TOWARDS QUANTIFICATION OF THE BRAIN’S SHEET STRUCTURE: EVALUATION OF THE DISCRETE LIE BRACKET

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Purpose: A three-dimensional Manhattan street grid or the intricate streets of Victorian London, which structure reflects our brain’s organization best? This central question added three Science publications to the diffusion MRI (dMRI) literature 1-3. Wedeen et al. (2012a,b) 1,3 conjectured that which structure reflects our brain’s organization best? This central question added three Science

Theory: From a set of diffusion or fiber orientation distribution functions (ODFs) on each position of the brain (a manifold $\mathcal{M} \subset \mathbb{R}^3$) obtained from any suitable dMRI reconstruction technique, one can obtain a smooth vector field $V: \mathcal{M} \to \mathbb{R}^3$ (with $\mathcal{M} \subset \mathcal{M}$) derived from ODF maxima. A single vector field can be integrated to obtain a family of streamlines (or integral curves) $s \mapsto \gamma_V(s)$ such that $d\gamma_V(s)/ds = V(\gamma_V(s))$, where $s$ denotes the arc-length parameter. This integration can be extended to two vector fields $V$ and $W$, resulting in an integral surface $S$ (the sheet) whose tangent plane at $p$ is spanned by $V_p$ and $W_p$. The requirements for such a surface to exist are formalized in the Frobenius theorem\footnote{The Frobenius theorem states that for a vector field $X$ on a manifold $\mathcal{M}$, if the set of all vector fields $Y$ that commute with $X$ (i.e., $[X,Y] = 0$) spans the tangent space at every point of $\mathcal{M}$, then there exists a submanifold of $\mathcal{M}$ on which $X$ and $Y$ are defined.}. The Lie bracket of vector fields $V$ and $W$ on $\mathcal{M}$ is a bilinear operator defining a third vector field $[V,W] = \mathcal{L}_V(W)$, with $\mathcal{L}_V(W)$ the Jacobian of a vector field $X$. The Frobenius theorem states that the sheet $S$ exists if and only if $[V,W]$ lies in the plane spanned by $V$ and $W$ (i.e. “the normal component of the Lie bracket”\footnote{The normal component of the Lie bracket is defined as $\gamma_V(s) \cdot \gamma_W(s)$, where $\gamma_V$ and $\gamma_W$ are the integral curves of $V$ and $W$, respectively.} should be zero) for all points $p \in S$ (Fig. 1).

Methods: Lie bracket calculations: Differential operators on vector fields are notoriously difficult to implement, often requiring considerable implicit smoothing. In Wedeen et al. (2012a) the authors opted instead to move around along the integral curves\footnote{In this work we have evaluated a method to calculate the discrete Lie bracket for the quantification of sheet structure.} and consider the difference vectors $D^\Delta_{\mathcal{L}_V}(h_1,h_2) = \gamma_{V}(h_2) - \gamma_{V}(h_1)$, where $q = \gamma_{V}(h_1) - \gamma_{V}(h_2)$ and $h_1$ and $h_2$ are step sizes, see Fig. 1. This difference vector at $p$ is related to the local Lie bracket according to $D^\Delta_{\mathcal{L}_V}(h_1,h_2) = h_1 h_2 \delta(\Delta h_1, \Delta h_2) + \delta(h_1, h_2)$, with $\delta(h_1, h_2)$ correction terms of third and higher orders in $h_1$ and $h_2$ (i.e. $O(h_1^2)$ and similar terms)\footnote{The correction terms are necessary because the local Lie bracket is a measure of the deviation of the flow from being linear.}.

Results: We compare for each of the vector field pairs the Lie bracket estimates $E_p(V,W)$ to the analytically calculated Lie bracket $[V,W]_p$, with $p$ the origin. Analogous to Wedeen et al. (2012a)\footnote{Wedeen et al. (2012a,b) investigated whether the grid pattern is most likely an artifact, biased by the limitations of the techniques used in Wedeen et al. (2012a). In order to prove or disprove the occurrence of sheet structure, more extensive quantitative analyses are needed. In this work, we aim for a formalization of the terminology, and evaluate the validity of the discrete Lie bracket (estimated as proposed in Wedeen et al. (2012a)) as a tool to quantify the occurrence of sheet structure on simulated vector fields as a function of noise and spatial resolution.}, we determine $E_p(V,W)$ by using the linear relationship between $D^\Delta_{\mathcal{L}_V}(h_1,h_2)$ and $h_1$ and $h_2$ (i.e. $\Delta h_1, \Delta h_2$) assumed to be small): the components $E_{\mathcal{L}}(V,W)$ equal the slope of the least squares fit to the scatter plots of $D^\Delta_{\mathcal{L}_V}(h_1,h_2)$ versus $[h_1,h_2]$ (see Fig. 2). The fit is very much dependent on the choice of maximum $[h_1,h_2]$, since for larger $[h_1,h_2]$ the influence of the correction terms $\delta(h_1, h_2)$ and the choice of ‘walking path’ (i.e. the signs of $h_1$ and $h_2$) in the different ‘branches’ in the scatterplot grows. Because $[V,W]_p^\Delta = 0$ only if sheet structure is present, $E_{\mathcal{L}}(V,W)$ can be used as an indicator of sheet structure. Fig. 4 shows the absolute error of $E_{\mathcal{L}}(V,W_2)$ (averaged over 50 noise iterations) as a function of maximum $[h_1,h_2]$ and noise level $\sigma$. For higher noise levels, a lower maximum $[h_1,h_2]$ gives the best estimate of $E_{\mathcal{L}}(V,W_2)$, as errors accumulate along pathways. Figs. 5 (a) and (b) show $E_{\mathcal{L}}(V,W)$ for pair 1 and 2 as a function of noise and voxel size, respectively. By looking at $E_{\mathcal{L}}(V,W)$, it is possible to distinguish sheet structure from non-sheet structure, except at high noise levels and large voxel size.

Discussion and Conclusion: In this work we have evaluated a method to calculate the discrete Lie bracket for the quantification of sheet structure. By considering the normal component, this approach is indeed capable of differentiating sheets from non-sheet structures being present in these simple vector field examples. Our experiments further show that its performance is dependent on noise level, voxel size, and maximal walking distance along the streamlines. The results will additionally depend on the dMRI reconstruction and tractography method used, and on a number of parameters (e.g. the step size and the stopping criterion), dependencies which we have not considered here. The optimal combination of methods and settings to make this approach as robust as possible, along with quantification of the presence of sheet structure in the brain, are future work.