Notes on binned 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 antipodal 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

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 $N \ll K$ 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:

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

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:

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

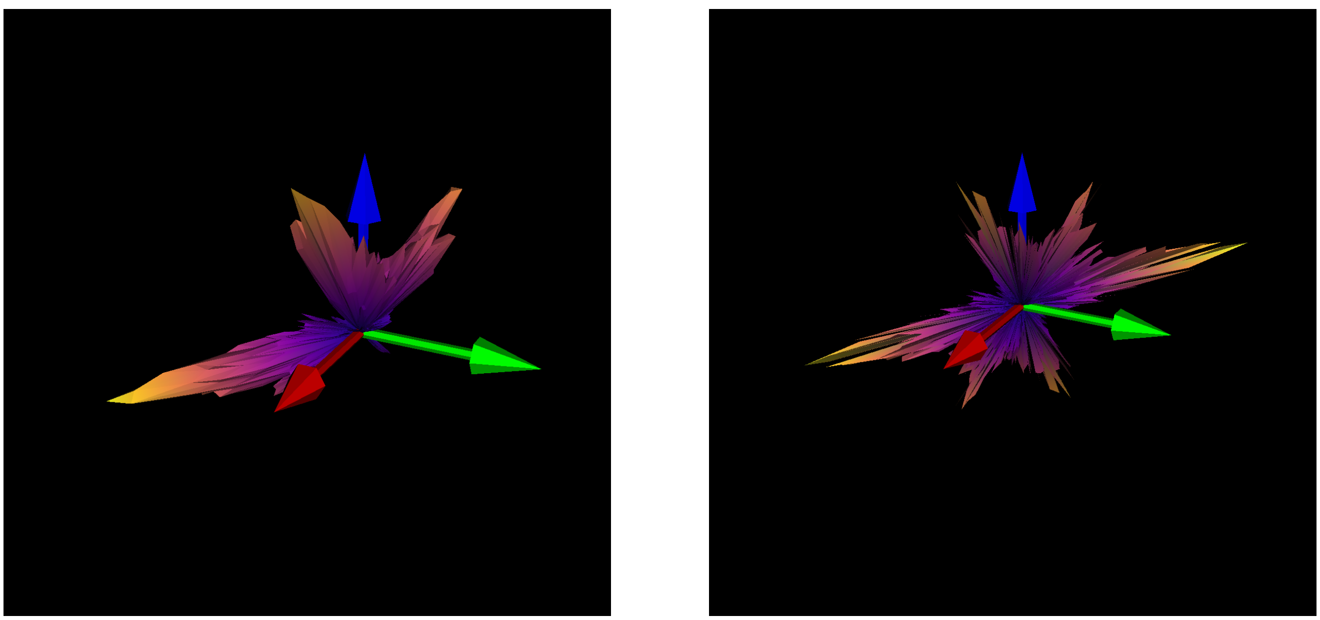
The same symmetries are exploited from Eqn 6.

4 Results

4.1 Raw FOD visualization

An MRI-voxel-sized ROI (125×125×125 voxels) was taken from μCT data, and the orientations at each voxel were estimated with structure tensor analysis. For the purposes of this report, orientations were not thresholded by FA or pixel value to mask out non-fiber voxels.

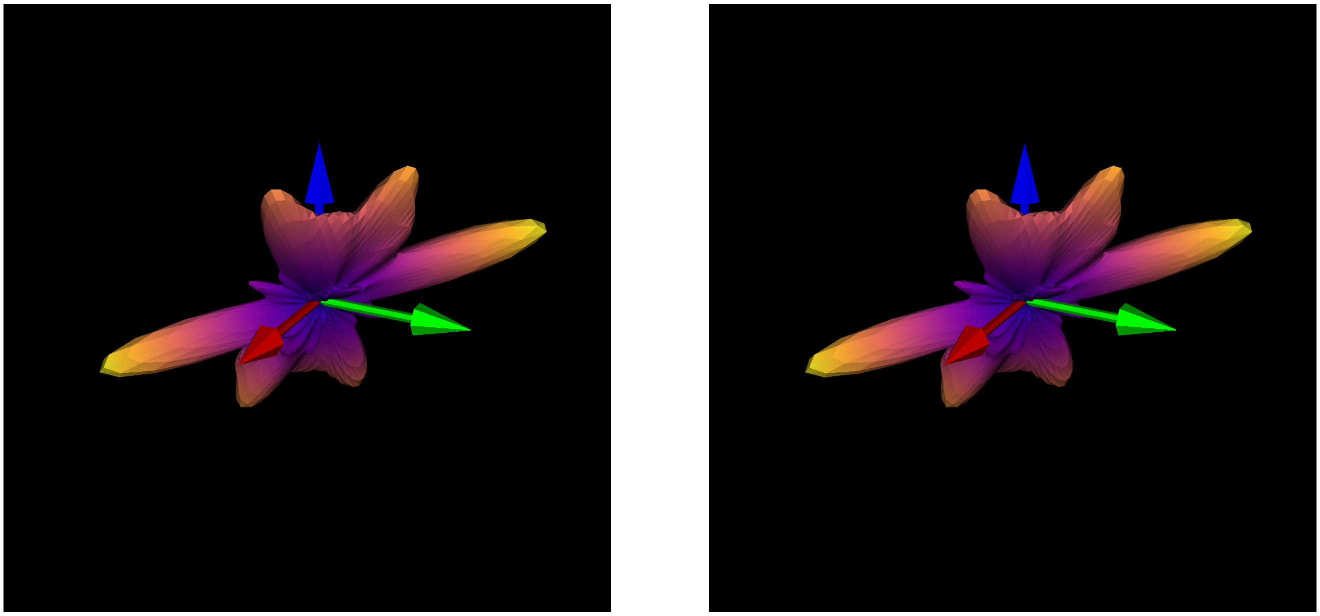
One advantage to the new binning method is that it allow us to directly visualize the raw FOD before expanding it onto spherical harmonics. Figure 1a is a plot of this FOD calculated according to Eqn 7 with $N = 6500$. Notably, the raw FOD does not have antipodal symmetry. This is not surprising — the orientations at each voxel are calculated as eigenvectors of a tensor. These normalized eigenvectors are unique within a minus sign; at each voxel, the opposite orientation might as well have been reported. Furthermore, the FODs calculated with the dMRI methods of interest will always have antipodal symmetry. Accordingly, the true μCT FOD we are interested in estimating is shown in Figure 1b, which was calculated by taking every point from Figure 1a and assigning the same bin count to the opposite point. Note that we are already enforcing this symmetry in the SH representation by only using even-ordered coefficients. I tested calculating the coefficients from the FODs in both Fig 1a and Fig 1b and they were identical.



(a) Raw orientations

(b) After enforcing antipodal symmetry

Figure 1: The "binned" μCT FOD



(a) Delta (b) Binned

Figure 2: SH FOD representations

4.2 Comparison of methods

Figure 2 shows a comparison of the SH representation of the FODs calculated with the delta function method (Fig 2a, Eqn 1) and the spherical binning method (Fig 2b, Eqn 7). The binned FOD was calculated using $N = 6500$ sample points, and both FODs were also plotted on a sphere with the same $N = 6500$ points. Bth SH representations look like spherically "blurred" versions of Figure 1b, as we expect.

Visually, the difference between the two FODs are negligible. This difference is quantified in Figure 3a as the root mean squared error (RMSE) of the SH coefficients, plotted as a function of the number of sampling points. The RMSE is calculated as

$$\mathrm{RMSE} = \sqrt{\frac{1}{N_{SH}} \sum_{l,m} \left[c^{\delta}_{lm} - c^{b}_{lm}(N)\right]^2}, \tag{9}$$

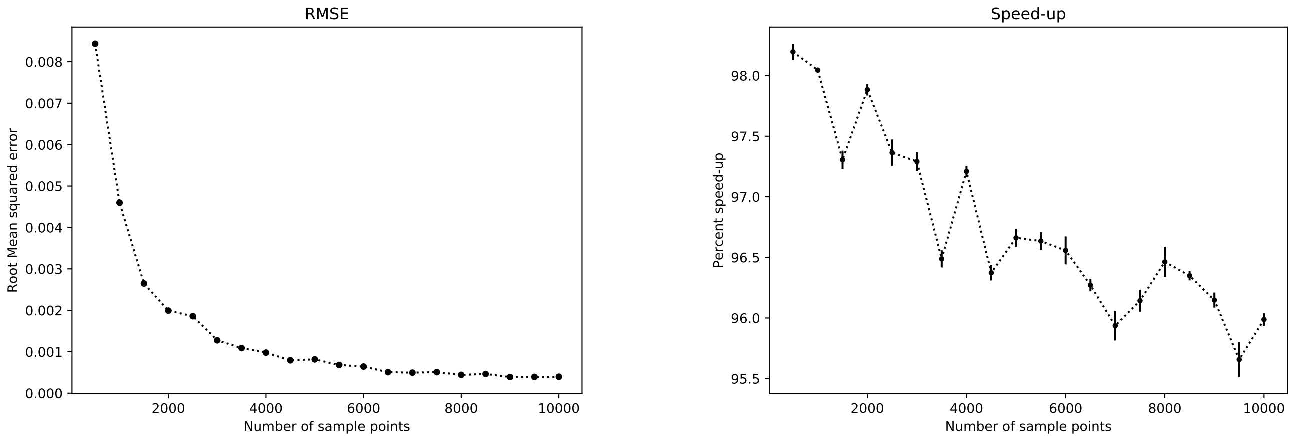
where $N_{SH} = 231$ is the total number of SH coefficients, c^{δ}_{lm} is the SH coefficient for l and m calculated with the delta function method and $c^{b}_{lm}(N)$ is the SH coefficient for l and m calculated with the binned method using N sample points.

Figure 3b shows the corresponding speed-up of computation time between the two methods. For each N, a single "best-case" time measurement was recorded as the lowest time of three separate executions. The average time $\bar{t}_N$ and error σ_N were taken as the mean and standard deviation of ten of these lowest times; thus, the coefficients were calculated a total of 30 times for each N, as well as for the delta method. The percent speed-up (SU_N) was then calculated as

$$\mathrm{SU}_N = \left(1 - \frac{\bar{t}_N}{\bar{t}_\delta}\right) \times 100, \tag{10}$$

where $\bar{t}_\delta$ is the mean execution time for the delta method. The error in SU_N was calculated by adding the relative errors of the binned and delta times:

$$\sigma_{SU,N} = \left(\frac{\sigma_N}{\bar{t}_N} + \frac{\sigma_\delta}{\bar{t}_\delta}\right) \times \mathrm{SU}_N \tag{11}$$



(a) RMSE

(b) Speedup

Figure 3: Performance metrics

5 Conclusion

Together, these plots show that for an adequate number of sampling points, the binned FOD method approaches a 100% speedup with very little loss in accuracy. The percent speedup generally decreases with increasing N, as expected, though it stays consistently over 95%. The RMSE seems to level off after around $N = 6500$. With this level of accuracy, the FODs could be calculated across the whole brain in a much more managable computation time of ~140 hours. Spread across multiple nodes, this could be completed in less than a day.

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.