Notes on faster spherical harmonic expansion implementation

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1 Introduction

The two major steps in the pipeline for constructing a fiber orientation distribution (FOD) from a cubic ROI of x-ray μCT data are (1) estimate the local orientation at each voxel using structure tensor analysis, and (2) express the distribution of these orientations using the spherical harmonics. Until now, calculating the relevant spherical harmonic coefficients has been the major computation bottleneck in this pipeline. This report details a new method for calculating these coefficients using a spherical binning algorithm that improves performance by nearly 100% with no significant drop in accuracy.

2 Previous implementation

2.1 From orientations to FOD

The output of the structure tensor analysis algorithm for an ROI with a total of K elements is an array of K vectors: $\{x_k, y_k, z_k\}$. With the current implementation, these K vectors are first converted into spherical coordinates: $\{\theta_k, \phi_k\}$ with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$. The FOD is then represented as a sum of dirac delta functions at these coordinates:

$$\mathrm{FOD}(\theta, \phi) = \frac{1}{K} \sum_{k=1}^{K} \delta(\theta - \theta_k)\delta(\phi - \phi_k). \tag{1}$$

2.2 Spherical harmonic representation

The spherical harmonics are defined as

$$Y_l^m(\theta, \phi) = N_l^m P_l^m(\cos\theta) e^{jm\phi}, \tag{2}$$

where N_l^m is a normalization coefficient, and P_l^m are the associated Legendre polynomials.

The SH form an orthonormal basis over $L_2(\mathbb{S}^2)$. Any square integrable function $g(\theta, \phi) \in L_2(\mathbb{S}^2)$ can be expressed as a linear combination of SH:

$$g(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} c_{lm} Y_l^m(\theta, \phi), \tag{3}$$

with coefficients c_{lm} given by

$$c_{lm} = \int_{\mathbb{S}^2} g(\theta, \phi) \bar{Y}_l^m(\theta, \phi) \mathrm{d}\mathbf{\Omega}, \tag{4}$$

where the overbar denotes conjugation.

If we substitute Eqn. 1 into Eqn 4, then the sifting property of the Dirac delta function can be used, and the integral reduces to:

$$c_{lm} = \frac{1}{K} \sum_{k=1}^{K} \bar{Y}_l^m(\theta_k, \phi_k). \tag{5}$$

A SH approximation $\hat{\text{FOD}}(\theta, \phi)$ can then be determined to an arbitrary band-limit L_{max} using Eqn 3.

Spherical harmonics are used extensively in the HARDI literature to represent FODs. Generally, it is assumed that diffusion has even symmetry, so odd-ordered SH components are assumed to be zero and ignored. Furthermore, since the diffusion-weighted signal and ODF are both real functions, their SH representations exhibit conjugate symmetry:

$$Y_l^m(\theta, \phi)_{real} \equiv \begin{cases} \sqrt{2}\text{Re}\left[Y_l^{|m|}(\theta, \phi)\right] & m < 0 \\ Y_l^0(\theta, \phi) & m = 0 \\ \sqrt{2}\text{Im}\left[Y_l^m(\theta, \phi)\right] & m > 0 \end{cases} \tag{6}$$

These simplifications hold true for the µCT FODs as well. In this work, we use a band-limit of $L_{max} = 20$, for a total number of 231 even-ordered SH coefficients.

2.3 Computational Expense

With our current data, the µCT voxels are 1.2 μm^3 isotropic, and the MRI voxels are 150 μm^3 isotropic. Accordingly, one MRI-voxel-sized ROI includes a total of $K = 125^3 \approx 2$ million µCT voxels. The above implementation thus requires each of the 231 even spherical harmonics up to $L_{max} = 20$ to be evaluated at 2 million points. Calculating all 231 of these coefficients with this method for one ROI typically takes around 100 seconds on the bigmem SIRAF nodes. There are approximately 500,000 voxels in the MRI data. In order to create a corresponding µCT FOD for each of these voxels with this method would thus take: 500,000 voxels $\times$ 100 seconds/voxel $\approx$ 14,000 hours of computation time, not including the additional time needed to estimate the orientations themselves.

3 New implementation: spherical binning

3.1 From orientations to FOD

The primary change comes in how the FOD is constructed from the orientation vectors. Representing the FOD as a sum of $K \approx 2 \times 10^6$ delta functions required each of the spherical harmonics to be evaluated at K points. With the new method, the FOD is instead constructed as a histogram on the sphere using N approximately uniform sampling points as the bin centers.

The N sampling points are chosen using a Fibonacci sampling algorithm [1]. The K vectors are sorted into the corresponding bins using a very fast nearest-neighbors search algorithm, implemented with a "ball tree" nested data structure in the `scikit-learn` Python package.

This "binned" FOD can be written as a weighted sum of N delta functions, where $N \ll K$:

$$\text{FOD}_b = \frac{1}{K} \sum_{n=1}^{N} b_n \delta(\theta - \theta_n)\delta(\phi - \phi_n), \tag{7}$$

where b_n is the bin count for the sampling point (θ_n, ϕ_n), and $\sum_n b_n = K$.

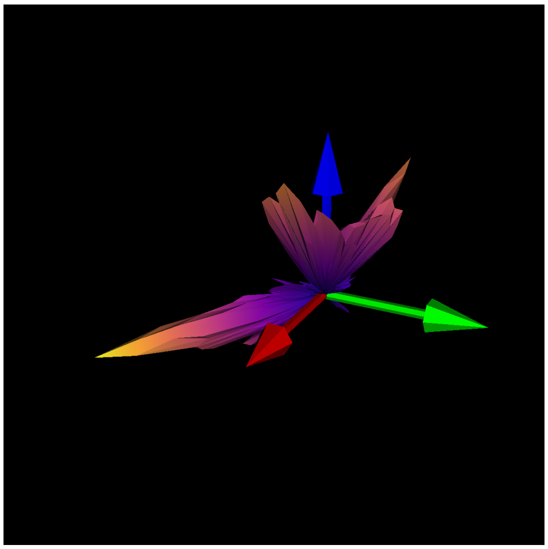
3.2 Spherical harmonic representation

The calculation of the spherical harmonic coefficients proceeds in the same way. The "binned" FOD is substituted into Eqn 4, which results in:

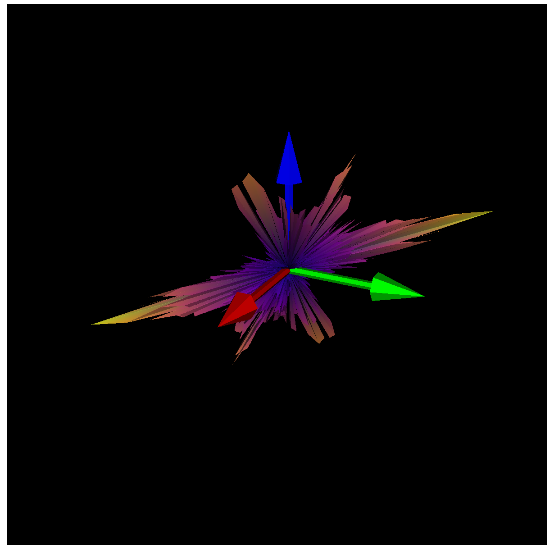
$$c_{lm} = \frac{1}{K} \sum_{n=1}^{N} b_n \bar{Y}_l^m(\theta_n, \phi_n). \tag{8}$$

The same symmetries are exploited from Eqn 6.

4 Results



(a) Raw



(b) "Forced-even"

Figure 1: The "binned" FOD

References

[1] J. H. Hannay and J. F. Nye, "Fibonacci numerical integration on a sphere," *Journal of Physics A: Mathematical and General*, vol. 37, pp. 11591–11601, dec 2004.