vector can be written $\pi = \kappa \mu_0$ where $\kappa \geq 0$ is a scalar concentration parameter and $\mu_0$ is a unit orientation vector. On the circle, it is sometimes convenient to write $\mu_0 = (\cos \theta_0, \sin \theta_0)^T$ in polar coordinates.

(b) For the data matrix $Z(n \times q)$, the sufficient statistic is the $q$-dimensional sample mean vector $\bar{z}$. The maximum likelihood estimate of $\mu_0$ is the unit vector $\hat{\mu}_0, \text{MLE} = z/||z||$ and is also the hybrid score matching estimator. Let $R$ be a $q \times q$ orthogonal matrix such that $R^T \hat{\mu}_0, \text{MLE} = e_1$, where $e_1$ is a unit vector along the first coordinate axis in $\mathbb{R}^q$, and let $Y = ZR$, i.e. $y_h = R^T z_h$ ($h = 1, \ldots, n$), denote the standardized data.

(c) As shown in Table 2, the reduced model for $Y$ involves just a single concentration parameter $\kappa$.

(d) For the reduced model, $W_n$ and $d_n$ in (12)–(13) are one-dimensional,

$$W_n = 1 - \frac{1}{n} \sum y_{h1}^2, \quad d_n = (q - 1) \sum y_{h1},$$

so that the hybrid score matching estimator of $\kappa$ becomes

$$\hat{\kappa}_{\text{SME, hybrid}} = d_n/W_n, \quad (14)$$

expressed in terms of the first two sample moments of the standardized data. All sums here and below range over $h = 1, \ldots, n$.

The score matching estimator for the von Mises distribution can also be derived from the two trigonometric moments,

$$E(\cos \nu \theta) = I_\nu(\kappa)/I_0(\kappa), \quad \nu \geq 0,$$

for $\nu = 1, 2$. Using the Bessel function identity

$$I_{\nu+1}(\kappa) = I_{\nu-1}(\kappa) - \frac{2\nu}{\kappa} I_\nu(\kappa) \quad (15)$$

with $\nu = 1$ and simplifying yields the population version of (14) for the circle, $q = 2$. Analogous results using Legendre polynomials yield the population version of (14) for larger values of $q$.

If $q = 2$ and the data are represented in polar coordinates, $(z_{h1}, z_{h2}) = (\cos \theta_h, \sin \theta_h)$ ($h = 1, \ldots, n$), then the score matching estimators can be recast in polar coordinates. In particular, the estimated orientation angle for the hybrid score matching estimator is
\[ \hat{\theta}_{0,\text{SME,hybrid}} = \hat{\theta}_{0,\text{MLE}} = \text{atan2}(\bar{S}, \bar{C}) = \hat{\theta}_0, \text{ say,} \] (16)

where \( \text{atan2}(.) \) is defined so that \( \text{atan2}(y, x) = \theta \) if and only if \( (\cos \theta, \sin \theta)^T \propto (x, y)^T \) for \( x^2 + y^2 > 0 \), and where

\[ \bar{C} = \frac{1}{n} \sum \cos \theta_h, \quad \bar{S} = \frac{1}{n} \sum \sin \theta_h, \quad \bar{R} = \sqrt{\bar{S}^2 + \bar{C}^2}. \]

The hybrid score matching estimator of \( \kappa \) can be re-expressed as

\[ \hat{\kappa}_{\text{SME,hybrid}} = \frac{\sum \cos(\theta_h - \bar{\theta})}{\sum \sin^2(\theta_h - \bar{\theta})} = \frac{n\bar{R}}{\sum \sin^2(\theta_h - \bar{\theta})}. \] (17)

The full score matching estimator on the circle is also straightforward to derive, with \( m = 2 \) and sufficient statistics \( t_1(\theta) = \cos \theta \) and \( t_2(\theta) = \sin \theta \). Set \( \bar{C}_2 = \frac{1}{n} \sum \cos 2\theta_h, \bar{S}_2 = \frac{1}{n} \sum \sin 2\theta_h, \bar{R}_2 = (\bar{C}_2^2 + \bar{S}_2^2)^{1/2} \). Then \( W_n \) and \( d_n \) have elements

\[ w_{11}^{(n)} = \frac{1}{2}(1 - \bar{C}_2), \quad w_{12}^{(n)} = -\frac{1}{2}\bar{S}_2, \quad w_{22}^{(n)} = \frac{1}{2}(1 + \bar{C}_2), \]

and \( d_1^{(n)} = \bar{C}, \ d_2^{(n)} = \bar{S} \). Since \( |W_n| = (1 - \bar{R}_2^2)/4 \), the full score matching estimator becomes

\[ \hat{\theta}_{0,\text{SME}} = \text{atan2}\{\bar{C}\bar{S}_2 + \bar{S}(1 - \bar{C}_2), \bar{C}(1 + \bar{C}_2) + \bar{S}\bar{S}_2\} \]

\[ \hat{\kappa}_{\text{SME}} = 2\{\bar{R}_2^2(1 + \bar{R}_2^2) + 2(\bar{C}^2 - \bar{S}^2)\bar{C}_2 + 4\bar{C}\bar{S}\bar{S}_2\}^{1/2}/(1 - \bar{R}_2^2). \]

After rotating the data so that \( \bar{S} = 0 \), the full score matching estimate of \( \kappa \) turns out to be the same as the hybrid estimate if \( \bar{S}_2 = 0 \).

### 7.2 Bingham distribution

(a) The parameter matrix \( A \) for the Bingham distribution in Table 2 is a symmetric \( q \times q \) matrix, where without loss of generality, the trace of \( A \) may be taken to be 0. If \( A = \Gamma \Lambda \Gamma^T \) is the spectral decomposition of \( A \), then the orthogonal matrix \( \Gamma = [\gamma_{(1)}, \ldots, \gamma_{(q)}] \), whose columns are eigenvectors of \( A \), represents the orientation parameters and the eigenvalues \( \Lambda = \text{diag}(\lambda_j) \) represent the concentration parameters, with \( \sum_{j=1}^q \lambda_j = \text{tr}(A) = 0 \).

(b) Given the \( n \times q \) original data matrix \( Z \) calculate the moment of inertia matrix \( T(Z) = (1/n)Z^TZ \) and find its spectral decomposition \( T(Z) = GLG^T \). Then the maximum likelihood estimate of \( \Gamma \) is \( G \). Define the standardized data matrix by \( Y = ZG \).

(c) In the reduced model, the matrix \( A \) simplifies to the diagonal matrix \( \Lambda \), with \( y^T \Lambda y = \sum_{j=1}^{q-1} \lambda_j (y_j^2 - y_j^2) \) since \( \sum_{j=1}^q \lambda_j = 0 \).
(d) For the reduced model \( \pi \) becomes the parameters \( \lambda_j (j = 1, \ldots, q - 1) \) and the estimates \( W_n \) and \( d_n \) have entries for \( i, j = 1, \ldots, q - 1 \),

\[
\begin{align*}
w_{ij}^{(n)} &= \begin{cases} 
\frac{4}{n} \sum \left(y_{hi}^2 + y_{hq}^2 - (y_{hi}^2 - y_{hq}^2)^2\right), & i = j \\
\frac{4}{n} \sum \left(y_{hq}^2 - (y_{hi}^2 - y_{hq}^2)(y_{hj}^2 - y_{hq}^2)\right), & i \neq j 
\end{cases} 
\end{align*}
\]

and

\[
d_i^{(n)} = \frac{2q}{n} \sum (y_{hi}^2 - y_{hq}^2).
\]

7.3 Kent distribution

The Fisher-Bingham distribution in Table 2 has \( q^2 + 3q - 2 \) parameters which can be estimated by the score matching estimator. However, this distribution has too many parameters to be of much interest in practice. Instead it is more useful to consider sub-families of this distribution. One such sub-family for \( S_2 \) is the 5-parameter FB5 distribution, also known as the Kent distribution, which forms a curved exponential family.

(a) For the Kent distribution, \( \mu = \kappa \gamma (1) \) is assumed to be an eigenvector of \( A = \Gamma \Lambda \Gamma^T \) with eigenvalue \( \lambda_1 = 0 \); the other two eigenvalues are assumed to be of equal size with opposite signs, \( \lambda_2 = -\lambda_3 = \beta \). The orthogonal matrix \( \Gamma \) contains the orientation parameters and there are two concentration parameters, \( \kappa \geq 0 \) and \( \beta \geq 0 \).

(b) Kent (1982) describes a moment estimator \( \hat{\Gamma} \) for the orientation matrix, which will also be used for the hybrid score matching estimator. After standardizing to \( Y = \tilde{Y} \hat{\Gamma} \), the sample mean vector becomes \( \bar{y} = (\tilde{R}, 0, 0)^T \) and the moment of inertia matrix \( T(Y) = (1/n)Y^TY \) satisfies \( (T(Y))_{23} = (T(Y))_{32} = 0 \) and \( (T(Y))_{22} - (T(Y))_{33} \geq 0 \).

(c) The reduced form of the distribution is given in Table 2 with \( \pi = (\kappa, \beta)^T \) having two components.

(d) The estimates \( W_n \) and \( d_n \) have entries

\[
\begin{align*}
w_{11}^{(n)} &= 1 - \sum y_{h1}^2, \quad w_{12}^{(n)} = w_{21}^{(n)} = \frac{2}{n} \sum y_{h1}(y_{h3} - y_{h2}^2), \\
w_{22}^{(n)} &= \frac{4}{n} \sum \left(y_{h2}^2 + y_{h3}^2 - (y_{h2}^2 - y_{h3}^2)^2\right) 
\end{align*}
\]

and

\[
d_1^{(n)} = \frac{2}{n} \sum y_{h1}, \quad d_2^{(n)} = \frac{6}{n} \sum (y_{h2}^2 - y_{h3}^2).
\]

7.4 Multivariate von Mises sine model on the torus

A general model on a product manifold \( M = \prod_{r=1}^k M^{(r)} = M^{(1)} \otimes \cdots \otimes M^{(k)} \), involving first order interaction terms, takes the form

\[
f(x; \pi) \propto \exp\left\{ \sum_{r=1}^k \pi^{(r)} T^{(r)}(x^{(r)}) + \sum_{r<s} \pi^{(r)} T^{(r)}(x^{(r)}) \Omega^{(r,s)} T^{(s)}(x^{(s)}) \right\}
\]
Different sufficient statistics, of possibly different dimensions, are allowed each manifold $M^{(r)}$. In principle it is also possible to include higher order interactions, and in some applications it may be desirable to consider submodels by setting some of the parameters to 0.

An important example of this construction is the general multivariate von Mises distribution on the torus $M = (S_1)^k$, for which $t^{(r)}(z^{(r)}) = (z_1^{(r)}, z_2^{(r)})^T = (\cos \theta^{(r)}, \sin \theta^{(r)})^T$ comprises the two Euclidean coordinates on each circle. See e.g. Jupp and Mardia, 1980 for the torus case. Mardia and Patrangenaru (2005) give an extension to a product of higher dimensional spheres, $q > 2$.

Even on the torus, this model has too many interaction parameters to be easily interpretable, so simplifications are often considered, including a sine model and two versions of a cosine model (e.g., Mardia, 2013, p. 501). For this paper we limit attention to the sine model on the torus; the cosine versions can be analyzed similarly.

(a) The density for the sine model takes the form in Table 2 where $\theta^{(r)} = \theta^{(r)} - \theta_0^{(r)}$, $\theta_0^{(r)}$ (for $r = 1, \ldots, k$), denote a set of orientation or centering parameters. The sine model forms a curved exponential family.

(b) The centering parameters can be estimated marginally by the sample mean directions $\hat{\theta}_0^{(r)}$ on each circle separately. Let $\phi_h^{(r)} = \theta_h^{(r)} - \bar{\theta}_0^{(r)}$ denote the standardized angles for the $n$ data points arranged as an $n \times k$ matrix $\Phi$. In this example, it is simpler to work in polar coordinates than in Euclidean coordinates.

(c) The reduced model takes the form

$$f(\phi) = \exp\left\{ \sum_{r=1}^{k} \kappa^{(r)} \cos \phi^{(r)} + \sum_{r<s} \lambda^{(rs)} \sin \phi^{(r)} \sin \phi^{(s)} \right\}$$

and forms a canonical exponential family with $m = k + k(k-1)/2$ parameters. The $m$-dimensional sufficient statistic, denoted $t(\phi)$, say, can be split into two blocks, $\cos \phi^{(r)}$ ($r = 1, \ldots, k$) and $\sin \phi^{(r)} \sin \phi^{(s)}$ ($r < s$).

(d) Working in polar coordinates, the $m \times k$ matrix of partial derivatives $\nabla^T t(\phi)$ can be similarly be partitioned into two blocks, where the nonzero elements are

$$(\nabla \cos \phi^{(r)})_j = -\sin \phi^{(r)}, \quad j = r$$

$$\left\{ \nabla (\sin \phi^{(r)} \sin \phi^{(s)}) \right\}_j = \begin{cases} \cos \phi^{(r)} \sin \phi^{(s)}, & j = r, \\ \sin \phi^{(r)} \cos \phi^{(s)}, & j = s, \end{cases}$$

for $j, r, s = 1, \ldots, k$, $r < s$. Then

$$W_n = \frac{1}{n} \sum \nabla^T t(\phi_h) \{ \nabla^T t(\phi_h) \}^T,$$
where \( \phi_h = (\phi_{h1}, \ldots, \phi_{hk})^T \) denotes the \( k \)-vector of angles for row \( h \) of the standardized data matrix.

The functions \( \cos \phi^{(r)} \) are eigenfunctions of the Laplace-Beltrami operator with eigenvalue \(-1\). Similarly, the product functions \( \sin \phi^{(r)} \sin \phi^{(s)} \) are eigenfunctions with eigenvalue \(-2\). Hence the elements of \( d_n \) have entries

\[
d_r^{(n)} = \frac{1}{n} \sum \cos \phi_h^{(r)} \quad (r = 1, \ldots, k),
\]
\[
d_{rs}^{(n)} = \frac{2}{n} \sum \sin \phi_h^{(r)} \sin \phi_h^{(s)} \quad (r < s).
\]

Figure 1: Comparison of two estimators of \( \kappa \) for the von Mises distribution with \( n = 2 \): maximum likelihood estimator (solid line) and score matching estimator (dashed line).

8 Efficiency study for the von Mises distribution

For the von Mises distribution on the circle, it is possible to study the behaviour of the score matching estimator in more detail, both empirically and analytically. The score matching estimators were described in [16] and [17]. The maximum likelihood estimator of \( \theta_0 \) is the same as hybrid score matching estimator. The maximum likelihood estimator of \( \kappa \) is \( \hat{\kappa}_{MLE} = A_1^{-1}(\bar{R}) \), where \( A_\nu(\kappa) = I_\nu(\kappa)/I_0(\kappa) \), \( \nu \geq 0 \).
Figure 2: Asymptotic relative efficiency (ARE), as a ratio of mean squared errors, for the estimation of $\kappa$ for the von Mises distribution, comparing the score matching estimator to the maximum likelihood estimator.

Table 3 gives the relative efficiency, as a ratio of mean squared errors, comparing the score matching estimator of $\log \kappa$ to the maximum likelihood estimator. Each entry is based on 100,000 simulated datasets. The log transformation is used to improve the numerical stability of the results, though in the final column for asymptotic relative efficiency, the use of a transformation makes no difference. The simulation from von Mises distribution was carried out in R (R Core Team, 2013) using the package CircStat (Jammalamadaka and Sengupta, 2001; Lund and Agostinelli, 2012). For all cases, the relative efficiency is at least 78% and is generally much closer to 100%.

The case $n = 2$ is interesting because it is possible to write the estimators in closed form and so compare their behaviour in detail. Further, the hybrid and full score matching estimators are identical in this setting. After centering, the standardized data take the form $\pm \theta$ for a single value of $\theta$, $0 < \theta < \pi/2$, where for simplicity we exclude the extreme possibilities $\theta = 0, \pi/2$. Then

$$\hat{\kappa}_{SME} = \frac{\cos \theta}{\sin^2 \theta}, \quad \hat{\kappa}_{MLE} = A_1^{-1}(\cos \theta).$$

The two estimators are compared in Figure 1 as a plot of the estimated $\kappa$ vs. $R = \arccos \theta$. Although (19) does not provide enough information to compute the relative efficiency, even in the extreme setting $n = 2$ the two estimators are
Table 3: Relative efficiency, as a ratio of mean squared errors, comparing the score matching estimator of log $\kappa$ to the maximum likelihood estimator. The final column ARE gives the asymptotic relative efficiency as $n \to \infty$, taken from (20).

| $\kappa$ | $n=2$ | $n=10$ | $n=20$ | $n=100$ | ARE |
|----------|-------|--------|--------|---------|-----|
| 0.5      | 100   | 89     | 93     | 95      | 95  |
| 1        | 98    | 88     | 86     | 85      | 85  |
| 2        | 98    | 92     | 85     | 79      | 78  |
| 10       | 100   | 100    | 99     | 99      | 99  |

Table 4: Great Whin Sill data on the sphere $S^2$, with sample size $n = 34$, and fitted by the Kent distribution. Estimates of $\kappa$ and $\beta$ are given by four different methods described in the text.

| Method               | $\hat{\kappa}$ | $\hat{\beta}$ |
|----------------------|-----------------|----------------|
| Hybrid SME           | 42.13           | 9.34           |
| Hybrid MLE           | 42.16           | 9.27           |
| Hybrid approximate MLE | 41.76         | 8.37           |
| Full MLE             | 42.41           | 9.28           |

reasonably similar, with the difference tending to 0 as $R \to 0$ and with the relative difference tending to 0 as $R \to 1$. The maximum difference between the two estimators is about $\hat{\kappa}_{MLE} - \hat{\kappa}_{SME} = 2.46 - 1.80 = 0.66$ when $R = 0.76$, i.e. $\theta = 41^o$.

In the limiting case $n \to \infty$, it is possible to compute analytically the asymptotic relative efficiency of the hybrid score matching estimator for $\kappa$, relative to the maximum likelihood estimator,

$$ARE = \frac{A^2_1(\kappa)}{(2\kappa - 3A_1(\kappa)) \left\{ \kappa - \kappa A^2_1(\kappa) - A_1(\kappa) \right\}}.$$  

A plot of (20) is given in Figure 2 and a proof is given in the Appendix.

9 Numerical examples

9.1 Kent distribution

The Great Whin Sill dataset was analyzed in Kent (1982) and is presented here to illustrate various estimates of the concentration parameters for the Kent distribution; see Table 4. The first three methods of estimation are hybrid estimators. Hence, as discussed in Section 7.3, the moment estimator is used for the orthogonal matrix representing the orientation parameters. After rotation of the data, the reduced model involves just the two concentration parameters.
Table 5: Isoleucine data, component 1, on the torus \((S_1)^4\), with sample size \(n = 23\), and fitted using the multivariate von Mises sine model. Estimates of the concentration parameters are given by three different methods: the hybrid score matching estimator (SME), the hybrid composite likelihood estimator and the hybrid approximate maximum likelihood estimator (AMLE).

|         | SME   | composite | AMLE  |
|---------|-------|-----------|-------|
| \(\kappa\) | 4.3   | -6.3      | 2.5   |
| \(\beta\)  | 4.9   | -7.3      | 4.0   |
| \(\lambda_{12}\) | 3.4   | 3.4       | 3.1   |
| \(\lambda_{13}\) | 6.6   | -5.3      | 3.1   |
| \(\lambda_{14}\) | 4.9   | -7.3      | 3.1   |
| \(\lambda_{23}\) | 45.4  | 24.5      | 6.0   |
| \(\lambda_{24}\) | 59.3  | -4.6      | 6.0   |
| \(\lambda_{34}\) | 2.2   | 2.5       | 3.6   |

Here are further details about the estimators in Table 4. The hybrid score matching estimator for \(\kappa\) and \(\beta\) was described in Section 7.3. The “hybrid maximum likelihood estimate” is the maximum likelihood estimate for the concentration parameters after rotating the data using the moment estimate of orientation (eqn. (4.8) in Kent (1982)). The “hybrid approximate maximum likelihood estimate” is the same, but using a normal approximation for the normalizing constant (eqn. (4.9) in Kent (1982)). The “full maximum likelihood estimate” involves maximizing the 5-parameter likelihood over both the orientation and concentration parameters; the estimated orientation is negligibly different from the moment estimator and is not reported here. All the estimates of the concentration parameters are close together.

9.2 Torus

In Mardia et al. (2012), \(k = 4\) angles from the amino acid isoleucine were modelled by a mixture of multivariate von Mises sine models and grouped into 17 clusters. Here we look at just one of those clusters, Cluster 1, and look at the fits to the concentration parameters from three estimation methods. All the methods are hybrid methods. Thus in each case location is estimated using the moment estimator given by the sample mean directions for each of the \(k = 4\) angles. After rotation the reduced model involves just the \(k(k+1)/2 = 10\) concentration parameters.

The hybrid score matching estimator was described in Section 7.4. The hybrid approximate maximum likelihood estimator uses a high concentration normal approximation for the normalizing constant in the reduced model; the numerical values were given in Mardia et al. (2012). The hybrid composite likelihood estimator is based on the conditional von Mises distribution in the reduced model for each angle given the remaining angles; the methodology is summarized in Mardia et al. (2009).

The estimated parameters are given in Table 5. The estimates are presented as a symmetric matrix: the diagonal elements are the \(\kappa^{(r)}\) and the off-diagonal elements are the \(\lambda^{(rs)}\) in (18), given for clarity just in the upper triangle. In general all the
estimates match reasonably closely.

10 Discussion

Methods of estimation for exponential families on manifolds can be divided into at least three broad categories:

- Maximum likelihood estimators, both the exact version and approximate versions. Although the exact version is preferred in principle, there may be problems in practice evaluating the normalizing constant. Hence approximations may be used, such as (a) saddlepoint (Kume et al., 2013), (b) holonomic (Sei and Kume, 2015), and (c) approximate normality under high concentration.

- Composite maximum likelihood estimation. Suppose a point on the manifold can be represented as a set of variables, such that the conditional distribution of each variable given the rest is tractable. Then the composite likelihood is the product of the conditional densities. In some cases this method can be very efficient (Mardia et al., 2009).

- Score matching estimators. As shown in this paper these estimators often reduce to the solution to a set of linear equations based on sample moments of the data. Hence the method is easy to implement and straightforward to apply to large datasets, including streaming data.

Strictly speaking, an approximate maximum likelihood estimator, at a fixed level of approximation, will not be consistent as the sample size $n \to \infty$. The score matching estimator is always consistent under the mild regularity conditions (A1)–(A2) on $f$ in Section 3 with an asymptotic variance at least as large as the maximum likelihood estimator. The the numerical examples here suggest the efficiency of the hybrid score matching estimator, compared to the maximum likelihood estimator, will often be close to 1.

Score matching estimators can also be developed for distributions on noncompact manifolds, including Euclidean spaces. The simplest example is the multivariate normal distribution (Hyvärinen, 2005) where it turns out that the score matching estimator is identical to the maximum likelihood estimator. Many directional distributions are approximately normal under high concentration. Hence we expect high efficiency of the score matching estimator in this setting. See Table 3 for confirmation in the von Mises case.

In the directional setting, the score matching estimator can often be interpreted as a “double moment estimator”. For example, for the von Mises-Fisher distribution the sufficient statistic is a linear function of $z$, but the matrix $W_n$ in the score matching estimator involves quadratic functions of $z$. Similarly, for the Bingham distribution the sufficient statistic is a quadratic function of $z$, but the matrix $W_n$ in the score matching estimator involves quartic functions of $z$.

This paper has emphasized the setting where $M$ is a sphere or a product of spheres. Work is in progress to investigate the score matching estimator for models
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11 Appendix

This section gives a proof of the asymptotic relative efficiency for the score matching estimator of $\kappa$ in (20). For simplicity the proof focuses on the estimator in the reduced model.

First, it can be shown that, asymptotically,

$$\text{var}(\hat{\kappa}_{\text{SME, hybrid}}) = \frac{\kappa}{A_1^2(\kappa)} \{2\kappa - 3A_1(\kappa)\}.$$  \hspace{1cm} (A1)

To verify this equation note that, treating $\theta$ as random from the von Mises distribution, \(\text{var}(\cos \theta) = 1 - A_1^2(\kappa) - A_1(\kappa)/\kappa\), \(\text{var}(\sin^2 \theta) = \frac{1}{8} \{3 + A_4(\kappa) - 4A_2(\kappa)\} - A_1^2(\kappa)/\kappa^2\) and \(\text{cov}(\cos \theta, \sin^2 \theta) = \frac{1}{4} \{A_1(\kappa) - A_3(\kappa)\} - A_1^2(\kappa)/\kappa\). Using the delta rule gives

$$\text{var}(\hat{\kappa}_{\text{SME, hybrid}}) = \frac{\kappa}{8nI_1A_1(\kappa)} \{\kappa(8 + 3\kappa^2)I_0 - 8I_1 - 4\kappa^2I_1 - 4\kappa^3I_2 + 4\kappa^2I_3 + \kappa^3I_4\},$$

with the shorthand notation $I_\alpha = I_\alpha(\kappa)$. Repeated use of (15) leads to (A1).

For the maximum likelihood estimator it can be shown that, asymptotically,

$$n \text{ var}(\hat{\kappa}_{\text{MLE}}) = \frac{1}{1 - A_1^2(\kappa) - A_1(\kappa)/\kappa}.$$  \hspace{1cm} (A2)

For both estimators the asymptotic variance converges to 2 as $\kappa \to 0$ and is asymptotic to $2\kappa^2$ as $\kappa \to \infty$. Hence for small and large $\kappa$, the asymptotic relative efficiency tends to 1. Combining (A1) and (A2) yields (20).

The discussion here has emphasized the hybrid score matching estimator and the maximum likelihood estimator for the full model with two unknown parameters. But in fact there are other models and estimators to consider, including three versions of the score matching estimator and two versions of the maximum likelihood estimator. The hybrid score matching estimator and the full score matching estimator are defined for the full model with two unknown parameters $\theta_0$ and $\kappa$. The score matching estimator can also be defined under the reduced model with just one unknown parameter. It turns out that all three estimators of $\kappa$ have the same asymptotic variance. Similarly, the maximum likelihood estimator of $\kappa$ can be
defined in the setting of the full model or the reduced model. Again both estimators
have the same asymptotic variance. Hence the asymptotic relative efficiency takes
the same value for all these possibilities.

References

Beran, R. (1979). Exponential models for directional data. *Ann. Statist.*, 7:1162–1178.

Chavel, I. (1984). *Eigenvalues in Riemannian Geometry*. Academic Press, Orlando.

Dawid, A. P. and Lauritzen, S. L. (2005). The geometry of decision theory. In *Proceedings of the Second International Symposium on Information Geometry and Applications*, pages 22–28. Univ. Tokyo.

Forbes, P. G. M. and Lauritzen, S. (2014). Linear estimating equations for exponential families with applications to Gaussian linear concentrations models. *Linear Algebra and its Applications*, 473:261–283.

Hyvärinen, A. (2005). Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning Research*, 6:695–709.

Hyvärinen, A. (2007). Some extensions of score matching. *Computational Statistics and Data Analysis*, 51:2499–2512.

Jammalamadaka, S. R. and Sengupta, A. (2001). *Topics in Circular Statistics*. World Scientific.

Jost, J. (2005). *Riemannian Geometry and Geometric Analysis, fourth edition*. Springer, Berlin.

Jupp, P. E. and Mardia, K. V. (1980). A general correlation coefficient for directional data and related regression problems. *Biometrika*, 67:163–73.

Kent, J. T. (1982). The Fisher–Bingham distribution on the sphere. *J. Roy. Statist. Soc. B*, 44:71–80.

Kume, A., Preston, S. P., and Wood, A. T. A. (2013). Saddlepoint approximations for the normalizing constant of Fisher–Bingham distributions on products of spheres and Stiefel manifolds. *Biometrika*, 100:971–984.

Lund, U. and Agostinelli, C. (2012). *CircStats*. R package version 0.2-4.

Mardia, K. V. (1975). Statistics of directional data (with discussion). *J. Roy. Statist. Soc. B*, 37:349–393.

Mardia, K. V. (2013). Statistical approaches to three key challenges in protein structural bioinformatics. *Applied Statistics*, 62:487–514.
Mardia, K. V., Hughes, G., Taylor, C. C., and Singh, H. (2008). A multivariate von Mises distribution with applications to bioinformatics. *The Canadian Journal of Statistics*, 36:99–109.

Mardia, K. V. and Jupp, P. E. (2000). *Directional Statistics*. Wiley.

Mardia, K. V., Kent, J. T., Hughes, G., and Taylor, C. C. (2009). Maximum likelihood estimation using composite likelihoods for closed exponential families. *Biometrika*, 96:975–982.

Mardia, K. V., Kent, J. T., Zhang, Z., Taylor, C. C., and Hamelryck, T. (2012). Mixtures of concentrated multivariate sine distributions with applications to bioinformatics. *J. Appl. Statist.*, 39:2475–2492.

Mardia, K. V. and Patrangenaru, V. (2005). Directions and projective shapes. *Ann. Statist.*, 33:1666–1699.

Parry, M., Dawid, A. P., and Lauritzen, S. (2012). Proper local scoring rules. *Ann. Statist.*, 40:561–592.

Patrangenaru, V. and Ellingson, L. (2016). *Nonparametric Statistics on Manifolds and Their Applications to Object Data Analysis*. CRC Press, Boca Raton.

R Core Team (2013). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.

Rosenberg, D. (1997). *The Laplacian on a Riemannian Manifold*. Cambridge University Press.

Sei, T. and Kume, A. (2015). Calculating the normalising constant of the Bingham distribution on the sphere using the holonomic gradient method. *Statistics and Computing*, 25:321–332.

Singh, H., Hinizdo, V., and Demchuk, E. (2002). Probabilistic model for two dependent circular variables. *Biometrika*, 89:719–723.

Stein, E. M. and Weiss, G. (1971). *Introduction to Fourier Analysis on Euclidean Spaces*. Princeton University Press.