A DTI TRACTOGRAPHY ALGORITHM DERIVED FROM THE DIFFUSION EQUATION AND QUANTUM-MECHANICAL CORRESPONDENCE: METHOD AND SIMULATION

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Target audience: Scientists interested in diffusion-based MRI tractography algorithm

Purpose: Diffusion tensor imaging (DTI) is a powerful tool to delineate the white matter fiber pathways. However, only diffusion tensor, instead of diffusion equation, plays an important role in most of the tractography methods. As an attempt, we derived a Lagrangian from the diffusion equation for our tractography algorithm, and applied it on simulated two-dimensional diffusion tensors to demonstrate its feasibility.

Methods: There is a well-known correspondence between diffusion equation and Schrodinger equation. [1] By replacing the Planck constant $\hbar$ with an imaginary number $-i$, we can utilize all the quantum-mechanical techniques if the corresponding Hamiltonian operator is hermitian. Now the momentum operator in position space is $\hat{p} = -\nabla$ which is not a hermitian operator. Fortunately, the "diffusion" Hamiltonian $\hat{H}_0 = \nabla \cdot D \cdot \nabla$ is a hermitian operator because it can be rewritten in the form of $-(\nabla/i)\cdot D \cdot(\nabla/i)$, where the diffusion tensor D is a real symmetric matrix. After using Hamilton's canonical equation and Legendre transformation, we acquire a Lagrangian $L_0 = (1/4)v \cdot D^{-1} \cdot v$, where v is a generalized velocity. We can append another term of Lagrangian L_1, which obeys the following equation:

$$\frac{d}{dt}\left(\frac{\partial L_1}{\partial v}\right) - \frac{\partial L_1}{\partial x} = \frac{1}{2}\beta v \ ,$$

where t is the generalized time, x is the coordinate, and β is a constant. Obviously, L_1 is pertaining to a damping force with a negative damping coefficient. Then the total Lagrangian of the system is $L_{total} = L_0 + L_1$. Solving the Euler-Lagrange equation, we have an equation of motion:

$$\frac{dv_i}{dt} = f \cdot \frac{1}{2} D_{ij}\partial_j\left(v_k D_{kl}^{-1} v_l\right) + \beta D_{ij} v_j \ , \qquad (1)$$

where f = 0 or 1 for further discussions, and Einstein notation is used for simplicity. This equation is the core of our tractography algorithm.

To show its viability, we calculated inverse tensors of structure tensors from a picture of magnetic lines with 168 x 168 pixels, [2] and divided it into 4 x 4 voxels. Tensor average in each voxel was constructed as the simulated diffusion tensor. Voxels of the fourth column were chosen as seeding voxels, and the initial velocity was in the direction of the principal axis in each voxel. Solving the Eq. (1) numerically, tracts were obtained. All the calculations were performed with MATLAB (The Mathworks), employing *ode45* function.

Results: The original picture and simulated diffusion tensors are shown in Fig.1 A and B. The calculated streamlines with (f, β) = (0, 3), (1, 0), and (1, 3) were shown in Fig.1 C, D, and E, respectively.

Discussion and conclusion: Since Eq. (1) is related to the tensor derivative, calculated tracts are able to turn in one voxel more easily. Simulated results show that turning in an acute angle is possible in only 4 ~ 6 voxels. Comparing Fig.1 C, D, and E with each other, it is clear that the first term in Eq. (1) contributes to turnings of tracts, and the second term in Eq. (1) contributes to the acceleration in the direction of the principal axis. [3] Tracts are consistent with the original picture, manifesting the feasibility of this method. The whole algorithm is also applicable in three-dimensional cases. On the other hand, because this method belongs to deterministic streamline algorithms, it can neither solve the fiber crossing problem nor eliminate the effect of noise. Nevertheless, this Lagrangian is full of potential applications. For one thing, it would be suitable for evaluating the correctness of a calculated tract. For another, it could include higher order terms, such as terms related to Kurtosis.

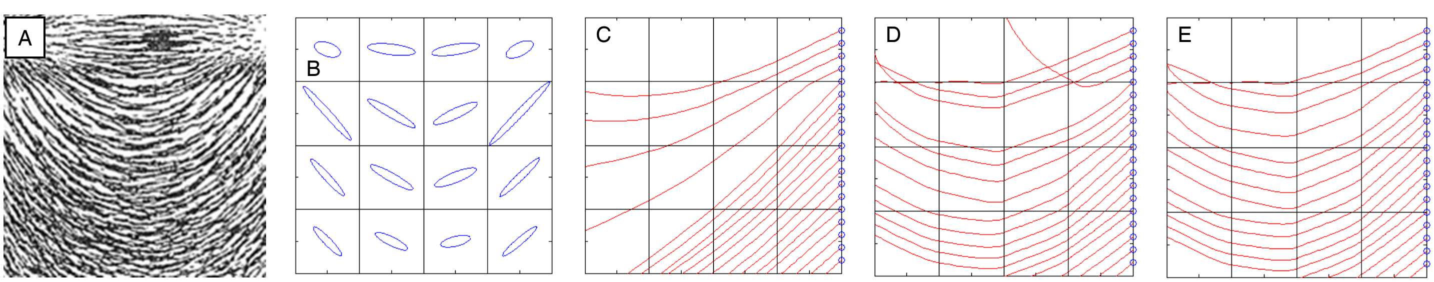

Fig.1 This figure shows **A.** original picture, **B.** simulated diffusion tensor, and **C, D, and E.** calculated tracts with parameters of (f, β) = (0, 3), (1, 0), and (1, 3), respectively. Blue circles are seeds, and red lines are resulting streamlines.

References:

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3. Lazar M, Weinstein DM, et al. White Matter Tractography Using Diffusion Tensor Deflection. Human Brain Mapping. 2003;18:306-321.