MicroLearn: Framework for machine learning, reconstruction, optimization and microstructure modeling

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Synopsis

MicroLearn is a Machine Learning and Model Fitting framework that enables modular construction of multi-compartment microstructure models in crossings with fast and accurate parameter estimation.

Introduction

Recent research attempting to probe the tissue microstructure using diffusion MRI (dMRI), has led to a variety of model fitting and machine learning based approaches to estimate the underlying model parameters accurately and quickly [1]. Both kinds of approaches construct multi-compartment models via combinations of intra- and extra- axonal spaces which are generally very hard to fit. MicroLearn aims at unifying these approaches with additional capabilities to interoperate between some state-of-the-art optimizers, machine learning methods and microstructure models. This framework is efficient in modeling regions of the brain with 0, 1, 2 and 3 fiber crossings alongside improved runtime performance and estimation accuracy. MicroLearn further helps underpin the mesostructure [2] (macro-level tissue organization) features necessary for reconstruction using Supervised Bayesian Learning of the tissue microstructure. The framework will be made available as a part of DIPY [3] with TensorFlow [4] integrations to easily switch between the training strategies, optimization methods and advanced regression algorithms. This novel framework includes transparent implementation of various models with a superquadrics-based visualization.

Methods

MicroLearn provides tools for estimating multi-compartment microstructure models by taking two different approaches: 1) Model Fitting based from Fiber Orientation Directions and 2) Machine Learning from Mesostructure. MicroLearn currently provides 4 different multi-compartment models, namely, ActiveAx [5], ZCD [6], NODDI [7], IVIM [8] in a modular manner without compromising on speed. These multi-compartment models can be fed into a model fitting module or into the machine learning module keeping the underlying microstructure model the same. For the Model Fitting paradigm, MicroLearn provides capabilities to switch between 0, 1, 2 and 3 fiber crossings for different tissues in specific regions of the brain. As shown in the figure, we can make use of the MTMS-CSD [9] (in combination with HMRF [10], SHORE [11], etc. from DIPY) to obtain the number of peaks in each voxel and fit the number of crossings accordingly (depicted in figure 2). In order to fit these complex biophysical models, MicroLearn provides tools for estimating parameters in manifold spaces using the Variable Projection [12] (VarPro) algorithm to find a global minima faster by constraining the non-linear parameters and separating them from the linear ones. This has been implemented in combination with differential evolution and convex optimizers to as a part of the MIX[13] framework. Apart from this we also provide tools to perform interior point optimization using a different set of algorithms as an alternative to the MIX optimizer. In contrast to the above multi-stage fitting procedures, the machine learning paradigm provides tools to perform supervised Bayesian learning by extensively simulating and training signals[2] from any of the above mentioned microstructure models. Along with a simple polynomial regression, MicroLearn provides advanced alternative training strategies via the TensorFlow API using Follow the regularized leader (Ftrl), Steepest Dual Coordinate Ascent (SDCA), Proximal AdaGrad and Adam optimizers for regressors such as Deep Neural Network (DNN), Boosted Trees and Linear Combined DNNs[4]. The learning approach is governed by a higher level mesoscopic structure to disentangle the meso- and micro- properties without having to use Fiber Orientation Distribution (FOD) as a prerequisite. This approach works with processed signal derivatives[2] and extensive simulations of the underlying tissue microstructure model. As an added capability, we also provide means to train the microstructure models from the features obtained from the model fitting module (explained in detail in Figure 1).

Results

This framework provides capabilities such as switching in and out from a machine learning to classical model fitting approach not currently available in any other toolbox. This implementation outperforms the estimation performances of NODDI, IVIM, ZCD and ActiveAx (by ~25X - 30X) with enhancements such as tools to fitting multiple fiber crossings. The experiments have been conducted on an intel i7 machine with no external GPUs required for computation. Contemporary toolboxes such as MDT [14], Dmipy [15], AMICO [16], and NODDI [7] implement microstructure toolboxes with modular and different approaches but do not provide flexible means to perform machine learning and direct model fitting at the same time.

Discussion and Conclusion

MicroLearn provides computational capabilities from different parameter estimation paradigms with an end-goal of continually supporting more algorithms for transparent and collaborative growth of the microstructure domain. The framework will be available as a part of DIPY with efficient software design to help the community with a capability to adopt new models and approaches. Furthermore, it includes tutorials and experiments to compare different models and try different combinations with the Human Connectome Project (HCP) data.

Acknowledgements

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Figures

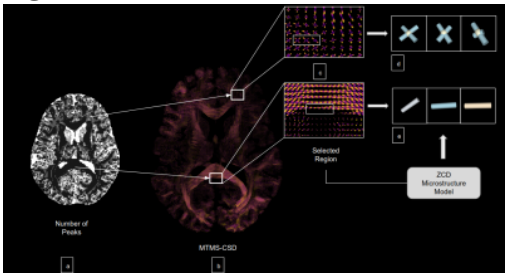

Figure 2: This depicts a sequence of parameter estimation in MicroLearn. First, the number of peaks (a) are calculated in conjunction with the MTMS-CSD (b). Three voxels have been selected from two particular regions (c) of the brain with 1 fiber (e) and 2 fiber crossings (d) using the ZCD microstructure model to estimate their parameters.

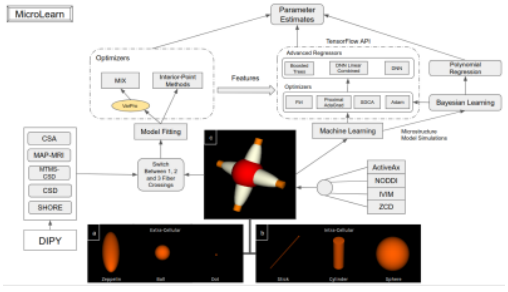

Figure 1: The flowchart explains the capabilities of MicroLearn. It consists of intracellular (a) and extracellular(b) components modeled via a superquadrics which can be added together to construct the microstructure model (c). The left hand flow denoted the classical model fitting approach whereas the right hand side denotes the machine learning approach.