
Supplementary material for: Harmonic Exponential Families

This document provides additional background and implementation details for the paper “Harmonic Exponential Families on Manifolds”.

Code will be released on the project webpage.

A simple test script for the harmonic density on the circle (the generalized von-Mises) is included. This density is not studied experimentally in the paper, but the script shows the simplicity and effectiveness of the algorithm.

1. Numerical stability: the log - Fourier - exp trick

When the distribution is highly peaked, the unnormalized probabilities $\varphi(g) = \exp(\eta \cdot T(g))$ can become extremely large, causing numerical instability or overflow. A similar problem is regularly encountered in probabilistic computations where one wishes to compute $\ln \sum \exp x_i$, for some log-probabilities x_i . The standard solution is to subtract the maximum $x^* = \max x_i$ before exponentiating:

$$x^* + \ln \sum_i \exp(x_i - x^*) = \ln \sum_i \exp(x_i) \quad (1)$$

This is stable because all numbers $\exp(x_i - x^*)$ are between zero and one.

Our situation is slightly different, because we want to compute the Fourier transform of exponentially large quantities. The Fourier transform is a linear transformation but not a plain sum, so the outputs (the moments) can be negative even when the inputs are all positive. The logarithm of a negative number is a complex number, so one way to make the computation stable is to use the log-Fourier-exp trick with a complex logarithm function.

Alternatively, we may notice that all we need is the *ratio* of large quantities, so we need not compute the logarithm at all. The algorithm becomes:

1. Compute $\ln \varphi = \mathcal{F}^{-1} \eta$.
2. Compute $m = \max_i \ln \varphi(g_i)$.
3. Compute $\bar{\varphi} = \exp(\ln \varphi - m)$.
4. Compute $M = \mathcal{F} \bar{\varphi}$.
5. Compute $\mathbb{E}_{p(g|\eta)} [T(g)] = M/M_{00}^0$.

The factor e^{-m} cancels in the division.

2. Fast and stable evaluation of spherical harmonics

In order to compute the empirical moments one must evaluate the sufficient statistics at the data. For a spherical harmonic density, these sufficient statistics are spherical harmonics Y_m^l (denoted T_{m0}^λ in the paper) of potentially high degree l . We found that the spherical harmonics implementation in SciPy has acceptable performance for evaluations of all spherical harmonics up to degree 50 – 80, but was much too slow to be used for orders up to 200. We also found that for large orders the SciPy function produces NaN values.

Faster and more stable algorithms for the evaluation of spherical harmonics have been developed recently, but they are quite complicated, involving code generators or extended floating point numbers (Sloan, 2013; Fukushima, 2011). We developed a very simple, stable, and fast algorithm for evaluation of all spherical harmonics up to order L . Our method uses the algorithm of Pinchon & Hoggan (2007) for computing real-valued Wigner D-functions $D_{mn}^\lambda(\alpha, \beta, \gamma) = T_{mn}^\lambda(g)$, and the fact that spherical harmonics Y_m^λ are the $n = 0$ column of this matrix:

$$Y_m^l(\phi, \theta) = D_{m0}^l(\phi, \theta, 0). \quad (2)$$

(up to an arbitrary scaling constant)

Pinchon and Hoggan decompose the D matrix as

$$D^l(\alpha, \beta, \gamma) = X^l(\alpha) J^l X^l(\beta) J^l X^l(\gamma), \quad (3)$$

where X are matrices with sinusoids on the diagonal and anti-diagonal, and J^l is a pre-computed symmetric orthogonal block matrix with 4 non-zero blocks.

Computing the entire matrix

$$D(\phi, \theta, 0) = \text{blockdiag}(D^0(\phi, \theta, 0), \dots, D^L(\phi, \theta, 0)),$$

and then selecting the $n = 0$ column from each block is not feasible because it involves the multiplication of $O(L)$ blocks of dimension $O(L)$, which makes the complexity $O(L^4)$.

A better approach is to construct a binary coefficient vector c with ones in the positions corresponding to $m = 0$ (one

for each value of l), and then compute

$$D(\phi, \theta, 0)c = X^l(\alpha)J^l X^l(\beta)J^l c \quad (4)$$

in the right-associative order.

The vector c for $L = 2$ would be:

$$c = (1; 0, 1, 0; 0, 0, 1, 0, 0)$$

(the semicolons are there for readability only). One way to think of c is as selecting the $n = 0$ columns from the blocks of D when left multiplied by D . Another way to understand this is to think of $c = Y(0, 0)$ as the evaluation of the spherical harmonics at the north-pole of the sphere, and then $D(\phi, \theta, 0)c$ rotates this vector to become the spherical harmonics evaluated at some other point (ϕ, θ) on the sphere.

By exploiting right-associativity, each multiplication is a matrix-vector multiplication with cost $O(L^2)$ instead of matrix-matrix multiplication with cost $O(L^3)$. Furthermore, the products involving $X(\cdot)$ take only linear time because X is very sparse (Pinchon & Hoggan, 2007). The total cost of computing spherical harmonics is thus $O(L^2)$ per degree or $O(L^3)$ for all degrees up to L . Since the number of spherical harmonics grows quadratically with the maximum degree L , the complexity of this algorithm when measured in terms of the number of spherical harmonics is $O(N^{3/2})$. Stability follows from the orthogonality of X and J , as demonstrated by Pinchon & Hoggan (2007).

3. A basis for $L^2(H)$

We claim in the paper that one can find a subset of matrix elements of irreducible unitary representations to span the space of square-integrable functions on a homogeneous space. This will be clarified in this section.

Let \mathcal{G}^λ be the finite-dimensional subspace of $L^2(G)$ spanned by the matrix elements U_{mn}^λ . Let \mathcal{H}^λ be the subset of \mathcal{G}^λ consisting of right invariant functions (i.e. for $f \in \mathcal{H}^\lambda$, we have $f(gk) = f(g), \forall g \in G, k \in K$). First, notice that \mathcal{H}^λ is indeed a subspace of \mathcal{G}^λ : Let $f', f'' \in \mathcal{H}^\lambda$ and set $f(g) = \alpha f'(g) + \beta f''(g)$ for scalars α, β . Then

$$f(gk) = \alpha f'(gk) + \beta f''(gk) = \alpha f'(g) + \beta f''(g) = f(g).$$

So $f \in \mathcal{H}^\lambda$ and hence \mathcal{H}^λ is a vector space.

Since \mathcal{H}^λ is a finite-dimensional subspace one can obtain a basis for it by taking linear combinations of matrix elements U_{mn}^λ . In fact, one may choose the matrix elements for the group in such a way that a subset of these form a basis for \mathcal{H}^λ .

4. Action of $SO(3)$ on the spherical harmonics expansion

We claim in the paper that the rotation group $SO(3)$ acts irreducibly on the spherical harmonics coefficients. That is to say, if x is a function on the sphere and $\hat{x} = \mathcal{F}x$ are its Fourier coefficients, then the Fourier coefficients of $x' = R(g)x(p) = x(g^{-1}p)$ are given by $\hat{x}' = \mathcal{F}x' = U(g)\hat{x}$, where $U(g)$ is a block-diagonal matrix with irreducible representations U^λ as blocks.

Recall that the spherical Fourier transform is the expansion of a function on the sphere in terms of spherical harmonics $Y_m^\lambda(p) = U_{m0}^\lambda(g_p)$, where U^λ are the irreducible unitary representation of $SO(3)$, and $g_p \in SO(3)$ is an element in the coset that represents p . In the following derivation, we will write a finite-dimensional vector of spherical harmonics evaluated at p as $Y(p) = (Y_0^0(p), \dots, Y_{\lambda_*}^{\lambda_*}(p))^T = U_{\cdot,0}(g_p)$. In full detail:

$$\begin{aligned} [R(h)x](p) &= x(h^{-1}p) \\ &= \hat{x} \cdot Y(h^{-1}p) \\ &= \hat{x} \cdot U_{\cdot,0}(h^{-1}g_p) \\ &= \hat{x} \cdot U(h^{-1})U_{\cdot,0}(g_p) \\ &= \hat{x} \cdot U(h^{-1})Y(p) \\ &= U^T(h^{-1})\hat{x} \cdot Y(p) \\ &= U(h)\hat{x} \cdot Y(p) \\ &= U(h)\mathcal{F}x \cdot Y(p) \\ &= \mathcal{F}^{-1}U(h)\mathcal{F}x \end{aligned} \quad (5)$$

The spherical harmonics are not always defined equal to U_{m0}^λ , but can have different scale factors depending on λ . The result above still holds for other scalings, though.

References

Fukushima, T. Numerical computation of spherical harmonics by extending exponent of floating point numbers. *J. Geodesy*, pp. 271–285, 2011. doi: 10.1007/s00190-011-0519-2.

Pinchon, D. and Hoggan, P. E. Rotation matrices for real spherical harmonics: general rotations of atomic orbitals in space-fixed axes. *Journal of Physics A: Mathematical and Theoretical*, 40(7):1597–1610, February 2007. ISSN 1751-8113.

Sloan, P.-p. Efficient Spherical Harmonic Evaluation. *Journal of Computer Graphics Techniques*, 2(2):84–90, 2013. URL <http://jcgt.org>.

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