Notes on diffusion MRI

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1 Representing spherical functions

1.1 Reproducing kernel

Here we'll present a derivation of the reproducing kernel representation for functions $f \in L^2\left(\mathbb{S}^2\right)$, where $\mathbb{S}^2$ is the unit sphere in $\mathbb{R}^3$. We start by defining the subspace of spherical harmonics

$$\mathcal{H}_N = \operatorname{span}\left\{Y_l^m : |m| \leq l,\ 0 \leq l \leq N\right\} \tag{1}$$

of maximum degree N. Let $f \in \mathcal{H}_N$. Then, by definition,

$$f\left(\omega\right) = \sum_{l=0}^{N} \sum_{|m|\leq l} f_l^m Y_l^m\left(\omega\right), \tag{2}$$

where

$$f_l^m = \int_{\mathbb{S}^2} \overline{Y}_l^m\left(\omega\right) f\left(\omega\right) d\omega, \tag{3}$$

with an over-bar denoting complex conjugation. In Eq. (2), we change the order of summation and integration to obtain4

$$\begin{aligned}
f\left(\omega\right) &= \sum_{l=0}^{N} \sum_{|m|\leq l} \int_{\mathbb{S}^2} \overline{Y}_l^m\left(\omega'\right) f\left(\omega'\right) d\omega' Y_l^m\left(\omega\right) \\
&= \sum_{l=0}^{N} \int_{\mathbb{S}^2} \sum_{|m|\leq l} \overline{Y}_l^m\left(\omega'\right) Y_l^m\left(\omega\right) f\left(\omega'\right) d\omega' \\
&= \sum_{l=0}^{N} \int_{\mathbb{S}^2} \frac{2l+1}{4\pi} P_l\left(\omega\cdot\omega'\right) f\left(\omega'\right) d\omega' \\
&= \int_{\mathbb{S}^2} \sum_{l=0}^{N} \frac{2l+1}{4\pi} P_l\left(\omega\cdot\omega'\right) f\left(\omega'\right) d\omega' \\
f\left(\omega\right) &= \int_{\mathbb{S}^2} K\left(\omega\cdot\omega'\right) f\left(\omega'\right) d\omega', \qquad (4)
\end{aligned}$$

where we used the Addition theorem to go from the second to third line and defined the reproducing kernel K as

$$K(\mu) = \sum_{l=0}^{N} \frac{2l+1}{4\pi} P_l(\mu). \tag{5}$$

If $f \in \mathcal{H}_N$, then operating on f with $\int_{\mathbb{S}^2} K(\omega' \cdot \omega) \cdot d\omega'$ reproduces f, hence the name reproducing kernel. We can now discretize Eq. (4) to get the representation

$$f(\omega) = \sum_{i=1}^{M} w_i K(\omega \cdot \omega_i) f(\omega_i), \tag{6}$$

where $\{\omega_i, w_i\}_{i=1}^{M}$ are quadrature nodes and weights. Note that the quadrature needs to be exact for spherical harmonics up to and including degree $2N$.

The function K is analogous to the sinc kernel on the line and, like the sinc kernel can be further localized by extending its spectrum to zero smoothly. Here we have the spectral representation in term of Legendre polynomials, instead of Fourier modes. We write

$$\tilde{K}(\mu) = \sum_{l=0}^{N} \frac{2l+1}{4\pi} P_l(\mu) + \sum_{l=N+1}^{N'} \frac{2l+1}{4\pi} a_l P_l(\mu) \tag{7}$$

and choose the filter coefficients to increase localization. One way to do this is by considering the following minimization problem. Given $-1 < \mu_0 < 1$ and N', solve

$$\min_{a_l} ||\tilde{K}||_{L^\infty(-1,\mu_0)},$$

where the norm is taken only over the interval $(-1, \mu_0)$. This has the effect of "pushing" the function $\tilde{K}$ into the region $(\mu_0, 1)$, i.e., concentrating it near a quadrature point. I found that by using $N' = 2N$ the resulting filter behaved nicely, going monotonically to zero. If one oversamples more, then you have to add constraints to the minimization problem to get a "nice" filter. I also found that $\mu_0 \sim 0.9 - 0.98$ worked well, depending on the value of N; the larger N is the closer one can get to $\mu_0 = 1$. It is some times convenient to write Eq. (7) as

$$\tilde{K}(\mu) = \sum_{l=0}^{N'} \frac{2l+1}{4\pi} a_l P_l(\mu),$$

where $a_l \equiv 1$ for $0 \le l \le N$ and $0 \le a_l < 1$ for $N+1 \le l \le N'$ are found by some minimization problem.

With the extended kernel Eq. (7), we lose the projection property of Eq. (4). Suppose $f \in L^2(\mathbb{S}^2)$ with

$$f \sim \sum_{l=0}^{\infty} \sum_{|m| \le l} f_l^m Y_l^m,$$

then we have

$$\begin{aligned}
\int_{\mathbb{S}^2} \tilde{K}(\omega \cdot \omega') f(\omega') d\omega' &= \int_{\mathbb{S}^2} \sum_{l=0}^{N'} \frac{2l+1}{4\pi} a_l P_l(\omega \cdot \omega') f(\omega') d\omega' \\
&= \int_{\mathbb{S}^2} \left(\sum_{l=0}^{N} \frac{2l+1}{4\pi} P_l(\mu) + \sum_{l=N+1}^{N'} \frac{2l+1}{4\pi} a_l P_l(\mu) \right) f(\omega') d\omega' \\
&= \int_{\mathbb{S}^2} K(\omega \cdot \omega') f(\omega') d\omega' + \sum_{l=N+1}^{N'} a_l \int_{\mathbb{S}^2} \frac{2l+1}{4\pi} P_l(\mu) f(\omega') d\omega' \\
&= f|_{\mathcal{H}_N} + \text{“tail/noise”}.
\end{aligned}$$

2 Funk-Radon transform

First we'll need the Funk-Hecke theorem (formula): For any continuous function $f : [-1,1] \to \mathbb{R}$

$$\int_{\mathbb{S}^2} Y_l^m(\omega) f(\omega \cdot \omega') d\omega = \lambda_l Y_l^m(\omega'),$$

where

$$\lambda_l = 2\pi \int_{-1}^{1} P_l(\mu) f(\mu) d\mu.$$

This says that the eigenfunctions of the integral operator $\int_{\mathbb{S}^2} f(\omega \cdot \omega') \cdot d\omega'$ are the spherical harmonics with eigenvalues λ_l.

The diffusion weighted MRI signal has the form

$$s(\mathbf{q}) = s_0 \int_{\mathbb{R}^3} p(\mathbf{r}) e^{-2\pi i \mathbf{q}\cdot\mathbf{r}} d^3 r, \tag{8}$$

where $p(\mathbf{r})$ is the PDF describing the probability of diffusion in a direction $\mathbf{r}$ and s_0 is the signal without gradients. Defining the projection (the orientation distribution function ODF)

$$\psi(\mathbf{u}) \equiv \int_0^\infty p(\alpha \mathbf{u}) d\alpha, \quad \mathbf{u} \in \mathbb{S}^2, \tag{9}$$

Tuch showed that

$$\psi(\mathbf{u}) \approx \mathcal{G}[s](\mathbf{u}), \tag{10}$$

where $\mathcal{G}[s](\mathbf{u})$ is the Funk-Radon transform of s defined by

$$\mathcal{G}[s](\mathbf{u}) \equiv \int_{\mathbb{S}^2} \delta(\mathbf{u}\cdot\mathbf{v}) s(\mathbf{v}) d^3 v, \tag{11}$$

i.e., the integral of s over the great circle defined by the equation $\mathbf{u}\cdot\mathbf{v} = 0$.

We expect the ODF Eq. (9) to have a sparse representation in the form Eq. (4), i.e. if

$$\psi(\omega) \approx \sum_{i=1}^{n} \psi_i K(\omega \cdot \omega_i),$$

then many of the ψ_i should be neglagable. To obtain the coefficients, consider Eq. (10) and, assuming for the moment than $\mathcal{G}^{-1}$ exists,

$$s(\omega) \approx \sum_{i=1}^{n} \psi_i \mathcal{G}^{-1}[K(\cdot\omega_i)](\omega),$$

which suggests that we approximate the signal using the above equation. We now need to find how the inverse spherical Radon transform acts on the kernel function K. To this end, consider how $\mathcal{G}$ acts on K:

$$\begin{aligned}
\int_{\mathbb{S}^2} \delta(x\cdot\omega) K(\omega\cdot\omega_i)\, d\omega &= \sum_{l=0}^{N} \sum_{|m|\leq n} \overline{Y}_l^m(\omega_i) \int_{\mathbb{S}^2} \delta(x\cdot\omega) Y_l^m(\omega)\, d\omega \\
&= \sum_{l=0}^{N} \sum_{|m|\leq n} \overline{Y}_l^m(\omega_i)\, 2\pi \int_{-1}^{1} P_l(\mu)\,\delta(\mu)\, d\mu Y_l^m(x) \\
&= \sum_{l=0}^{N} 2\pi P_l(0) \sum_{|m|\leq n} \overline{Y}_l^m(\omega_i) Y_l^m(x) \\
& \sum_{l=0}^{N} 2\pi P_l(0) \frac{2l+1}{4\pi} P_l(x\cdot\omega_i) \\
& \sum_{l=0}^{N} \frac{2l+1}{2\pi} P_l(0) P_l(x\cdot\omega_i),
\end{aligned}$$

with

$$P_l(0) = \frac{1}{2^l} \sum_{k=0}^{l} (-1)^k \binom{l}{k}^2.$$

Note that if l is odd, then $P_l(0) = 0$, identically. Thus $\mathcal{G}$ filters out only the even harmonics of K (and scales them). Thus,

$$\mathcal{G}^{-1}[K(\cdot\,\omega_i)](\mathbf{u}) = \sum_{l=0,even}^{N} \frac{2l+1}{4\pi} \left(\frac{1}{2\pi P_l(0)}\right) P_l(\mathbf{u}\cdot\omega_i).$$

We define this function as

$$\tilde{K}(\mathbf{u}\cdot\omega_i) \equiv \mathcal{G}^{-1}[K(\cdot\,\omega_i)](\mathbf{u}) = \sum_{l=0,even}^{N} \frac{2l+1}{4\pi} \left(\frac{1}{2\pi P_l(0)}\right) P_l(\mathbf{u}\cdot\omega_i)$$

and expand the signal s as

$$s(\mathbf{u}) \approx \sum_{i=1}^{M} \psi_i \tilde{K}(\mathbf{u} \cdot \omega_i).$$

Assuming J measurements, we construct the system of equations

$$s(\mathbf{u}_j) \approx \sum_{i=1}^{M} \psi_i \tilde{K}(\mathbf{u}_j \cdot \omega_i) \qquad j = 1, 2, ...J$$

and solve it in a least-squares sense using an L_1 penalty term to promote sparsity in the solution:

$$\min||s(\mathbf{u}_j) - \sum_{i=1}^{M} \psi_i \tilde{K}(\mathbf{u}_j \cdot \omega_i)||_{L^2} + \lambda||\psi||_{L^1},$$

where λ is a regularization parameter and is related to the noise level. For $\lambda \to \infty$, the solution converges to zero, and as $\lambda \to 0$, the solution converges to the standard least-squares solution.

Once we have solve the above minimization problem, the ODF can be computed

$$\psi(\omega) \approx \sum_{i=1}^{n} \psi_i K(\omega \cdot \omega_i).$$

Note that the coefficients tell you the direction of the fiber orientation; there is no need to solve a maximum problem like in a spherical harmonic expansion. A word of caution: currently our quadratures do NOT have anti-podal symmetry and hence the don't respect the construction of having only even harmonics in the expansion. For this formulation of the problem, we'll need to develop quadratures that have symmetry with respect to inversion.