## Recovering Detailed Intra-voxel White Matter Structure by using an Adaptive Diffusion Dictionary

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Background: On the analysis of the Diffusion-Weighted Magnetic Resonance Imaging (DW-MRI), the multi-compartments (MC) models overcome the limitations of the well-known Diffusion Tensor (DT) model for estimating the axonal bundle orientations at voxels with partial volume effects. Some successful MC methods are based on Diffusion Dictionaries (DD). The DD methods assume that the observed MR signal at each voxel is a linear combination of atoms (fixed signals generated from a set of basis functions). The atoms are generated along predefined orientations and keep

fixed diffusion properties. For those reasons, the atoms do not necessarily correspond to the actual fiber bundle features (orientations or diffusion properties) for all the voxels. In spite of those limitations, the performances of the DD methods have presented very competitive results by using a reduced number of DW-MR samples [1]. To reduce the impact of the limitations of the DD methods, there are methods to build and design dictionaries [2][3]. However, those methods need a training data-set and the learned dictionary is still fixed for all voxels in the brain. Here, we present a voxel-wise Adaptive Diffusion Dictionary (ADD) method to overcome the limitations of the DD methods: the discrete nature of predefined diffusion orientations and their inability to estimate correct diffusivity shapes.

Methods: Our proposal is based on the DBF model [2]. The dictionary of the DBF method is based on the DT model, i.e., the j-th atom has associated a single fixed base tensor,  $\bar{T}_i = V_i \Sigma_i V_i^{\mathsf{T}} (V_i \text{ and } \Delta_i \text{ define})$ the orientation and the shape of the tensor, respectively). To modify the orientation and the diffusion properties of each atom, we define a new DBF formulation as:  $\varphi_{ij} = S_0 \exp\{-b_i g_i^T R_{\theta_i} [V_j(\Sigma_i + E_i)]\}$  $\delta_j V_j^{\mathsf{T}} R_{\theta_i}^T g_i$ , where  $\varphi_{ij}$  is the *ij*-th element of the *adaptive dictionary* generated from the acquisition

parameters  $b_i$  and the magnetic gradient  $g_i$  (for i = 1, ... M), and  $\bar{T}_j$  (for j = 1, ... N).  $R_{\theta_i}$ and  $\delta_i = \text{diag}[\delta_{1i}, \delta_{2i}, \delta_{2i}]$  are the 3D re-orientation matrix (defined by the angles with  $\theta_j = [\theta_{xj}, \theta_{yj}, \theta_{zj}]$ ) and the change on the tensor's shape used to modify the *j*-th atom, respectively. To compute those changes, we solve  $\min_{\Theta,\Delta,\alpha} U(\alpha,\Theta,\Delta) = \|\Phi(\Theta,\Delta)\alpha-S\|_2^2$ s.t.  $\alpha \ge 0$ ,  $R_{\theta_j} = R_{\theta_j}^{-1}$ ,  $\det\left(R_{\theta_j}\right) = 1$  and  $\Sigma_j + \delta_j \ge 0$  (for j = 1, 2, ...N). With  $\Theta =$  $\left\{\theta_{j}\right\}_{j=1,2...N}\text{ and }\Delta=\left\{\delta_{j}\right\}_{j=1,2...N},\ \Phi(\Theta,\Delta)=\left\{\phi_{ij}\right\}_{i=1,...M,j=1,...N}\text{ and }S=\left\{s_{i}\right\}_{i=1,...,M}\text{ are the }A=1,...M$ DW signals. The direct minimization of the previous problem can be complicated mainly because of R<sub>0</sub>. Therefore, we propose an iterative surrogate approach using mathematical approximations that simplify the problem and avoid the non-linear constrains on  $\Theta$ . First, we iteratively compute small changes for the unknowns involved for the atoms one by one  $(\alpha, \Theta, \Delta)$  until convergence, similarly to the coordinate descent strategy. For the case of  $\Theta$ , we rewrite  $R_{\theta_i}$  as the product of three rotation matrices around the canonical axes. Then, if we constrain the rotational angles,  $\theta_{wj}$  (for  $w \in \{x, y, z\}$ ), to be small (for instances less than  $8^{\circ}$ ), we can use the following approximations:  $\cos \theta_{wj} \approx 1$  and  $\sin \theta_{wi} \approx \theta_{wi}$ . Now, if only one of the three rotation matrices is applied at each time, the problem is reduced to three problems easer-to-solve with linear constrains (s.t.  $|\theta_{wi}|$  < 8°); for instance, to solve the angular displacements  $\theta_{xj}$ , we fix the values for  $\theta_{yj}$  and  $\theta_{zj}$ . Note that although we only allow small orientational changes, the effect of several iterations produce large reorientations. We highlight that by solving three problems for  $\Theta$ instead of one, our proposal avoids the non-linear constraints on  $R_{\theta_i}$ .

Experiments and Results: 1) Synthetic Data: This experiment was performed on the publicly available multi-shell data-set used in the 2012 HARDI Reconstruction Challenge (HRC). Figure 1 shows the Angular Error (AR), the Success Rate (SR) (as in [1]) and the Mean Square Error (MSE) of the signal fitting for ADD and DBF. We see that ADD presents better results than DBF. 2) In vivo Data: A single healthy volunteer was scanned on a Philips Achieva TX 3.0 scanner with 16 channels. We acquire four  $S_0$  images and 64 multi-shell DW images with  $b_i \in \{2000, 2500\} s/mm^2$  with voxel dimension equals to  $2 \times 2 \times 2$  mm<sup>3</sup>. Figure 2 depicts the estimations of the intra-voxel structure on the intersection of the Sensory-Motor tracts (SMT), superior fronto-occipital tracts (SFOT) and the cortical-spinal tracts (CST). Here, ADD achieves to capture up to 4 spatially coherent compartments without imposing spatial regularization, while DBF up to 3. Additionally, we can see that ADD estimates, in general, more coherent complex structures than DBF. Figure 3 shows the MSE for the DBF and ADD approaches: ADD presents a better data fitting than DBF. This behavior is explained as ADD voxel-wise modifies the dictionary to estimate a correct intra-voxel structure.

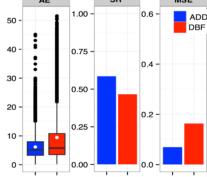


Fig. 1: Comparison between ADD and DBF over the HRC data-set with SNR=20.

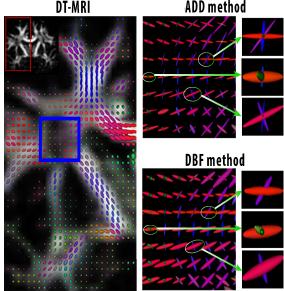


Fig. 2: Qualitative comparison of ADD and DBF estimations around the intersection of the SFOT, CST and SMT.

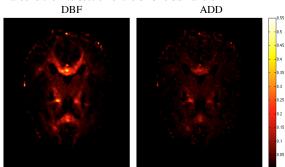


Fig. 2: Quantitative comparison of the signal fitting (MSE) between DBF and ADD.

Conclusions: One of the advantages of the DD methods is the ability to compute accurate reconstructions on clinically-realistic imaging protocols. Our framework presents an important benefit over the DD methods, while keeping the convenient features of them, because it iteratively adapts the dictionary properties in order to estimate accurate tissue features. The improvements in the correct estimation of the tissue structure benefit brain research, because they may help to the disease characterizations and allow obtaining better tractography estimations, hence, it results in an accurate computation of the brain connectivity patterns.

References: [1]. A. Daducci et. al., IEEE TMI, 2014; 33:384-399. [2]. J. Sun et. al., IPMI, 2013; 7917:619-631. [3]. S. Merlet et. al., MIA, 2013; 17:830–843. [3]. A. Ramírez-Manzanares et. al., IEEE TMI, 2007; 26: 1091-1102.