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► **To cite this version:**

Andreas Abildtrup Hansen, Yanis Aeschlimann, Samuel Deslauriers-Gauthier, Anna Calissano. Permutation equivariant structure-function mapping. 2023 Annual Meeting of the Organization for Human Brain Mapping, Jul 2023, Montreal (Canada), Canada. hal-04390750

HAL Id: hal-04390750

<https://hal.science/hal-04390750v1>

Submitted on 12 Jan 2024

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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)**.

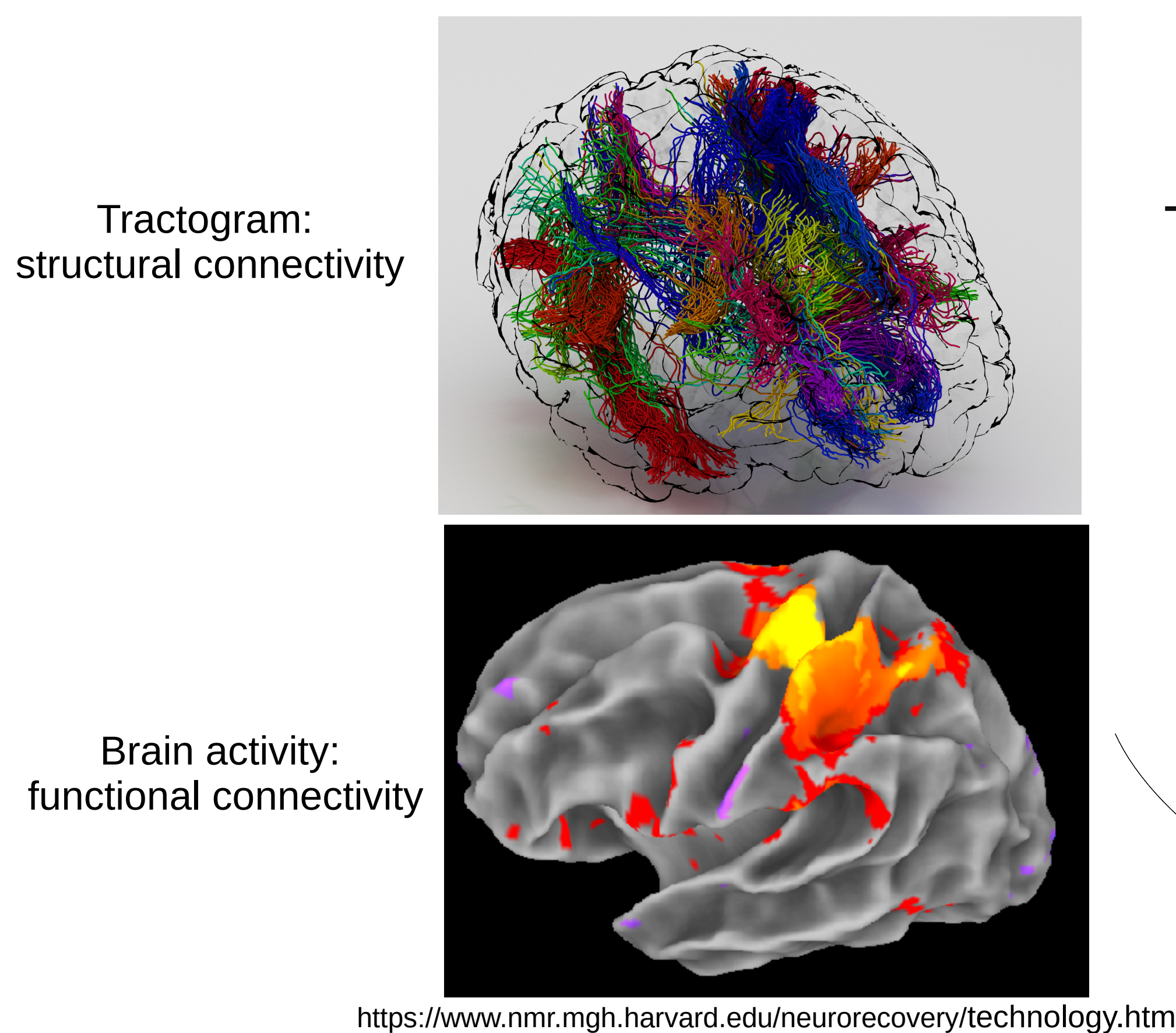
Key finding:

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.

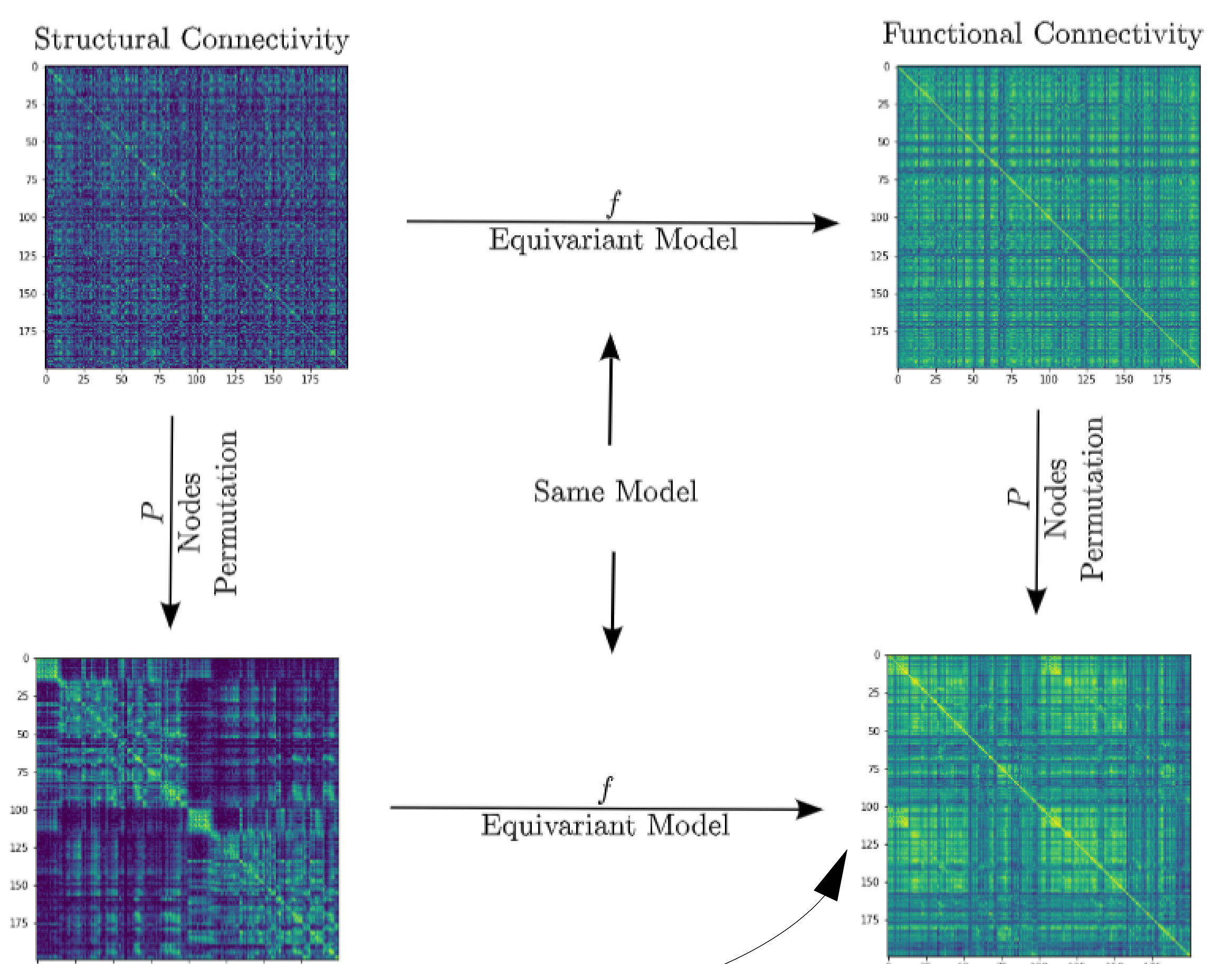


2 Why a permutation equivariant model?

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**.

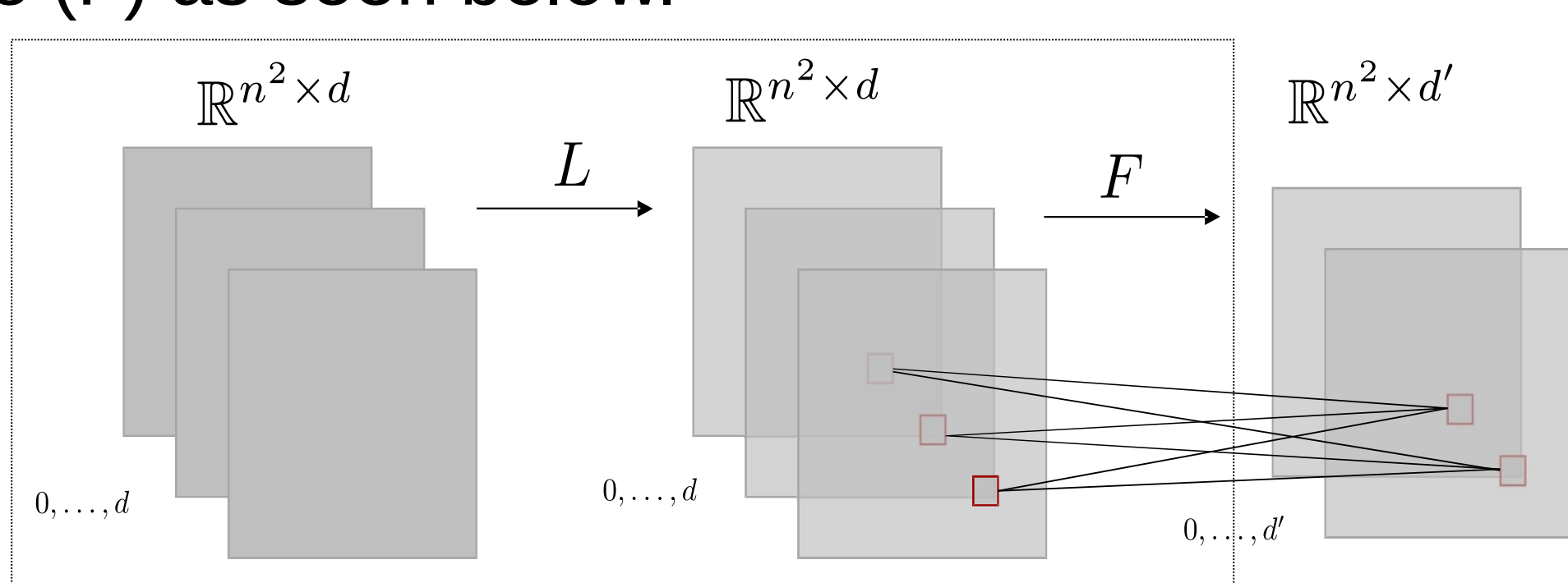


3 Methods

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

The research leading to this poster was funded by the Independent Research Fund Denmark (project no. 1032-00349A), and supported in part by the Novo Nordisk Foundation through the Center for Basic Machine Learning Research in Life Science (grant no. NNF20OC0062606)

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