Predicting brain functional connectivity from structural connectivity using fully connected neural networks

Identifying the link between brain structure and brain function is one of the open challenges of modern neuroscience. To this end, a common representation of the brain is that of an undirected network or graph, where nodes represent cortical and sub--cortical gray matter structures and edges represent the strength of structural or functional connectivity. The structural network is usually derived from diffusion magnetic resonance imaging (MRI) via tractography, a process that identifies white matter structures linking distant gray matter. On the other hand, the functional network is obtained by correlating the resting state functional MRI blood oxygenation level--dependent (BOLD) signal of cortical regions. The underlying assumption being that correlation is a measure of connectivity strength, i.e. cortical regions that activate synchronously are likely connected. Together, the structural and functional networks provide two different points of view on brain connectivity.

Recently, a number of studies have shown that the network structure of the white matter shapes functional connectivity. While the relationship is not local or one to one, simple linear models may be sufficient to characterize resting state dynamics. These results support the hypothesis that the structural network acts as a substrate on which functional connectivity is deployed. Therefore, it should be possible to predict, at least partially, functional connectivity given the structural network. Existing models relating the structural and functional connectivity matrices are based on explicit modeling [1] and very few machine learning approaches have been explored [2,3]. In this work, we investigated whether fully connected neural networks can be used to predict the functional connectivity matrix, given the structural connectivity matrix. Specifically, we considered fully connected neural networks whose input are the vectorized entries of the structural connectivity matrix and whose output are the predicted corresponding functional connectivity entries.

The data was provided by the Human Connectome Project (HCP) and our processing started from the minimally processed data for both diffusion and functional MRI data. For 1050 subjects, two million streamlines were generated, using a modern probabilistic anatomically--constrained tractography pipeline. The cortical surface extracted with FreeSurfer was then parcellated using the Desikan--Killiany atlas into 68 regions. Given the parcellation and the streamlines, a structural connectome was built by counting the number of streamlines connecting all pairs of cortical regions while ignoring self connections. The resting state functional MRI data was preprocessed following recommended practices, including bandpass filtering, detrending, movement regression, and motion scrubbing. The mean signal for each cortical region of the atlas was computed and used to build the functional connectivity matrix using Pearson correlation across regions. Finally all negative entries of the matrix, corresponding to anticorrelations between cortical regions, were set to zero.

Using a leave one out strategy, several neural network configurations were trained on 1049 subjects with a 70-30 training-validation split and evaluated on the remaining subject. All networks minimized the mean square error between the predicted and true function connectivity matrix using the Adam algorithm over 2000 epochs. The final performance of a network is evaluated by computing the correlation between the predicted and measured functional connectivity matrix on the left out subject. Overall, the performance of several configurations is close to state of the art models, with and average correlation of 0.7.

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