Diffusion Tensor Representations and Their Applications to DTI Error Propagation

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INTRODUCTION The diffusion tensor is a 3x3 positive definite matrix and, therefore, possesses several distinct matrix decompositions, e.g. the Cholesky, and the Eigenvalue decompositions. To date, the Eigenvalue decomposition has been used only in computing tensor-derived quantities [1-4] but not as a parametrization (or equivalently, a representation) in DTI error propagation [5]. Treating a matrix decomposition of the diffusion tensor as a representation is a very useful strategy not only in tensor estimation, constrained or otherwise, [1-4,6-8] but also, as we will show, in DTI error propagation. Specifically, we propose to use the Eigenvalue decomposition as a representation in DTI error propagation and show how the proposed technique can address important questions related to the uncertainty of the eigenvalues and, more importantly, of the eigenvectors. For completeness, we introduce three representations to DTI error propagation — the ordinary, the Cholesky, and the Euler representations. This work provides a unified framework in which the uncertainty of any tensor-derived quantity such as eigenvalues, eigenvectors, trace, fractional anisotropy (FA), and relative anisotropy (RA) can be analytically derived and estimated. Although the diffusion representations are essentially equivalent when dealing with the tensor estimate itself, the variances of interests derived from them may be different. In other words, one representation may be more accurate than the other in variance estimation. Furthermore, one representation may be more convenient and analytically tractable than the other. Theoretical analysis and simulations are carried out to investigate this issue.

METHODS Within the framework of least squares estimation [8], the nonlinear least squares (NLS) objective function in the ordinary tensor representation can be expressed as: $f_{NLS}(\gamma) = \frac{1}{2}\sum_i (s_i - \exp(\sum_j W_{ij}\gamma_j))^2$. In this representation, we have $\boldsymbol{\gamma} = [\ln(S_0), D_{xx}, D_{yy}, D_{zz}, D_{xy}, D_{yz}, D_{xz}]^T$ where the parameter for the non-DW signal is S_0. Similarly, we have $\boldsymbol{\rho} = [\rho_1, \cdots, \rho_7]$ [8] for the Cholesky representation and $\xi = [\ln(S_0), \lambda_1, \lambda_2, \lambda_3, \theta, \phi, \psi]$ for the Euler representation, which consists of the eigenvalues and the Euler angles. In DTI error propagation [5], the key object to compute is the covariance matrix with respect to γ, which will be denoted as Σ_γ. It has been shown in [5] that Σ_γ is related to the Hessian matrix of $f_{NLS}(\gamma)$ [8]: $\Sigma_\gamma = \sigma_{DW}^2 [\nabla^2 f_{NLS}(\hat{\gamma})]^{-1}$, where $\hat{\gamma}$ is the NLS estimate of γ, and σ_{DW}^2 is the variance estimate of the DW signals. In a similar vein, we can also obtain covariance matrices with respect to $\boldsymbol{\rho}$ and ξ, which we shall denote as $\Sigma_\rho = \sigma_{DW}^2 [\nabla_{\boldsymbol{\rho}}^2 f_{NLS}(\gamma(\hat{\boldsymbol{\rho}}))]^{-1}$ and $\Sigma_\xi = \sigma_{DW}^2 [\nabla_\xi^2 f_{NLS}(\gamma(\hat{\xi}))]^{-1}$, respectively. Once we have variance-covariance matrices in different representations, any uncertainty of interest related to DTI can be computed. For example, the covariance matrix of the components of the major eigenvector of the diffusion tensor can be constructed most easily in the Euler representation and the eigenvectors of this covariance matrix whose eigenvalues are nonzero are exactly the major and minor axes of the ellipse of the cone of uncertainty. To investigate the issue of accuracy of the variance estimate derived from different representations, we examine the transformation between the covariance structures. For example, Σ_γ can be constructed from Σ_ξ, which we shall denote as $\Sigma_{\gamma(\hat{\xi})}$. Then, it can be shown that $\Sigma_{\gamma(\hat{\xi})}$ has the following expression: $\Sigma_{\gamma(\hat{\xi})} = \sigma_{DW}^2 \left[\left(\nabla^2 f_{NLS}(\gamma(\hat{\xi})) + \varepsilon\right)\right]^{-1}$ where ε is a square matrix that is generally not zero because it depends on the residuals of the fit and the first and second order derivatives between the representations. It is clear that $\Sigma_{\gamma(\hat{\xi})}$ is different from $\Sigma_\gamma = \sigma_{DW}^2 [\nabla^2 f_{NLS}(\hat{\gamma})]^{-1}$ by the additional error term, ε. The implication is that the variance estimate of any tensor-derived quantity that is derived from representations other than the ordinary representation in a nonlinear fashion will introduce additional error in the final estimate.

RESULTS Simulations similar to those of [4] were carried out to validate the above analysis. A known ordinary diffusion tensor representation is used; $\gamma = [\ln(1000) \times 10^{+4}\, s/mm^2, 10.2, 6.7, 4.0, 1.3, -0.6, 2.1]^T \times 10^{-4} mm^2/s$ with $FA = 0.52$ and $Trace = 0.0021\, mm^2/s$. At SNR=15, 50000 NLS estimates of the diffusion tensor were generated from a set of 30 gradient directions and 4 b-values, (0, 500, 1000, and 1500 s/mm^2) based on the modified full Newton method [7]. Then, 50000 variance estimates of FA and of Trace with respect to both the ordinary and the Euler representations were derived. Figures 1A and 1B show the histograms of these variance estimates together with the sample variances. It is clear that the ordinary and Euler representations are equally accurate in estimating variance of Trace since Trace is a linear function in both of these representations. But, the Euler representation is less accurate than the ordinary representation in estimating the variance of FA because FA is a nonlinear function of the eigenvalues.

DISCUSSION AND CONCLUSION Different representations of the diffusion tensor can provide new insights about the variability in many tensor-derived quantities and the diffusion tensor itself. Within the proposed framework, the uncertainty of all relevant tensor-derived quantities can be estimated. Particularly, the covariance structures of the major eigenvector of the diffusion tensor can be constructed within this framework and it can be used to construct the cone of uncertainty for DTI tractography [9-11]. While the cone of uncertainty has been presumed to be circular in cross section in previous studies, the analysis presented here suggests that it is generally elliptical, Figure 1B. We also showed how the residuals from the nonlinear least squares fit affect the covariance structures, and consequently, the variance estimate in various representations.

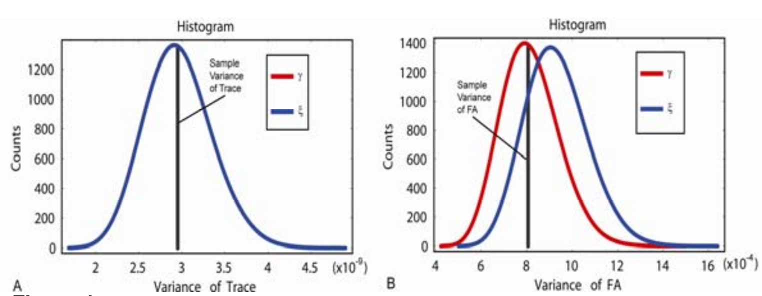

Figure 1

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