A Framework for Joint Diffusion Modelling and Orientation Estimation

Marco Reisert[1] and Valerij G. Kiselev[1]
[1]*Medical Physics, University Medical Center Freiburg, Freiburg, Germany*

TARGET AUDIENCE: Diffusion-Modelers who want to do fiber tracking, and researchers from the fiber tracking community who want to do diffusion modeling.

PURPOSE AND INTRODUCTION: Diffusion-Weighted Magnetic Resonance Imaging can reveal the microstructural organization of human brain white matter. There is a multitude of different models that try to address the signal formation, starting from simple single tensor models to complex three-compartment models. Although these models are not limited to voxels containing just one prominent fiber bundle, the complexity and ambiguities of the models usually exclude the application in multi-fiber voxels (apart from some simple ones[1,2]). To solve this problem we formulate in this work the model fitting as one global problem assuming spatial coherence of the underlying diffusion parameters. In this way, we are able to find voxel-wise the orientations of fibers and their model parameters. The decision for single or multi-fiber voxels is directly integrated into the optimization process by using the Bayesian information criterion (BIC). The problem is quite hard from a computational point of view as it is non-convex and combinatorial. Ordinary gradient-based approaches are prone to get trapped in local minima and are hard to be combined with the combinatorial nature of the problem. At the heart of our approach lies a reversible jump Monte-Carlo Markov-Chain (RJMCMC) sampling strategy, which is known to be computationally very expensive. Hence, the main technical contribution of this work is the proposal of an efficient way to compute certain energy differences which are required by the RJMCMC.

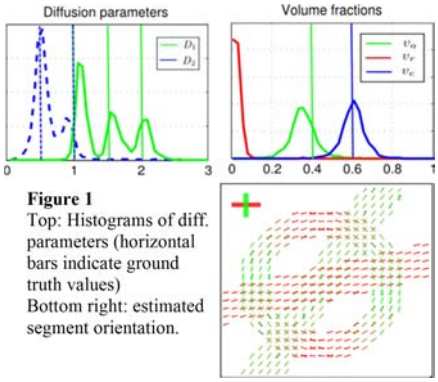

Figure 1
Top: Histograms of diff. parameters (horizontal bars indicate ground truth values)
Bottom right: estimated segment orientation.

METHOD: Our framework is illustrated with a three-compartment model, which is the stick-cylinder-dot model in terms of Panagiotaki's taxonomy[3]. This model is sufficiently complicated although the common axial diffusivity in the intra- and extraaxonal compartments might be unphysical[4]. The model signal is composed of a set of segments. Each segment contributes with the following signal:

$$M_i(\mathbf{r},\mathbf{q}) = w_i \left(v_r(\mathbf{r}) + v_a(\mathbf{r}) e^{-\mathbf{q}^T \mathbf{D}^i_a \mathbf{q}} + (1 - v_a(\mathbf{r}) - v_r(\mathbf{r})) e^{-\mathbf{q}^T \mathbf{D}^i_e \mathbf{q}} \right) I(\mathbf{r},\mathbf{r}_i)$$

where $\mathbf{r}$ is the voxel position and $\mathbf{q}$ the q-space coordinate (rescaled by diffusion time). Each segment carries 8 variables: position $\mathbf{r}_i$, orientation $\mathbf{n}_i$, two diffusivities D_1 and D_2, and the total volume fraction w_i. The relative volume fractions v_r ,v_a and v_e=1-v_r-v_a are not properties of the segment, but of the location, i.e. all segments within a voxel contribute with the same relative volume fractions. The intra-axonal tensor $\mathbf{D}^i_a$ and extra-axonal $\mathbf{D}^i_e$ have principal direction $\mathbf{n}_i$, where $\mathbf{D}^i_a$ has D_1 as eigenvalue in parallel direction and $\mathbf{D}^i_e$ has D_1 in parallel direction and D_2 in perpendicular direction. The function $\mathbf{I}(\mathbf{r},\mathbf{r}_i)$ is an indicator function, giving contribution if $\mathbf{r}=\mathbf{r}_i$. The total energy that we minimize is:

$$E = \frac{1}{\sigma^2} \| \sum_{i=1}^{N} M_i - S \|^2 + \lambda_0 N + \lambda_1 \|\nabla v\|^2 + \lambda_2 \sum_{i=1}^{N} \sum_{j \in \mathcal{N}(i)} ((D_1^i - D_1^j)^2 + (D_2^i - D_2^j)^2)(\mathbf{n}^i \cdot \mathbf{n}^j)^{2p}$$

The first term is the Gaussian data-likelihood, the second term refers to the BIC, the third term fosters smoothness of the volume fraction maps v_r and v_a, and the last term prefers smoothness of the diffusivities along aligned segments ($\mathcal{N}$(i) denotes the neighbouring voxels of voxel $\mathbf{r}_i$).

The optimization is carried out by a RJMCMC algorithm, where the possible moves of the algorithm are: creation/deletion of segments, changing orientation/position/diffusivities and changing volume fractions. The critical, time consuming part of the optimization is the data-likelihood. We found that correlations of the signal with the exponential model functions can very well approximated by inverse power series like $\Sigma_i\, s_i \exp(b_i\, D) = \Sigma_k\, a_k\, (A + D)^{-k}$. This kind of approximations sped up our algorithm by a factor of about 30, which leads to running times of about 25 minutes for whole brain reconstructions.

RESULTS: Experiments were performed for synthetic data and in-vivo measurements. The in-vivo measurements were acquired on a Siemens 3T TIM Trio using an SE EPI sequence, with a TE of 117 ms and a TR of 7.1 s. The whole brain was covered with contiguous 2-mm slices in an in-plane resolution of 2x2 mm^2. The diffusion encoding was performed on two b-shells with 61 directions with an effective b-value of 1000 s/mm^2 and 2000 s/mm^2 . The simulations were performed with the same scheme at an SNR of 20 (Rician noise). Three fiber bundles were arranged (see Fig.1) and to each bundle specific diffusivities were assigned (D_1, D_2)=(1, 0.5), (2, 0.5), (1.5, 0.5) µm^2/ms and the same volume fractions of (v_r ,v_a) = (0,0.4). The parameters of the priors were set empirically to (λ_0, λ_1, λ_2, p) = (0.1,0.1,1,8). Figure 1 shows results of the simulation in terms of two histograms and the segments' orientations. For the in-vivo measurements the same parameter setting was chosen. The reconstruction was performed inside a white matter mask (segmented via SPM8). Figure 2 shows first-order and second-order statistics of the parameters over the whole brain, spatial parameter maps (maps for D_1,D_2 are obtained by averaging) for several transversal slices and segment orientations for a section of a coronal slice.

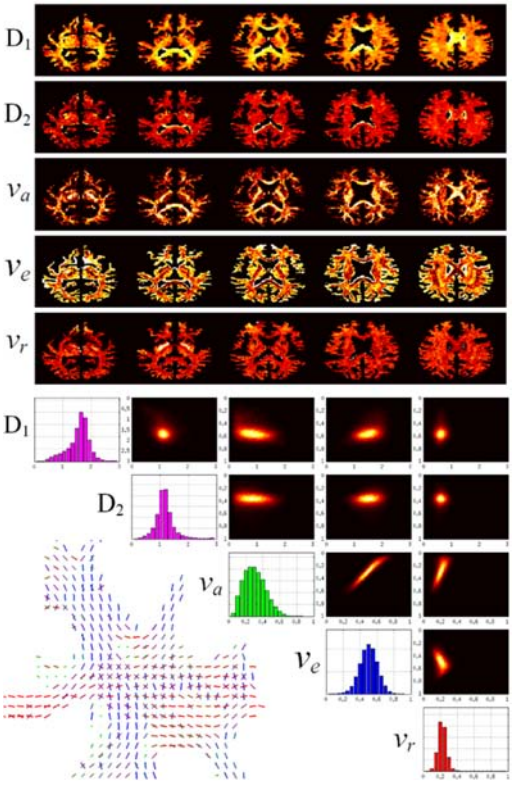

Figure 2: Top: Transversal maps of spatial parameter distributions. Bottom right: Single and joint histograms of parameters. Bottom left: Segment orientations in a coronal slice.

DISCUSSION: The simulation shows that the proposed algorithm does a nearly unbiased reconstruction of the diffusion parameters, although we use the compromised Gaussian data likelihood. In fact, the Rician noise floor is partially accounted for by the restricted water (dot). Additionally, the simulations show that already quite low b-values are enough to cope with the bi-exponential stick-cylinder-dot model due to the full orientation coverage. The approach is also able to disentangle the 45°-crossing and infer the right diffusion parameters, which is only possible due to the introduced spatial regularizer. The in-vivo experiments give plausible results, e.g. in the Corpus Callosum we have: D_1=1.8 µm^2/ms, D_2=0.9 µm^2/ms, v_r = *0.1,* v_a = 0.6. One can nicely see an increase of the extra-axonal fraction at the borders of the white matter mask. In frontal regions, where our head coil array has low sensitivity, the dot-compartment v_r has slightly increased values, which might be explained by a low SNR in these regions. The perpendicular diffusivity D_2 is quite homogeneously distributed apart from the area adjacent to ventricles. On the other hand, the parallel diffusivity D_1 shows a more heterogeneous pattern, e.g. higher values in the Corpus Callosum. The reconstructed segment orientations coincide quite well with the expected pattern that is known from traditional approaches like spherical deconvolution[3].

REFERENCES: **1.** Kreher et al., MRM 2005, 54(5):1216-25, **2.** Tournier et al., NeuroImage 2008, 42(2):617-25, **3.** Panagiotaki et al., NeuroImage 2012, 59(3):2241-54, **4.** Fieremans et al., NeuroImage. 2011 Sep 1;58(1):177-88

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