Optimal Reduction of Dirac Mixture Densities on the 2-Sphere

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Abstract: This paper is concerned with optimal approximation of a given Dirac mixture density on the $S^2$ manifold, i.e., a set of weighted samples located on the unit sphere, by an equally weighted Dirac mixture with a reduced number of components. The sample locations of the approximating density are calculated by minimizing a smooth global distance measure, a generalization of the well-known Cramér-von Mises Distance. First, the Localized Cumulative Distribution (LCD) together with the von Mises–Fisher kernel provides a continuous characterization of Dirac mixtures on the $S^2$ manifold. Second, the $L^2$ norm of the difference of two LCDs is a unique and symmetric distance between the corresponding Dirac mixtures. Thereby we integrate over all possible kernel sizes instead of choosing one specific kernel size. The resulting approximation method facilitates various efficient nonlinear sample-based state estimation methods.

Keywords: Probability density function, function approximation, optimization problems, least-squares approximation, parameter estimation, Dirac mixture approximation, samples, manifolds, target tracking, system state estimation, Kalman filters, density approximation

1. INTRODUCTION

Context: Exact Bayesian state estimation for nonlinear systems is a nontrivial task, because analytic representations of the occurring densities can become arbitrarily complex over time, or closed-form expressions may not even exist. Therefore, samples instead of density functions are often used as stochastic state representation in applications of state estimation and control.

In the prediction step, samples can simply be inserted individually into any nonlinear generative state transition model. However, incorporating additive or non-additive noise multiplies the number of samples in every time step. To keep the algorithm tractable, the number of samples must be reduced for further processing, while maintaining as much information as possible. In the update step, one method is to re-weight state samples according to the measurement likelihood. Over time, repeated re-weighting will result in samples with vanishing weight, i.e., sample degeneration. Thus, individually weighted samples should be re-approximated by equally weighted samples for further processing. In this context, our method could provide a more faithful resampling than many existing bootstrap resamplings.

State variables that describe directions or orientations, cannot be faithfully described in the Euclidean space $\mathbb{R}^D$. They require spaces with different topologies, for example the 2-sphere $S^2$. As a manifold, it is locally homeomorphic to $\mathbb{R}^2$, so for small uncertainties, linearization of the space (“tangent plane”) at the point of interest is actually an adequate approximation. Of course, probability mass far apart from this linearization point will increasingly deteriorate estimation results.

In general, wherever a cloud of many randomly drawn samples is employed, be it in assumed density filters or sequential Monte Carlo (SMC) state estimators, similar results can be achieved with far less deterministically chosen samples, see Fig. 1.

![Fig. 1. A von Mises–Fisher density with $\kappa = 7$ (black mesh) is defined on a 2-sphere (green object). Initially, 5000 samples (blue points) are drawn randomly from this density. Using the proposed method, a reduction to 30 samples (red points) is performed.](image-url)

Directional estimation problems occur in many practical problems, for example crystal orientation estimation using electron backscatter diffraction, Bingham et al. (2010), fiber tracking in biomedical image analysis, Zhang et al. (2009), or path planning in robotics, Sánchez and Latombe (2002).
State of Art: Measures to compare two continuous density functions are for example the Kullback-Leibler-divergence, Kullback and Leibler (1951), or simply the $L_2$ norm of the difference of the density functions. If at least one of the densities is discrete, i.e., a Dirac mixture density, and the samples are not equidistant, said distance measures cannot be applied anymore: the local concentration of samples must be involved in some way into the distance measure, in addition to the sample weight. The Cramér-von Mises distance as the $L_2$ norm of the difference of the cumulative distribution functions, see Darling (1957) and Choi and Bulgren (1968), is well suited to compare discrete densities on a one-dimensional domain. However for multivariate densities, the definition of the cumulative distribution is ambiguous, and the Cramér-von Mises distance cannot be employed directly.

Hanebeck and Klumpp (2008) proposed a localized cumulative distribution (LCD). Given a continuous or discrete density function, it provides a representation of that density that is unique and symmetric also in the multivariate case. The LCD of continuous or discrete densities is always continuous, so the $L_2$ norm of the difference of two LCDs can be calculated. This is called the modified Cramér-von Mises distance, and serves as an objective function to match two multivariate densities, regardless whether they are continuous or discrete. It has been used to vastly reduce numbers of samples while keeping most of the relevant information, see Eberhardt et al. (2010) and Hanebeck (2015). On the other hand, the LCD has been applied to obtain deterministic samples of given multivariate Gaussian densities in Hanebeck et al. (2009). Using these deterministic samples, some Gaussian filtering algorithms have been developed, for example the Smart Sampling Kalman Filter ($S^2$KF) in Steinbring and Hanebeck (2013) and Steinbring et al. (2016), or progressive Gaussian filters in Steinbring and Hanebeck (2014) and Hanebeck and Pander (2016).

All of the publications mentioned so far applied the LCD in $D$-dimensional Euclidean space $\mathbb{R}^D$. Now the question arises whether the LCD can also be used for sample reduction on non-Euclidean manifolds. The first idea was proposed in Li et al. (2019a), where the LCD was applied in the Euclidean tangent space $\mathbb{R}^{D-1}$ of a hypersphere $S^{D-1}$. Deterministic samples were placed on the principle axes only. This limitation was overcome in Li et al. (2019b), as samples were placed not only on the principle axes but in the entire tangent space of the hypersphere. The resulting Bingham filter can bee seen as spherical equivalent to the $S^2$KF. The linearization point for the tangent space was always placed at the mode of the spherical (Bingham) distribution, and various projection methods were used to transform samples between hypersphere and tangent space.

Finally we want to address some of the literature about non-parametric density function estimation on manifolds. Methods for spheres, Ruymgaart (1989), or more generally, closed manifolds, Hendriks (1990), have been proposed based on Fourier expansions, for example. Furthermore, there are Bayesian nonparametric density estimators based on mixtures of parametric densities like the vMF for spheres (Bhattacharya and Bhattacharya, 2012, Sec. 13.2), Bhattacharya and Oliver (2019). These methods allow to compute an adequate continuous representation of a given set of samples.

Contribution: We propose a definition of the LCD for DMDs directly on the $S^2$ sphere. We choose the vMF density as kernel function and it will become obvious that it can be seen as a spherical equivalent to the Gaussian kernel. Furthermore, a modified Cramér-von Mises distance is formulated on the sphere. It provides a scalar distance measure between two spherical LCDs. With these tools, we propose a distance measure between two sets of samples on the sphere. This distance measure is then minimized using nonlinear optimization. Altogether, a deterministic method for optimal sample reduction on the $S^2$ sphere is proposed, see Fig. 1 for an example.

Outline: In a first step, a distance measure between two DMDs, i.e., sets of samples, that are located on the unit sphere, is introduced. The numbers of samples are fixed beforehand, as well as the sample locations of one of the sets. In a second step, by minimizing the distance measure we propose a deterministic resampling method. Thereby it is possible to i) reduce the number of samples, and/or to ii) approximate weighted samples with unweighted ones. No local linearization of $S^2$ is necessary to calculate the distance measure. The distance measure is given in closed form as a nonlinear function of the sample locations. The computational effort lies in numerical optimization of the distance measure. The unknown variables to be optimized are the sample locations of the smaller set of samples.

2. PROBLEM FORMULATION

Consider a given and fixed Dirac mixture density (DMD) $f(\tilde{x})$, $\tilde{x} \in S^2 \subset \mathbb{R}^3$, with $M$ components, given by

$$ f(\tilde{x}) = \sum_{j=1}^{M} w_j^y \delta(\tilde{x} - y_j) ,$$

with positive weights $w_j^y$, i.e., $w_j^y > 0$ for $j \in \{1, 2, \ldots, M\}$, and $\sum_{j=1}^{M} w_j^y = 1$. Samples are located at

$$ y_j = \begin{bmatrix} y_{j,x} \\ y_{j,y} \\ y_{j,z} \end{bmatrix}, \quad y_j = \begin{bmatrix} y_{j,\phi} \\ y_{j,\theta} \end{bmatrix}$$

on the unit sphere, in Cartesian and spherical coordinates, respectively. This density is approximated by another DMD $f(\tilde{x})$ with $L$ components, given by

$$ f(\tilde{x}) = \sum_{i=1}^{L} w_i^x \delta(\tilde{x} - x_i) ,$$

again with positive weights $w_i^x$ that sum up to one. Sample locations on the unit sphere are

$$ x_i = \begin{bmatrix} x_{i,x} \\ x_{i,y} \\ x_{i,z} \end{bmatrix}, \quad x_i = \begin{bmatrix} x_{i,\phi} \\ x_{i,\theta} \end{bmatrix}$$

in Cartesian and spherical coordinates, respectively. Typically, the approximating density $f(\tilde{x})$ has much less components than the approximated density $f(\tilde{x})$, i.e., $L \ll M$.

The goal is to select the location parameters $x_i$, $i \in \{1, 2, \ldots, L\}$ of the approximating density $f(\tilde{x})$ such that a distance measure $D$ between the true density $f(\tilde{x})$ and its approximation $f(\tilde{x})$ is minimized. $L$ is assumed to be given and fixed. The corresponding weights $w_i^x$ are assumed to be either given or set to be equal, i.e., $w_i^x = 1/L$. 

1305
The true DMD $\tilde{f}(x)$ might already have equally weighted components, so that the information is solely stored in the component locations. In this case, the goal of the approximation is a pure reduction of the number of components. On the other hand, the components of $\tilde{f}(x)$ might have different weights, e.g. as a result of weighting some prior DMD with a likelihood function in a Bayesian filtering setup. In that case, the approximation replaces an already weighted DMD by an equally weighted one.

3. LOCALIZED CUMULATIVE DISTRIBUTION

DMDs cannot easily be compared to each other, especially when they do not share a common support. Not the “vertical” difference of density values can be considered here, but the “horizontal” distance between samples and clusters of samples is essential. Therefore each DMD, $f(x)$, is first transformed to its LCD, $F(m,b)$, which is a continuous characterization of the DMD. Intuitively, a kernel function $K(x,m,b)$ is placed on each component of the DMD. The kernel attains a maximum at $x = m$ (location parameter), and $b$ controls the kernel size (scale parameter). We consider the LCD as cumulative distribution because we take $b$ as an equivalent to the “upper integration limit” of the traditional scalar cumulative distribution $\int_{-\infty}^{x} f(t) \, dt$. Instead from $-\infty$, we integrate around $m$ in the LCD.

We propose to define the LCD $F(m,b)$ for arbitrary densities $f(x)$ on $\mathbb{R}^2$ as

$$F(m,b) = \int_{-\infty}^{\infty} f(x) K(x,m,b) \, dx .$$

In particular, the LCD $F(m,b)$ of the approximating DMD $f(x)$ from (2) is

$$F(m,b) = \int_{-\infty}^{\infty} \left( \sum_{i=1}^{L} w_i^x \delta(x - x_i) \right) K(x,m,b) \, dx = \sum_{i=1}^{L} w_i^x \int_{-\infty}^{\infty} \delta(x - x_i) K(x,m,b) \, dx .$$

With the Dirac delta distribution for spheres

$$\delta(x - x_i) = \frac{\delta(x_\theta - x_i,\theta)}{\sin(x_\theta)} ,$$

by just using the general definition of the Dirac delta distribution for any manifold

$$\int_{\mathcal{M}} f(x) \delta(x - x_i) \, dx = f(x_i) ,$$

the LCD (3) becomes

$$F(m,b) = \sum_{i=1}^{L} w_i^x K(x_i,m,b) .$$

Similarly, the LCD $\tilde{F}(m,b)$ of the true density $\tilde{f}(x)$ (1) is

$$\tilde{F}(m,b) = \sum_{j=1}^{M} w_j^y K(y_j,m,b) .$$

The LCDs $\tilde{F}(m,b)$ and $F(m,b)$ are continuous in $m$ and $b$ and can thus be used to easily calculate a distance between $\tilde{f}(x)$ and $f(x)$.

4. A MODIFIED CRAMÉR-VON MISES DISTANCE

A straightforward distance measure $D$ between two LCDs $\tilde{F}(m,b)$ and $F(m,b)$ is their $L_2$ norm. We also integrate this over $b$, thereby becoming independent of a specific choice of kernel width and instead using the information from all possible kernel widths,

$$D^2 = \int_{\mathbb{R}_+} w(b) \int_{\mathbb{R}^2} (\tilde{F}(m,b) - F(m,b))^2 \, dm \, db$$

with

$$D_{xx} = \int_{\mathbb{R}_+} w(b) \int_{\mathbb{R}^2} F^2(m,b) \, dm \, db$$

$$D_{xy} = \int_{\mathbb{R}_+} w(b) \int_{\mathbb{R}^2} F(m,b) \tilde{F}(m,b) \, dm \, db$$

$$D_{yy} = \int_{\mathbb{R}_+} w(b) \int_{\mathbb{R}^2} \tilde{F}^2(m,b) \, dm \, db .$$

Inserting the definitions (4) and (5) of the particular LCDs, the products between any two LCDs yields

$$F^2(m,b) = \sum_{i=1}^{L} \sum_{j=1}^{M} w_i^x w_j^y K(x_i,m,b) K(y_j,m,b) ,$$

$$\tilde{F}^2(m,b) = \sum_{i=1}^{L} \sum_{j=1}^{M} \tilde{w}_i^x \tilde{w}_j^y K(x_i,m,b) K(y_j,m,b) .$$

The following integral $D_s(x,y)$, depending on the locations $x$ and $y$ of one pair of samples,

$$D_s(x,y) = \int_{\mathbb{R}_+} w(b) \int_{\mathbb{R}^2} K(x,m,b) K(y,m,b) \, dm \, db$$

conveniently encapsulates most of the complexity and allows for a very concise representation of the three main parts (7) of the modified Cramér-von Mises distance (7)

$$D_{xx} = \sum_{i=1}^{L} \sum_{j=1}^{M} w_i^x \tilde{w}_j^y D_s(x_i,y_j) ,$$

$$D_{xy} = \sum_{i=1}^{L} \sum_{j=1}^{M} \tilde{w}_i^x \tilde{w}_j^y D_s(x_i,y_j) ,$$

$$D_{yy} = \sum_{i=1}^{L} \sum_{j=1}^{M} \tilde{w}_i^x \tilde{w}_j^y D_s(y_i,y_j) .$$

Obviously, in order to get an analytic representation of the modified Cramér-von Mises distance (7), a closed form solution of the integral (9) must be available. The inner and outer part of the integral will be denoted separately as

$$D_s(x,y) = \int_{\mathbb{R}_+} w(b) D_s(x,y,b) \, db$$

and

$$D_s(x,b) = \int_{\mathbb{R}_+} K(x,m,b) K(y,m,b) \, dm$$

(10)

and

$$D_s(x,y) = \int_{\mathbb{R}_+} w(b) D_s(x,y,b) \, db$$

(11)
5. SYMMETRIC KERNEL FUNCTIONS

Only symmetric kernel functions will be considered from now on. That means, the value of the kernel function \( K(\vec{x}, \vec{y}, b) \) depends, except for \( b \), only on the geodesic arc length \( d(\vec{x}, \vec{y}) \) between \( \vec{x} \) and \( \vec{y} \), and not on their absolute location on the sphere,

\[
K(\vec{x}, \vec{y}, b) = K(d(\vec{x}, \vec{y}), b). 
\]

In this case, due to symmetry also the sample distance \( D_s \) will depend solely on the geodesic between the samples

\[
D_s(\vec{x}, \vec{y}) = D_s(d(\vec{x}, \vec{y})). 
\]

(12)

\[
D_{s,b}(\vec{x}, \vec{y}, b) = D_{s,b}(d(\vec{x}, \vec{y}), b). 
\]

In order to obtain the geodesic of a pair of samples, the dot product is calculated first. The value of the dot product of two unit vectors \( \vec{u}, \vec{v} \) is

\[
d_c(\vec{u}, \vec{v}) = \cos(d(\vec{u}, \vec{v})) \\
= \vec{u}^\top \vec{v} \\
= u_x v_x + u_y v_y + u_z v_z 
\]

from their Cartesian representation \( \vec{u} = [u_x, u_y, u_z]^\top \), and

\[
d_c = \sin(u_\varphi) \sin(v_\varphi) \cos(u_\varphi - v_\varphi) + \cos(u_\varphi) \cos(v_\varphi) 
\]

from their spherical coordinates.

6. VON MISES-FISHER KERNEL

The LCD has previously been developed for densities in \( \mathbb{R}^N \), where a Gaussian kernel

\[
K(\vec{x}, \vec{m}, \sigma) = \exp \left\{ -\frac{1}{2\sigma} (\vec{x} - \vec{m})^\top (\vec{x} - \vec{m}) \right\}, 
\]

\[
K(d(\vec{x}, \vec{m}), \sigma) = \exp \left\{ -\frac{1}{2\sigma} (d(\vec{x}, \vec{m}))^2 \right\} 
\]

provided good results together with the weighting function \( w(\sigma) = \sigma^{1/2} \) in the two-dimensional case, see Hanebeck (2015).

Following (8), the integral over the product of two such Gaussian kernel functions and said weighting factor is

\[
\int_{\sigma=\sigma_1}^{\sigma=\sigma_2} w(\sigma) K(d_1(\sigma), \sigma) K(d_2(\sigma)) \, d\sigma \\
= \int_{\sigma=\sigma_1}^{\sigma=\sigma_2} \frac{1}{\sigma} \exp \left\{ -\frac{1}{2} \left( \frac{d_1^2 + d_2^2}{\sigma^2} \right) \right\} \, d\sigma.
\]

By substitution

\[
b = \sigma^{-2}, \quad \sigma = b^{-\frac{1}{2}}, \quad \sigma' = -\frac{b^{-\frac{1}{2}}}{2},
\]

this can be transformed into

\[
\int_{b=\sigma_1^{-2}}^{b=\sigma_2^{-2}} \frac{1}{b^{-\frac{1}{2}}} \exp \left\{ -\frac{1}{2} \left( \frac{d_1^2 + d_2^2}{b^{-\frac{1}{2}}} \right)^2 \right\} \left( -\frac{b^{-\frac{1}{2}}}{2} \right) \, db
\]

\[
= \frac{1}{2} \int_{b=\sigma_1^{-2}}^{b=\sigma_2^{-2}} \frac{1}{b} \exp \left\{ b \cdot \left( -\frac{d_1^2 + d_2^2}{2} \right) \right\} \, db.
\]

While the dot product in the exponent of (13) is a natural squared distance of points in Euclidean space, the cosine with its periodicity is tailored for spherical geometries.

Incorporating \( (\cos(d) - 1) \) as the “spherical version” of \((-d^2)/2\),

\[
-\frac{d^2}{2} \approx \cos(d) - 1,
\]

where the approximation stands for second order Taylor polynomial, one obtains

\[
\int_{b=\sigma_1^{-2}}^{b=\sigma_2^{-2}} \frac{1}{b} e^{-2b} e^b \cos(d_1) e^b \cos(d_2) \, db
\]

\[
= \int_{b=\sigma_1^{-2}}^{b=\sigma_2^{-2}} w(b) K(d_1, b) K(d_2, b) \, db,
\]

with the vMF kernel function

\[
K(d, b) = e^b \cdot \cos(d)
\]

\[
K(d, \vec{m}, b) = e^b \cdot \cos(d(\vec{x}, \vec{m}))
\]

and the weighting factor

\[
w(b) = \frac{1}{b} e^{-2b}.
\]

(14)

Thus, the vMF kernel with \( w(b) = b^{-1} e^{-2b} \) can be seen as the spherical equivalent to the Gaussian kernel with \( w(\sigma) = \sigma^{1/2} \). See also Fig. 2 for a visual comparison between Gaussian and vMF kernel. Note that the kernel function is scaled such that it has a maximum value of one, as opposed to the vMF distribution, which is normalized such that it integrates to one, see Fisher (1953).

Having established the choice of kernel function and weighting factor, the function \( D_{s,b}(\vec{u}, \vec{v}, b) \) will be calculated by integrating the product of two vMF kernels on the sphere according to (10).
Fig. 3. Different examples for sample reduction on the 2-sphere. a) Mixture of three vMF distributions. 1000 random samples with \( b = 50 \) in the upper left, 1500 samples with \( b = 30 \) in the upper right, and 500 samples with \( b = 70 \) in the center, altogether approximated by 30 samples (red dots). b) vMF distribution with \( b = 7 \), where three strips of samples are removed. The remaining 3333 samples are approximated by 30 deterministic samples. c) Bingham distribution with \( Z = \text{diag}(-40, -3, 0) \). 5000 stochastic samples are reduced to 30 deterministic samples.

For the vMF distribution, the stochastic sampling method by Kurz and Hanebeck (2015) was used, and for the Bingham distribution Kent et al. (2013). In both cases, the integral can be solved analytically. Then \( D_s(d) \) for the vMF kernel calculates to

\[
D_s(d) = \frac{\pi}{\cos(d/2)} \int_{b_1}^{b_2} e^{-2b} \sinh(2b \cos(d/2)) \, db .
\]

Multiplication with the weighting function (14) and integration (11) over \( b \) yields the sample distance function \( D_s(d) \)

\[
D_s(d) = \frac{\pi}{\cos(d/2)} \int_{b_1}^{b_2} \frac{e^{-2b}}{b^2} 2 \sinh(2b \cos(d/2)) \, db .
\]

Using the relationships from Zeidler (2013)

\[
\frac{d}{dx} \text{Ei}(x) = \frac{e^x}{x} ,
\]

the integral can be solved analytically. Then \( D_s(d) \) for the vMF kernel calculates to

\[
D_s(d) = \frac{\pi}{\cos(d/2)} \left[ \frac{4 \text{Ei}(-4b) + \frac{1}{b} (e^{-4b} - 1)}{b_1} \right]^{b_2}_{b_1} , \quad d = 0 , \]

\[
D_s(d) = \frac{\pi}{\cos(d/2)} \left[ c_1 \text{Ei}(c_1 b) - c_2 \text{Ei}(c_2 b) + \frac{1}{b} \left( e^{c_2 b} - e^{c_1 b} \right) \right]^{b_2}_{b_1} , \quad d \in (0, \pi) , \]

where

\[
c_1 = +2 \cos(d/2) - 2 ,
\]

\[
c_2 = -2 \cos(d/2) - 2 .
\]

Bounds of integration were set to \( b_1 = 0.001 \) and \( b_2 \to \infty \).

7. EVALUATION

In order to demonstrate and visualize the performance of this method, various sets of samples were first randomly drawn by stochastic sampling, see blue points in Fig. 3. For the vMF distribution, the stochastic sampling method by Kurz and Hanebeck (2015) was used, and for the Bingham distribution Kent et al. (2013). In both cases,
the implementation in the \texttt{libDirectional} library, Kurz et al. (2015) and Kurz et al. (2019) was employed. Each DMD (1) consisting of $M = 3000 \ldots 5000$ stochastic points $y_i$ was then compared to a DMD (2) of $L = 30$ points $x_i$, that were as well randomly chosen as an initial guess, using the distance measure (6). The $(2 \times L)$ parameters $x_{i,\theta}$ and $x_{i,\phi}$ were subsequently optimized using Matlab’s \texttt{fminunc}. Analytical gradients were provided for better optimization performance. The code of the presented method will be published as part of \texttt{libDirectional} as well and can be found in the class \texttt{AbstractHypersphericalDistribution}.

8. CONCLUSION

We propose a distance measure between two sets of samples on the sphere. Minimizing this distance using off-the-shelf numerical optimization algorithms provides an efficient method for optimal sample reduction, deterministic sampling, and resampling of weighted samples by unweighted samples.

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