A Joint PDF for the Eigenvalues and Eigenvectors of a Diffusion Tensor

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Purpose: To derive a joint parametric probability density function (pdf) of the eigenvalues and eigenvectors of 2nd-order tensors conforming to the isotropic tensor-variate normal (ITVN) pdf [1], to show (using a perturbation expansion of this pdf) that it decouples into a product of pdfs of the eigenvalues and eigenvectors, and to derive simple expressions for these pdfs.

Introduction: Finding a general analytical distribution of eigenvectors and eigenvalues is challenging. For moderate SNR, perturbation approaches can be employed [2], as well as other schemes [3]. Here we show that for an important special case of the ITVN pdf [1], approximately satisfied in well-designed DTI experiments, we can obtain the analytical form of the joint pdf of the three eigenvalues and three eigenvectors of an estimated diffusion tensor. A simple analytical expression for the pdf of the eigenvalues has already been derived [1]; here we derive, assuming small deviations, a simple analytical expression for the pdf of the eigenvectors, too.

Theory: Using the 3x3 eigenvector (orthogonal) and eigenvalue (diagonal) matrices of the tensor random variable (E and Λ, respectively) and of the mean tensor (E_0 and Λ_0=diag($\lambda_1, \lambda_2, \lambda_3$)) the ITVN pdf can be written as:

$$P(\Lambda, \Lambda_0, E, E_0) = \sqrt{\frac{4\mu^5(2\mu + 3\rho)}{\pi^6}} \exp\left(-\frac{1}{2}\mathrm{F}(\Lambda, \Lambda_0, E, E_0)\right), \tag{1}$$

where $\mathrm{F}(\Lambda, \Lambda_0, E, E_0) = \mathrm{A}(\Lambda, \Lambda_0) - 4\mu \mathrm{B}(\Lambda, \Lambda_0, E, E_0)$, $\mathrm{A}(\Lambda, \Lambda_0) = \rho(\mathrm{Tr}(\Lambda - \Lambda_0)^2 + 2\mu\,\mathrm{Tr}(\Lambda^2 + \Lambda_0^2)$, $\mathrm{B}(\Lambda, \Lambda_0, E, E_0) = \mathrm{Tr}[\mathrm{E}\Lambda E^T E_0 \Lambda_0 E^T]$, and ρ and μ are the two parameters that characterize the 4th-order covariance tensor. The variability of the eigenvalues and eigenvectors are intrinsically coupled through $\mathrm{B}(\Lambda, \Lambda_0, E, E_0)$. We perform the perturbation expansion of $\mathrm{A}(\Lambda, \Lambda_0)$ and $\mathrm{B}(\Lambda, \Lambda_0, E, E_0)$ using the substitutions $\Lambda = \Lambda_0 + \delta\Lambda$, and $E = E_0 + \delta E$. The variability in eigenvectors to first-order can be expressed in terms of infinitesimal rotations (small angles), where we use the Cardan rotation matrix, R, whose three rotation angles are pitch, ω_1, roll, ω_2, and yaw ω_3. For small angles $R = I + \Omega_p$, where I is the identity matrix and Ω_p is the infinitesimal part of the rotation matrix. Up to second-order in angles, Ω_p can be approximately written as $\Omega_p = [0, -\omega_2^2/2 - \omega_3^2/2, \omega_1\omega_2 + \omega_3; -\omega_2 - \omega_3, 0, -\omega_1^2/2 - \omega_3^2/2; -\omega_1 + \omega_2\omega_3, -\omega_1^2/2 - \omega_3^2/2, 0]$. It is necessary to include second-order terms of ω_1, ω_2, and ω_3 since the expansion of $\mathrm{B}(\Lambda, \Lambda_0, E, E_0)$ produces terms $\Omega_p + \Omega_p^T$ which are zero to first-order. After substituting this expression for Ω_p in the perturbation expansion of $\mathrm{B}(\Lambda, \Lambda_0, E, E_0)$ we obtain $\mathrm{B}(\Lambda, \Lambda_0, \delta\mathrm{E}, \mathrm{E}_0) \cong \mathrm{B}(\Omega_p, \Lambda_0) = -(\lambda_2 - \lambda_3)^2 \omega_1^2 - (\lambda_1 - \lambda_3)^2 \omega_2^2 - (\lambda_1 - \lambda_2)^2 \omega_3^2$. Hence, the final expression for $\mathrm{F}(\delta\Lambda, \Lambda_0, \delta E, E_0) = \rho\mathrm{Tr}(\delta\Lambda^2) + 2\mu\mathrm{Tr}(\delta\Lambda^2) + 4\mu((\lambda_2 - \lambda_3)^2 \omega_1^2 + (\lambda_1 - \lambda_3)^2 \omega_2^2 + (\lambda_1 - \lambda_2)^2 \omega_3^2)$ becomes decoupled, i.e.,

$$\mathrm{P}(\delta\Lambda, \omega_1, \omega_2, \omega_3) \approx e^{-\frac{1}{2}\rho(\mathrm{Tr}(\delta\Lambda))^2 + 2\mu\mathrm{Tr}(\delta\Lambda^2)}\, e^{-2\mu\left((\lambda_2 - \lambda_3)^2 \omega_1^2 + (\lambda_1 - \lambda_3)^2 \omega_2^2 + (\lambda_1 - \lambda_2)^2 \omega_3^2\right)} \tag{2}$$

Besides the eigenvalues and eigenvectors being independent, the rotation angles themselves are independently distributed according to

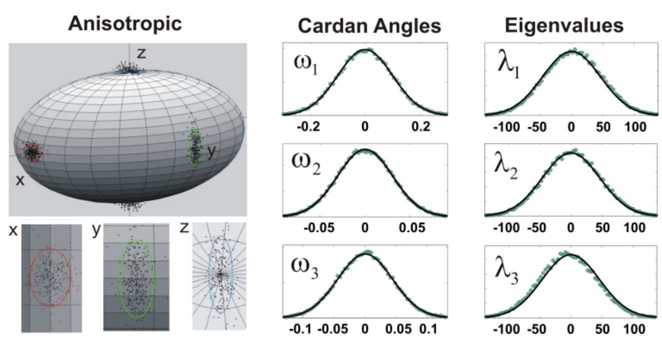
$$\mathrm{PDF}(\omega_i) \approx e^{-2\mu(\lambda_j - \lambda_k)^2 \omega_i^2}, \qquad i \neq j \neq k,\ \lambda_j \neq \lambda_k \text{ for } j \neq k, \tag{3}$$

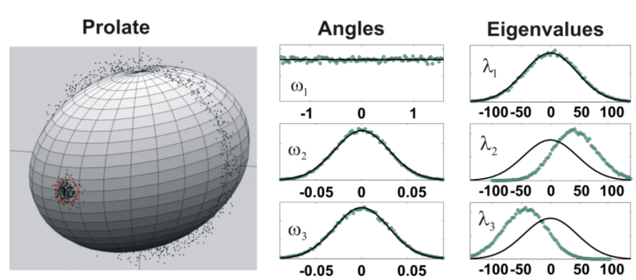
which is a zero-mean normal distribution with standard deviation

$$\sigma_i = \frac{1}{2\sqrt{\mu}\left|\lambda_j - \lambda_k\right|}, \qquad i \neq j \neq k \tag{4}$$

Methods: We perform Monte Carlo simulations using fully asymmetric (anisotropic), prolate and oblate mean 2nd-order tensors to generate ITVN distributed tensor samples. Eigenvectors and eigenvalues are computed for each simulated tensor. From these samples the empirical pdfs are obtained.

Results: Figure 1a shows the simulation results for a fully asymmetric tensor, with sample points displayed along with the "mean" ellipsoid. The inset magnifies the scatter around each axis with uncertainty ellipses plotted at three SDs to compare with the model predictions based on Eq. 4. In Figures 1b and 1c, the empirical pdfs (circles) are in a very good agreement with the predictions of Eqs. 2 and 3. For the symmetric tensors (prolate, oblate, or spherical) similar results are also obtained (Figure 2), but with the exception that the axes that violate the condition $\lambda_j \neq \lambda_k$ for $j \neq k$ in Eq. 3, show a uniform distribution of angles. The differences in the eigenvalue pdfs in these cases are due to the sorting bias so that larger/smaller eigenvalue pdfs are skewed and shifted to the right/left.





Discussion/Conclusion:

This new pdf for the eigensystem of an estimated diffusion tensor moves us closer to developing statistical hypothesis tests valid for measured DTI data.

References: **[1]** PJ Basser, S Pajevic, IEEE Trans Med. Img, 22, 785 (2003); **[2]** GR Hext, Biometrika, 50, 353 (1963); **[3]** CG Koay et al, IEEE Trans Med. Img, 26, 1017 (2007).