Simulation-driven machine learning framework to estimate brain microstructure using diffusion MRI

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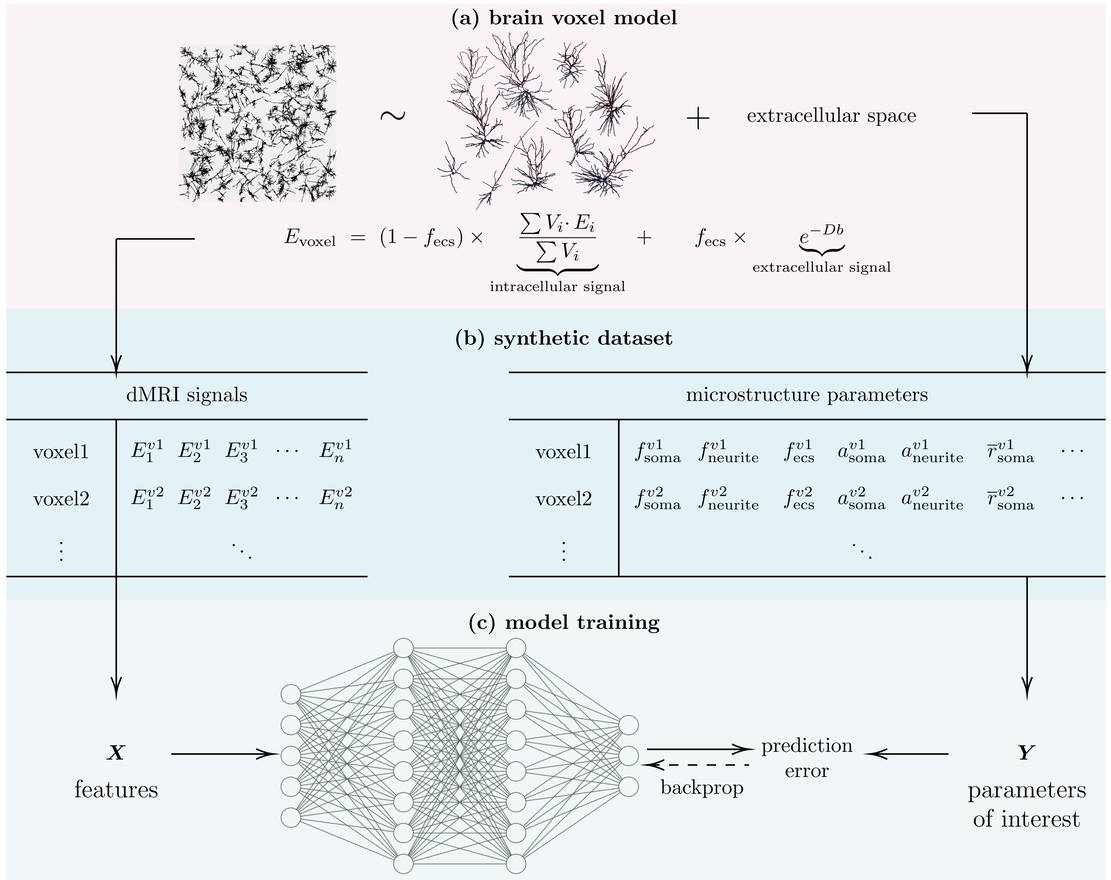
Abstract

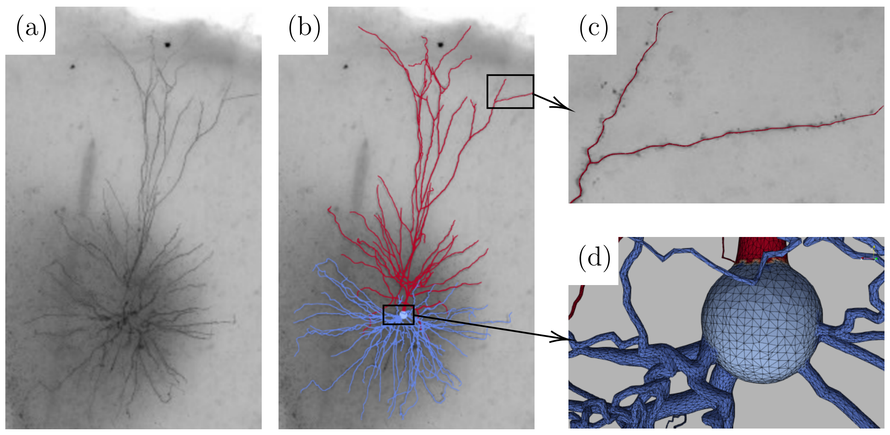
Existing methods that estimate brain microstructure parameters by diffusion MRI (dMRI) often use biophysical models that are based on analytical expressions of the diffusion MRI signal arising from oversimplified geometrical models of neuronal tissue. This study proposes a novel framework for in vivo brain microstructure estimation using a simulation-driven methodology. We perform the numerical matrix formalism simulation and the neuroanatomical measurements on *1213* realistic neuron meshes. Then, a synthetic dataset containing dMRI signals and ground-truth microstructure parameters can be built and used to train multilayer perceptrons (MLPs). The microstructure estimation of the trained MLP presents an excellent sensitivity to soma, neurite, and ECS volume fractions. Most importantly, the dependence of parameter maps on diffusion time is minimal.

I. Framework Illustration



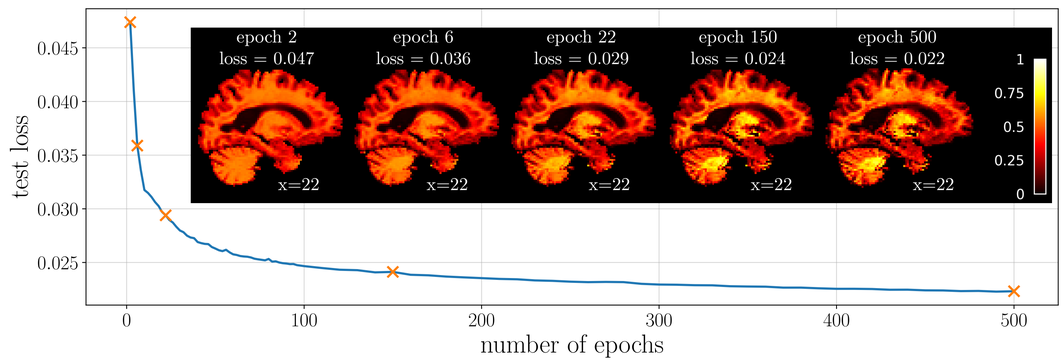
II. Cornerstones

1. An ultra-fast GPU-based matrix formalism implementation in SpinDoctor [1]. It now takes 10 minutes to simulate 1,000 dMRI signals on a neuron.
2. Over 1,000 realistic cellular meshes built from digitally reconstructed neurons and glia stored in NeuroMorpho.Org [2].



III. Model Training

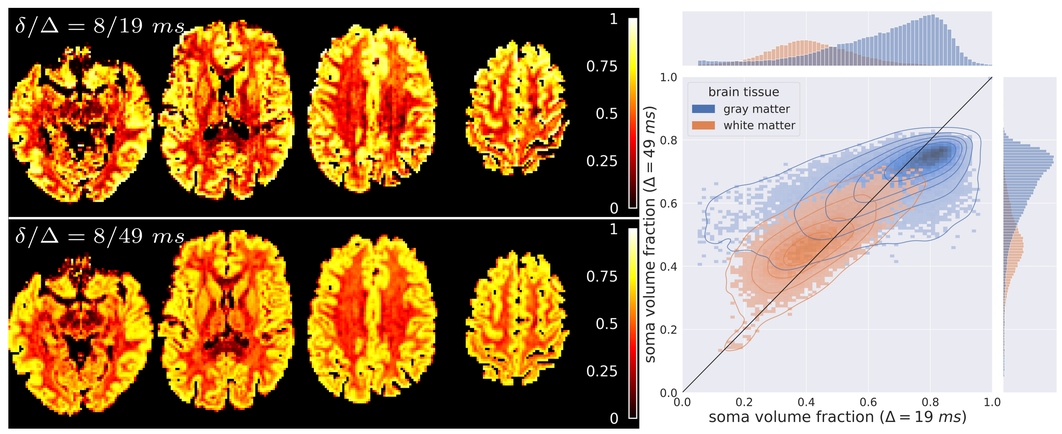
The neurite volume fraction is estimated by an MLP at different training stages. As the test error decreases, the contrast of, for example, the cerebellar white matter becomes more pronounced. The experimental dMRI signals are from the MGH CDMD dataset [3].



Training settings: four-layer MLPs are trained with Adam optimizer with an initial learning rate being 0.01; the loss function is the mean squared error, and the batch size is 10,000.

IV. Results & Conclusion

The parameter maps present the soma volume fraction estimation at two diffusion times. The voxelwise joint distribution demonstrates that the dependence of parameter maps on diffusion time is minimal, which is a very desirable property.



References

1. Li JR, et al. NeuroImage. 2019 Nov 15;202:116120.
2. Ascoli GA, et al. Journal of Neuroscience. 2007 Aug 29;27(35):9247-51.
3. Tian Q, et al. Scientific Data. 2022 Jan 18;9(1):1-1.

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