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Permutation equivariant structure-function mapping

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Predicting the brain's function given its structure (**structure-function mapping**^{1,2}) is no easy task. In this work, we observe the problem through the lens of a **permutation equivariant graph neural network (PE-GNN)**.

Key finding:

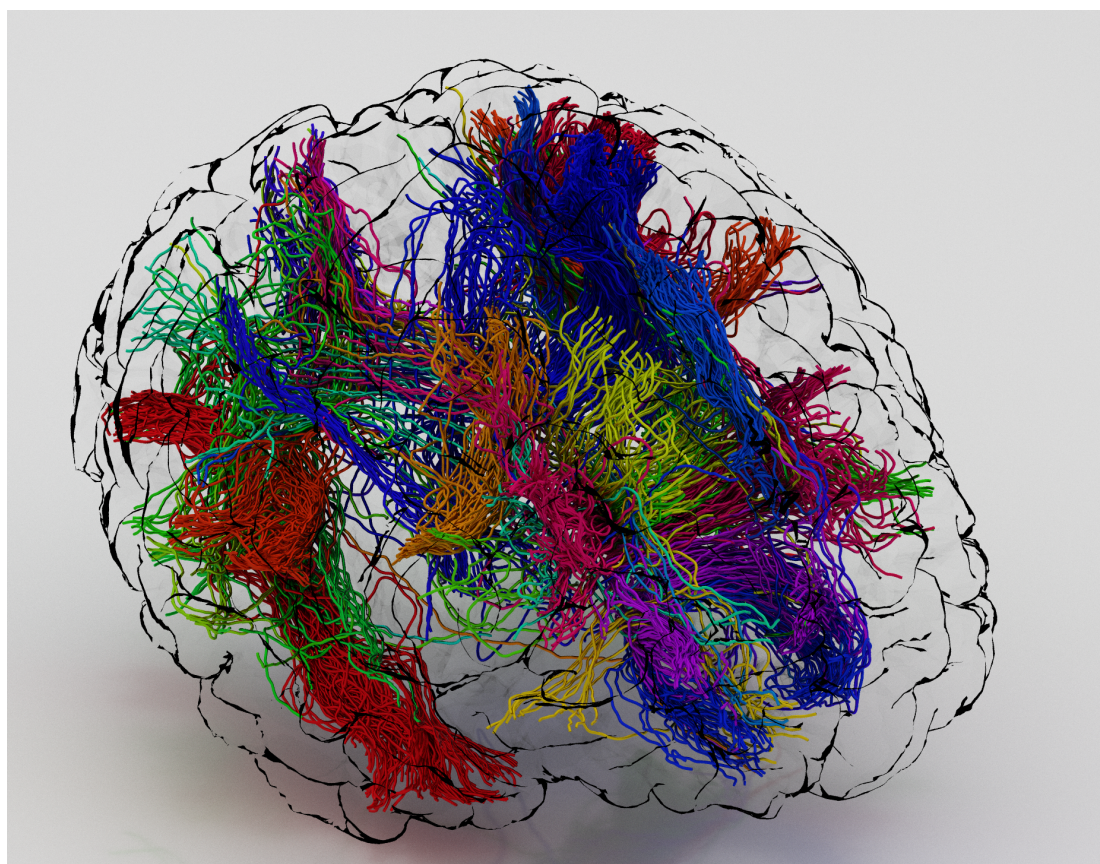
A PE-GNN achieves performance similar to a naive mean-estimator even though information on parcel-ordering is discarded during the modelling procedure.

1 Why structure-function mapping?

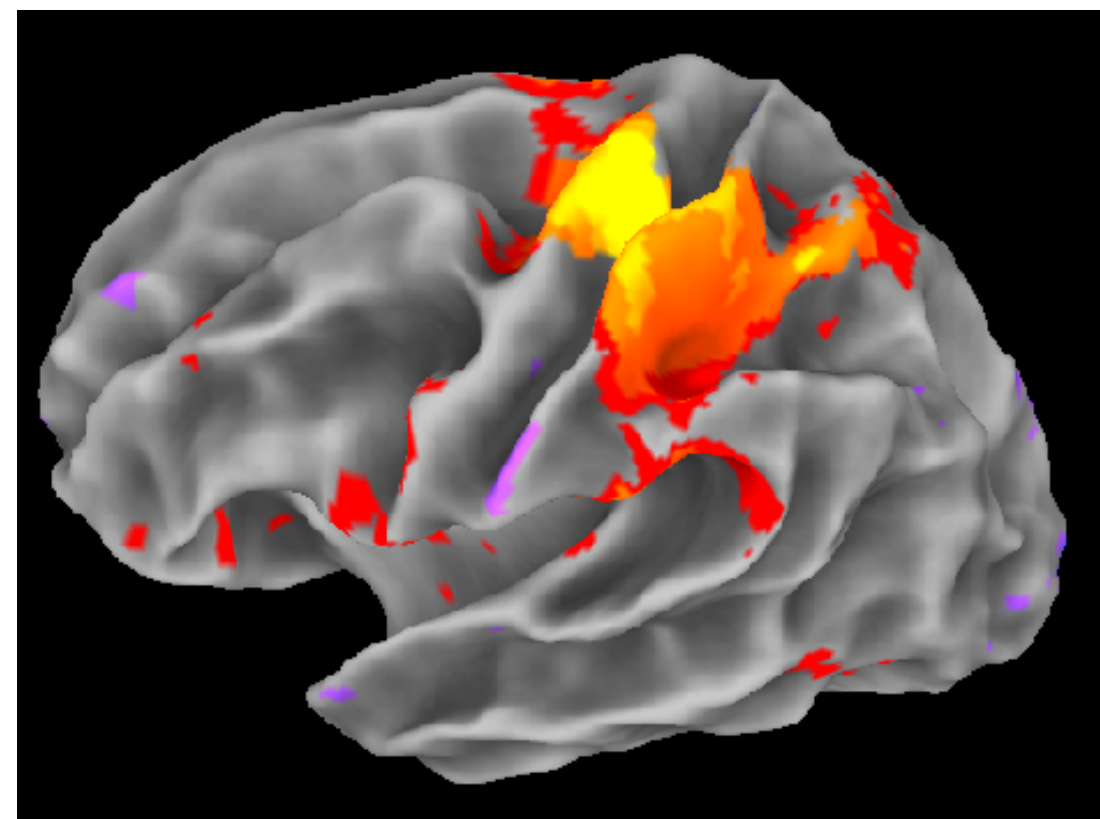
Brain structure-function mapping addresses the problem of predicting the brain's functional connectivity measured through (**rs-fMRI**) from the structural connectivity measured through (**dMRI**). The modelling procedure is built on two main assumptions:

1. Given the structure of a subject, it should be possible, at least partially, to predict his function.
2. The structure and function of specific sub-regions of the brain are matched across all subjects.

Tractogram:
structural connectivity



Brain activity:
functional connectivity



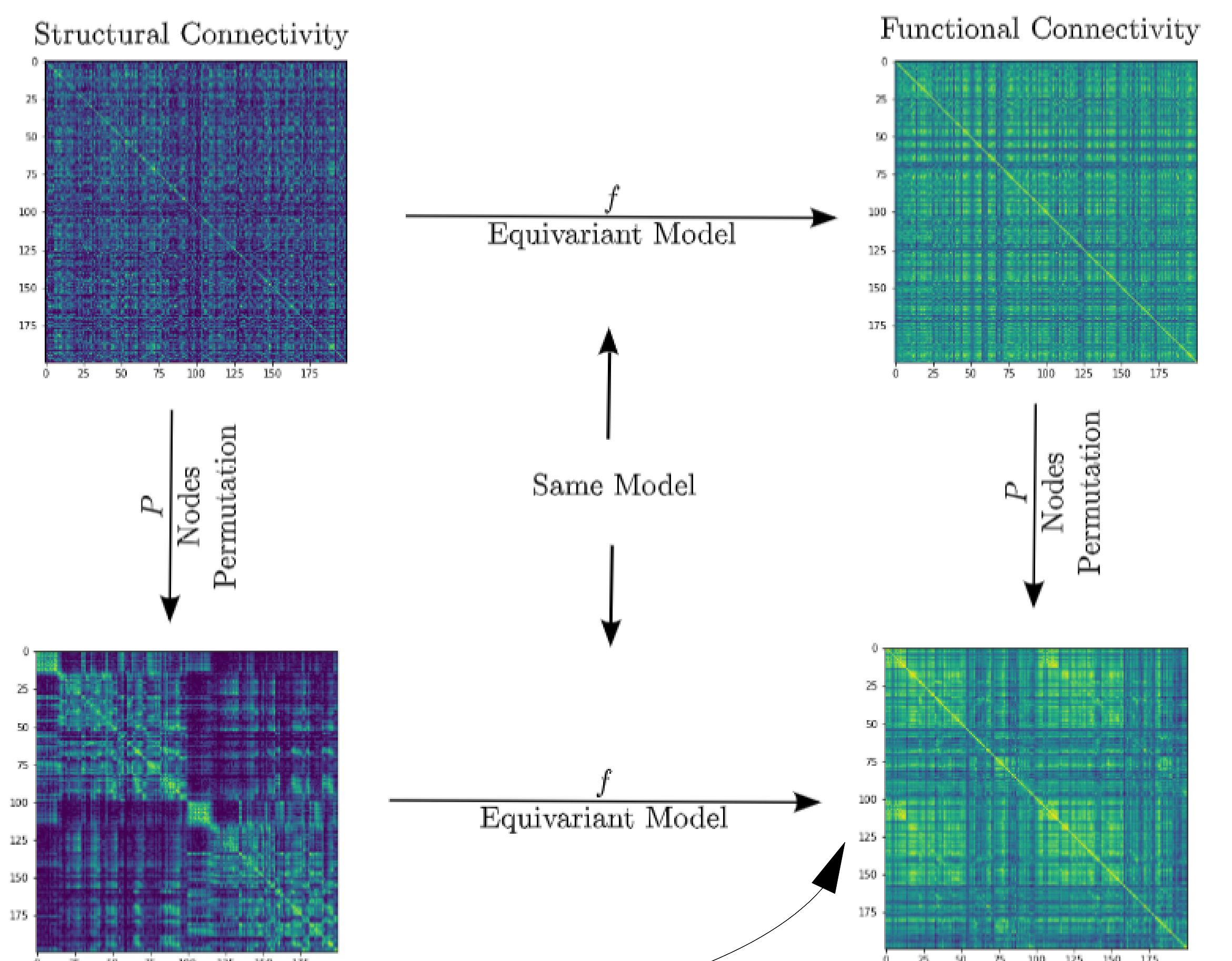
<https://www.nmr.mgh.harvard.edu/neurorecovery/technology.htm>

2 Why a permutation equivariant model?

Assume that X is a $n \times n$ matrix and P is an arbitrary $n \times n$ permutation matrix. Then a function $f: \mathbb{R}^{n \times n} \rightarrow \mathbb{R}^{n \times n}$ is permutation equivariant if

$$f(PXP^T) = Pf(X)P^T$$

Modelling the relation between structure and function by incorporating permutation equivariance ensures that the model behaves similarly for all parcel-orderings, and therefore **relaxes the second assumption**.

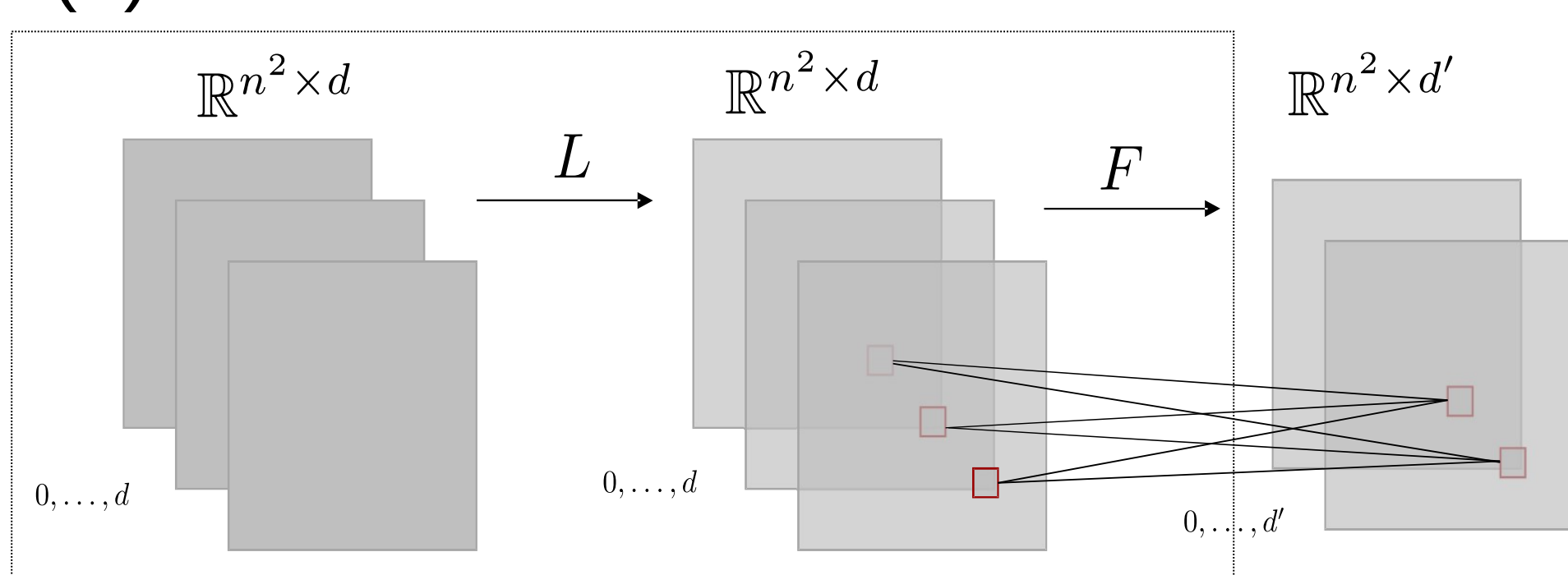


3 Methods

This work considers dMRI and rs-fMRI of **1050 young and healthy adults from the Human Connectome Project**³. For each subject, we derived a pair of structural and functional connectivity matrices. Two parcellations of the brain are considered; one containing 68 parcels (Desikan-Killiany), and one containing 200 parcels (Gallardo⁴).

Architecture

The architecture consists of 3 equivariant modules. The most important components in each module are the linear equivariant layers (L)⁵, and the 2D convolution with a 1×1 kernel size (F) as seen below.



The **PE-GNN is compared**, using 10-fold cross-validation, **to the mean functional connectivity matrix**, which is used as a reference estimator of the functional connectivity¹. We compute this predictor on both the training data (M-FC) and a second version of the training data where the rows and columns have been randomly permuted (PM-FC).

Number of parcels	PE-GNN	PM-FC	M-FC
68	0.0472 ± 0.0013	0.0750 ± 0.0017	0.0459 ± 0.0015
200	0.0378 ± 0.0026	0.0489 ± 0.0017	0.0346 ± 0.0021

The mean squared error (MSE) plus-minus the standard-deviation obtained from a 10-fold cross validation for each estimator. Each estimator is tested for atlases containing 68 and 200 parcels respectively.

Acknowledgments

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