Graph neural networks for classification and task-conditioned brain connectivity estimation of electrophysiological data

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Master Thesis – M.Sc. in Artificial Intelligence and Robotics

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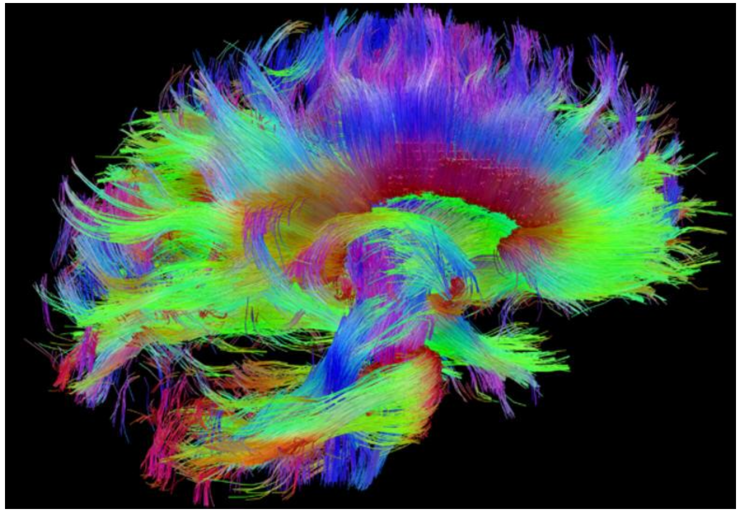
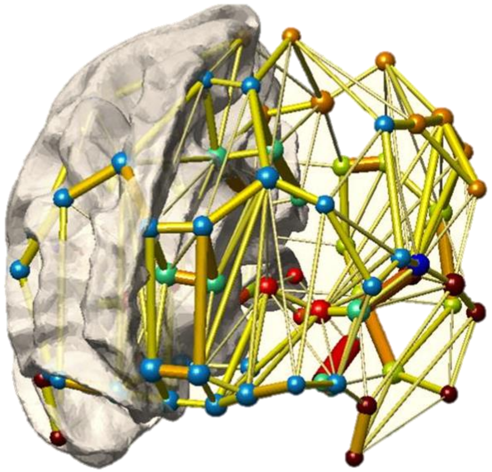
Introduction – Neuroscience and AI

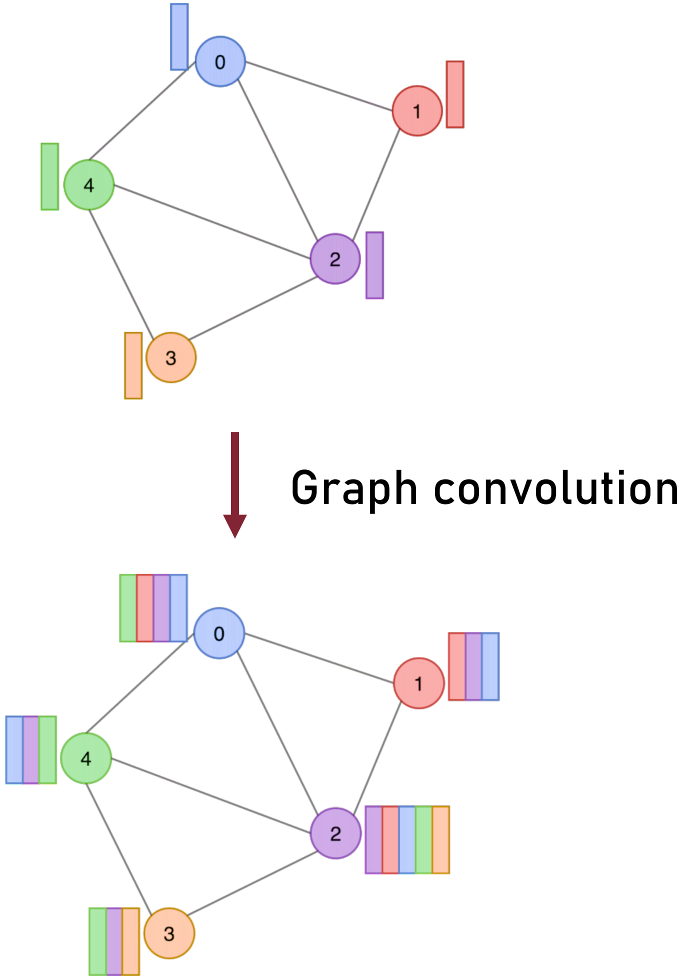


- The use of AI to support neuroscience is getting more and more attention
- Most of the efforts are devoted to brain disorder diagnosis
- Particular focus on the use of CNN and RNN



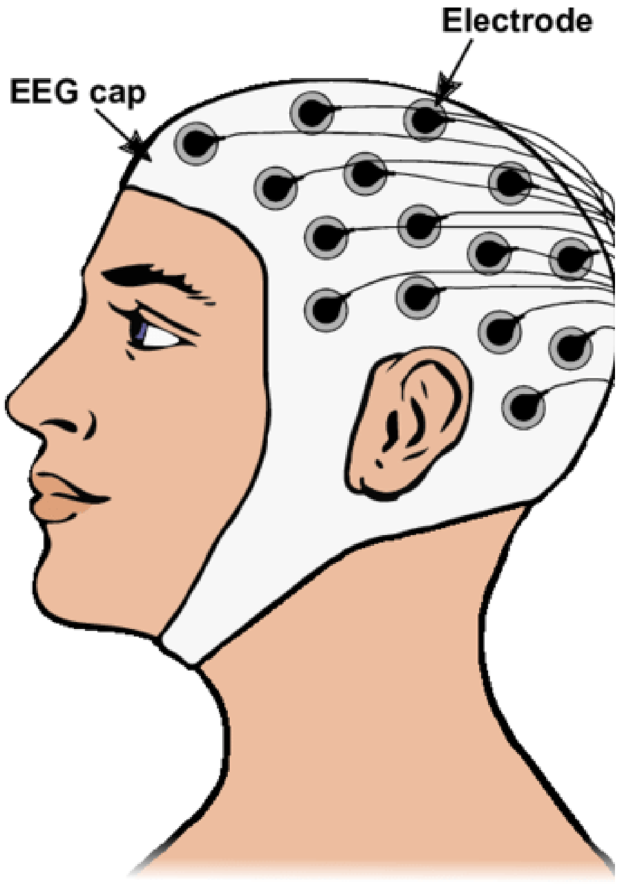
Graph neural networks – Introduction

- Increasing number of fields based on graph-structured data (social networks, chemistry, neuroscience)
- Extension of the classical convolution operation to graphs
  - Spatial convolutions
  - Spectral convolutions



Scalp electroencephalography (EEG)

- Measures electrical signals of the brain
- **Advantages:**
  - Non invasive
  - Cost effective
  - Excellent time resolution
- **Limitations:**
  - Sensitive to noise and artifacts
  - Spatial blur



Aims of the thesis

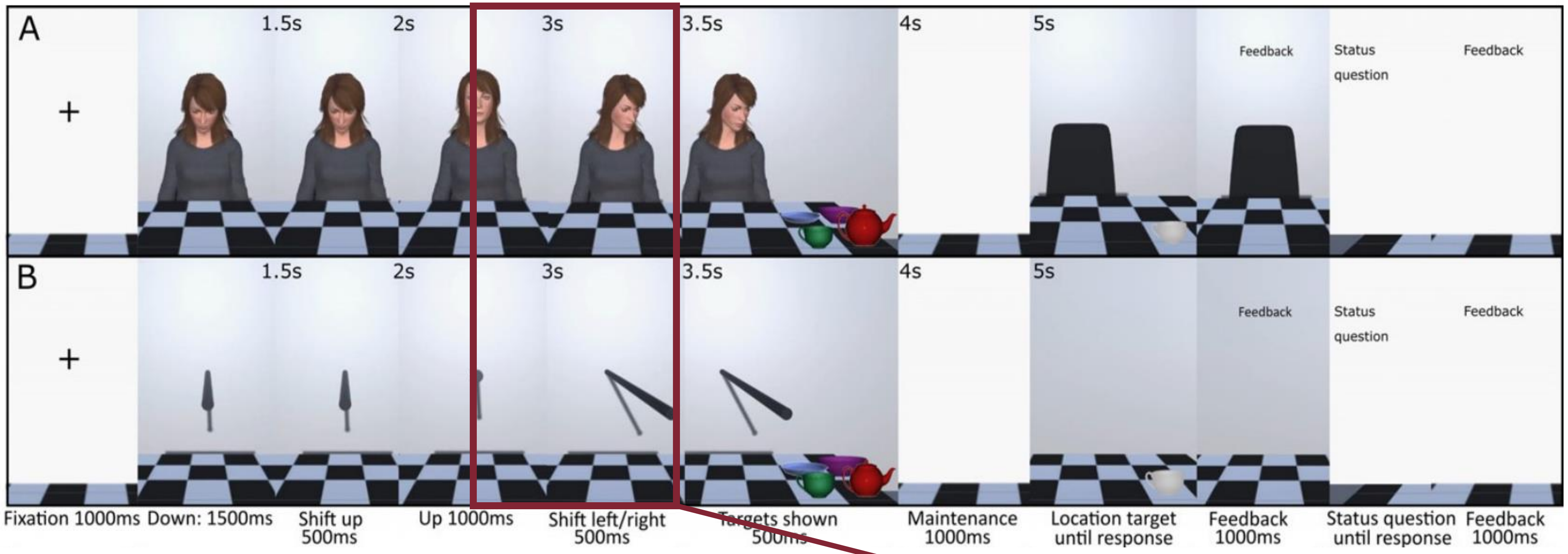
General aim: to investigate the effectiveness of GNN applied to real EEG data collected in human subjects.

Specific aims:

1. to build an effective classification pipeline based on GNN architectures and meaningful features extraction;
2. to develop an automatic mechanism for graph structure learning to avoid the arbitrariness of the choice about graph edges, with the purpose to improve the interpretability of the results.

Dataset description

VISUAL STIMULATION ADMINISTERED TO THE SUBJECTS



Cueing window: 2.5s -3.5s
Healthy subjects: 47
Trials per subject: 224
Social/Non-social condition trials: 112/112

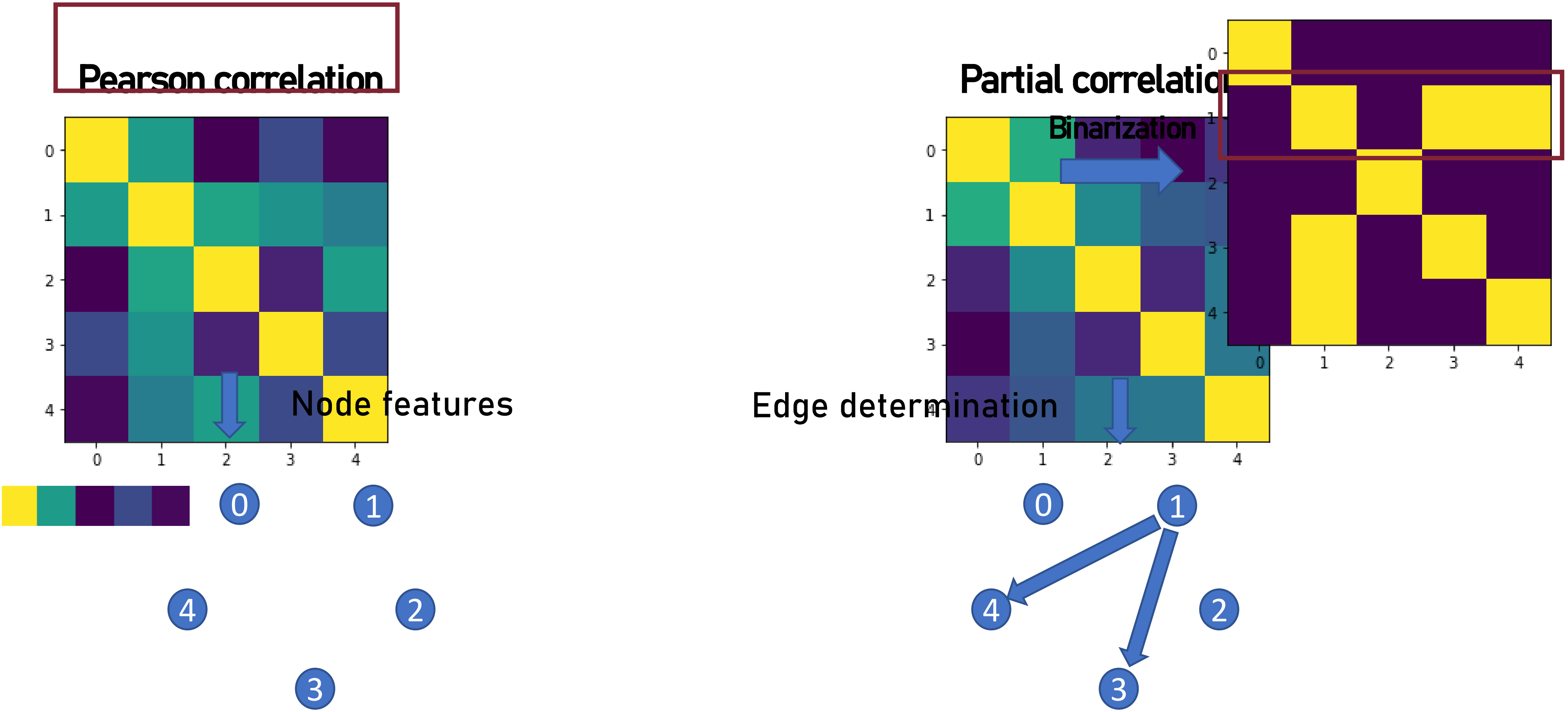
Cognitive task: Working Memory with a cue:

- a **human avatar** (social condition)
- a **stick** (non-social condition)

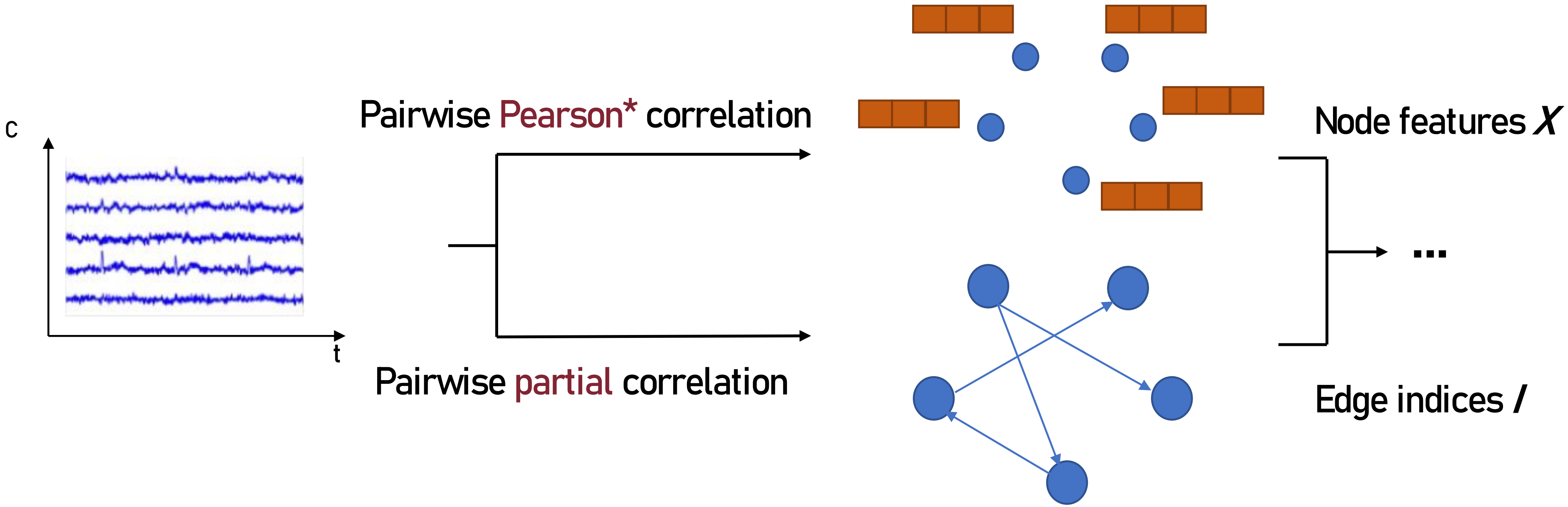
1st study

Building an effective pipeline based on GNN architectures and meaningful features extraction for the single trial, subject-dependent classification of the social/non-social content

Preprocessing and feature extraction



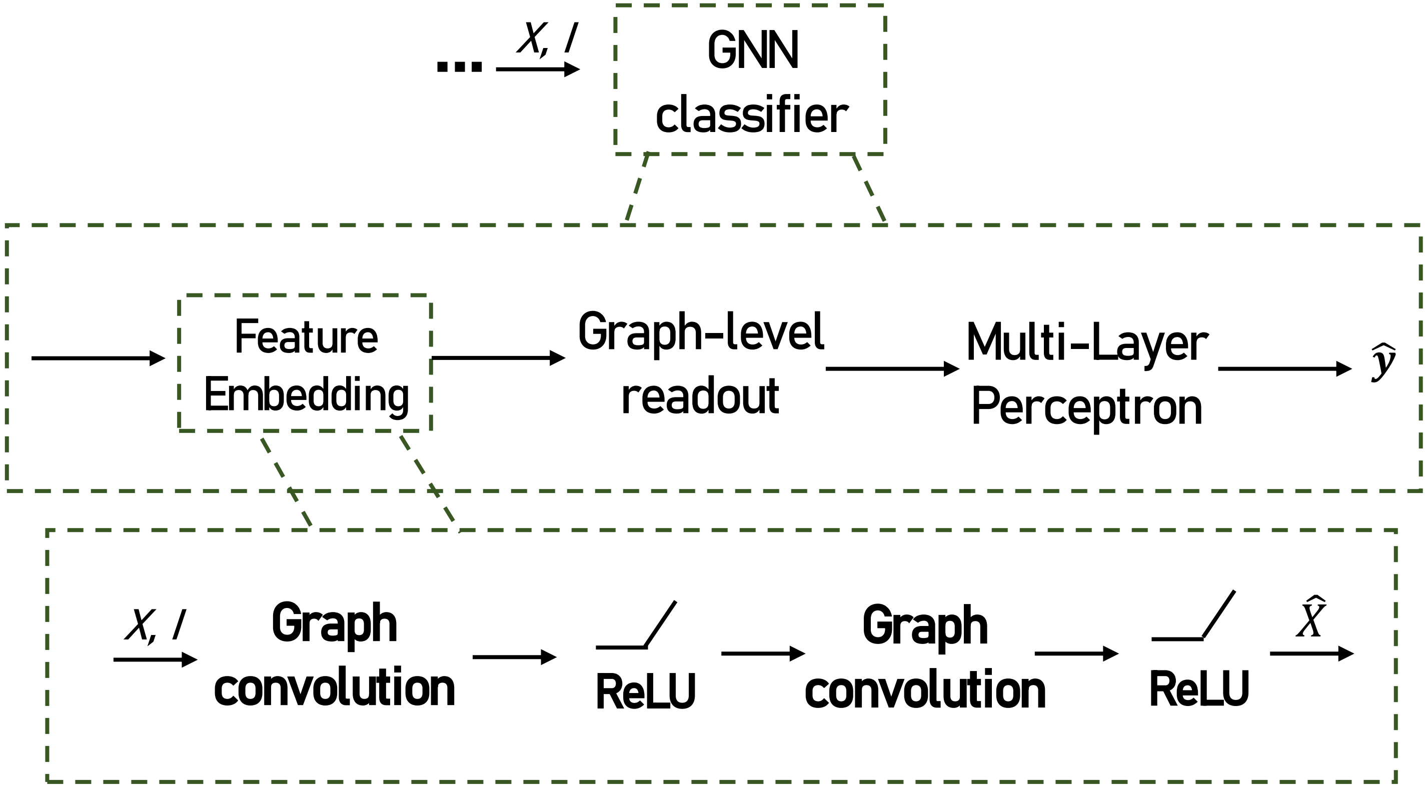
Preprocessing and feature extraction – summary



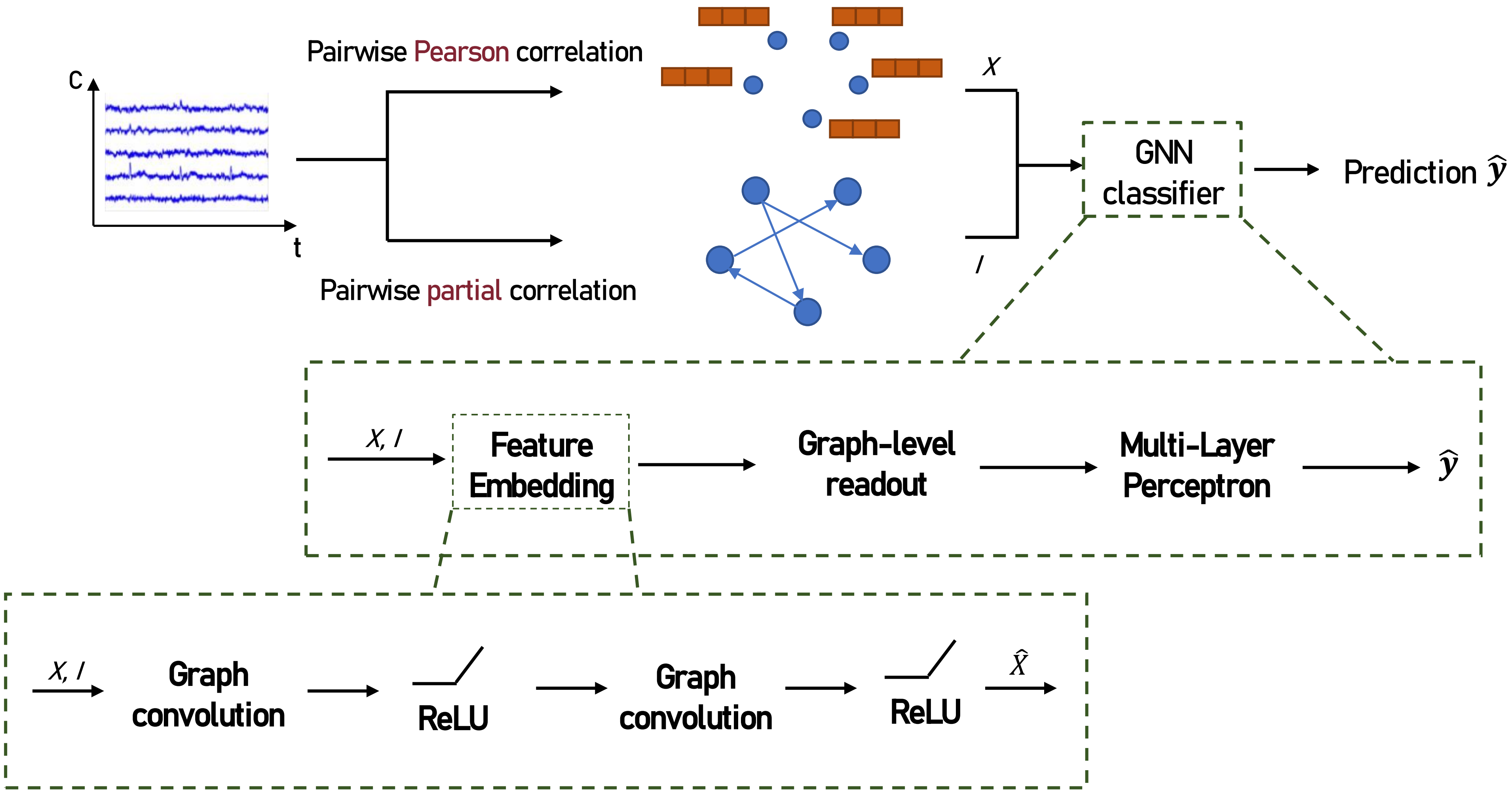
*Phase Locking Value (PLV) as an alternative

Graph neural networks – Classifiers

- Three different convolution operator tested:
  - Graph-SAGE
  - Graph Isomorphism Network (GIN)
  - Graph Convolution Network (GCN)
- Readout function to obtain graph level embedding
- Final multi-layer perceptron



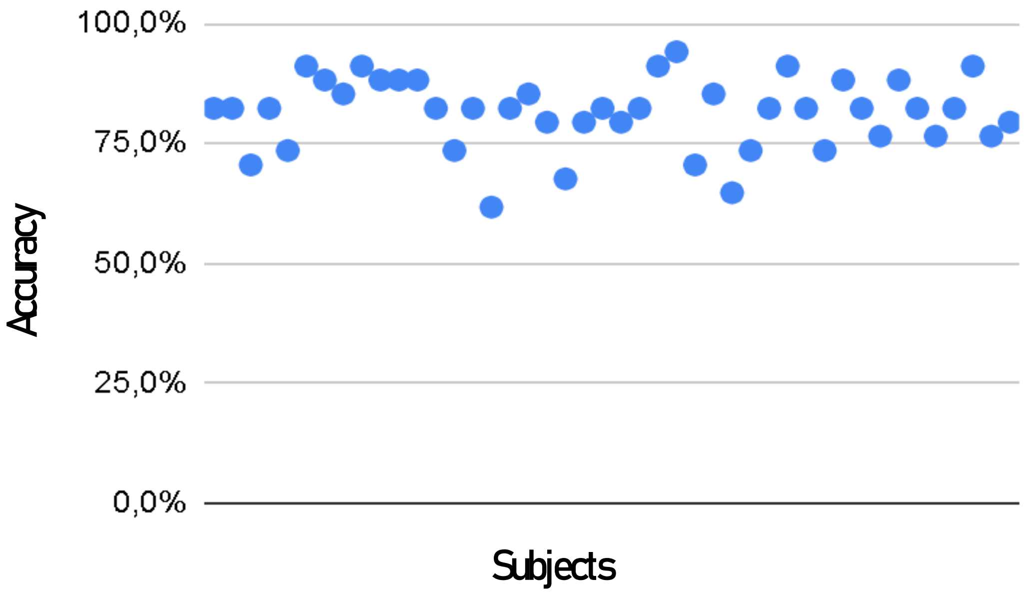
Graph neural networks – Complete classification pipeline



Results – Machine learning baselines

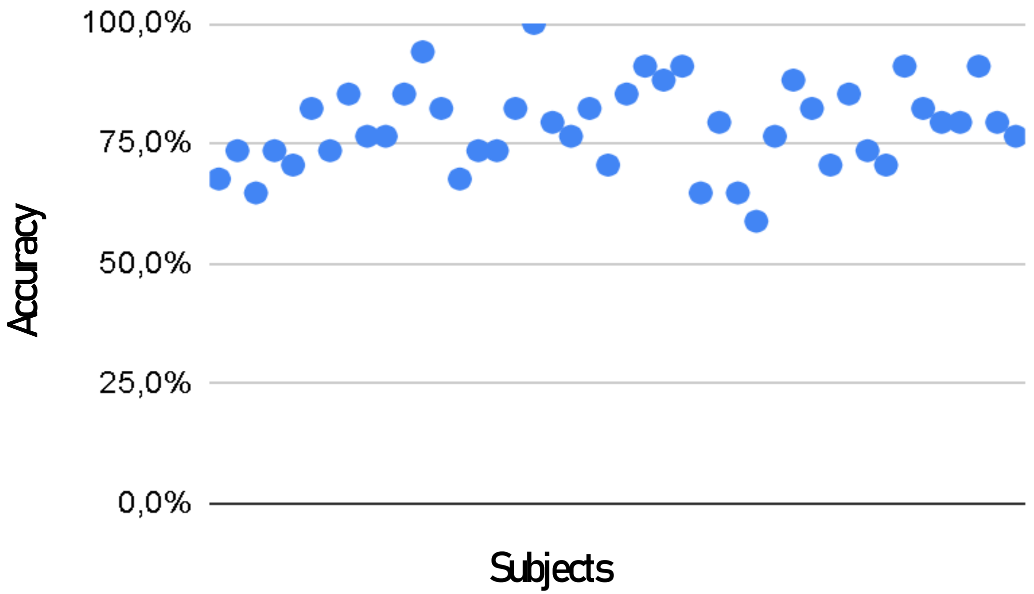
SVM – Linear kernel

Avg. Accuracy: 81.4% ± 7.5%

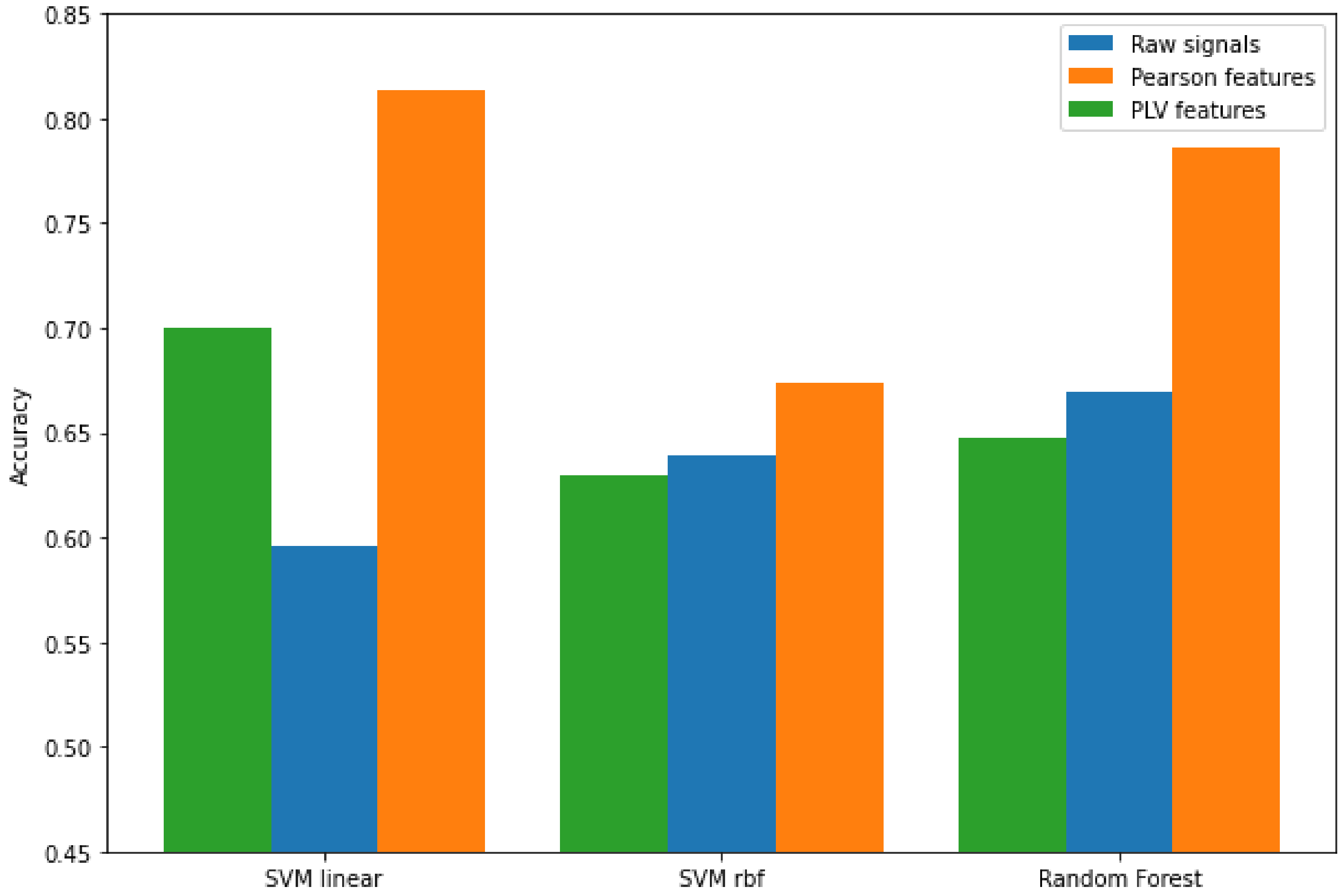


Random Forest

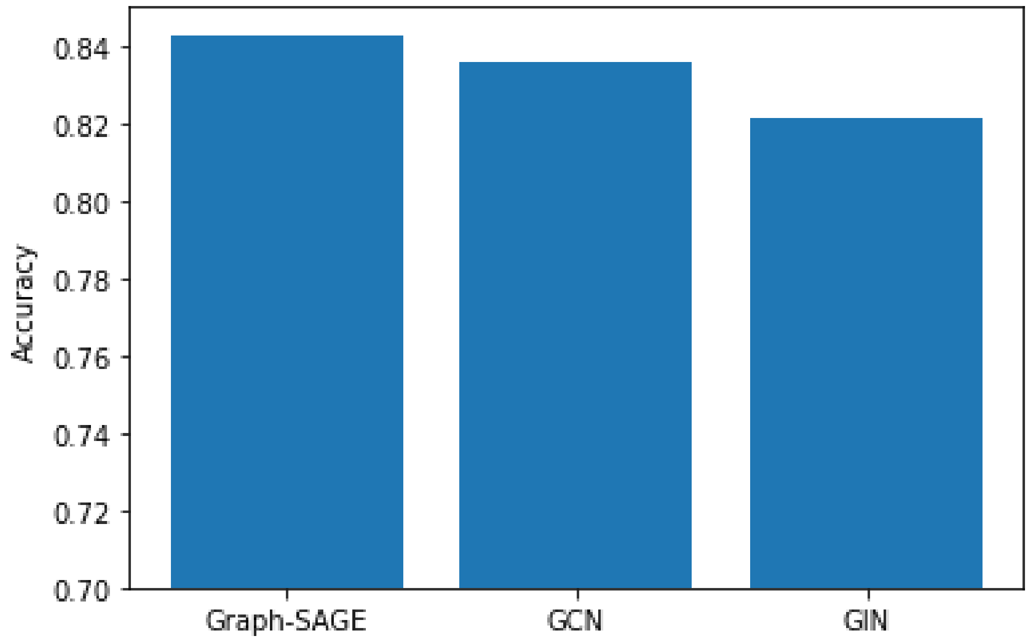
Avg. Accuracy: 78.6% ± 8.9%



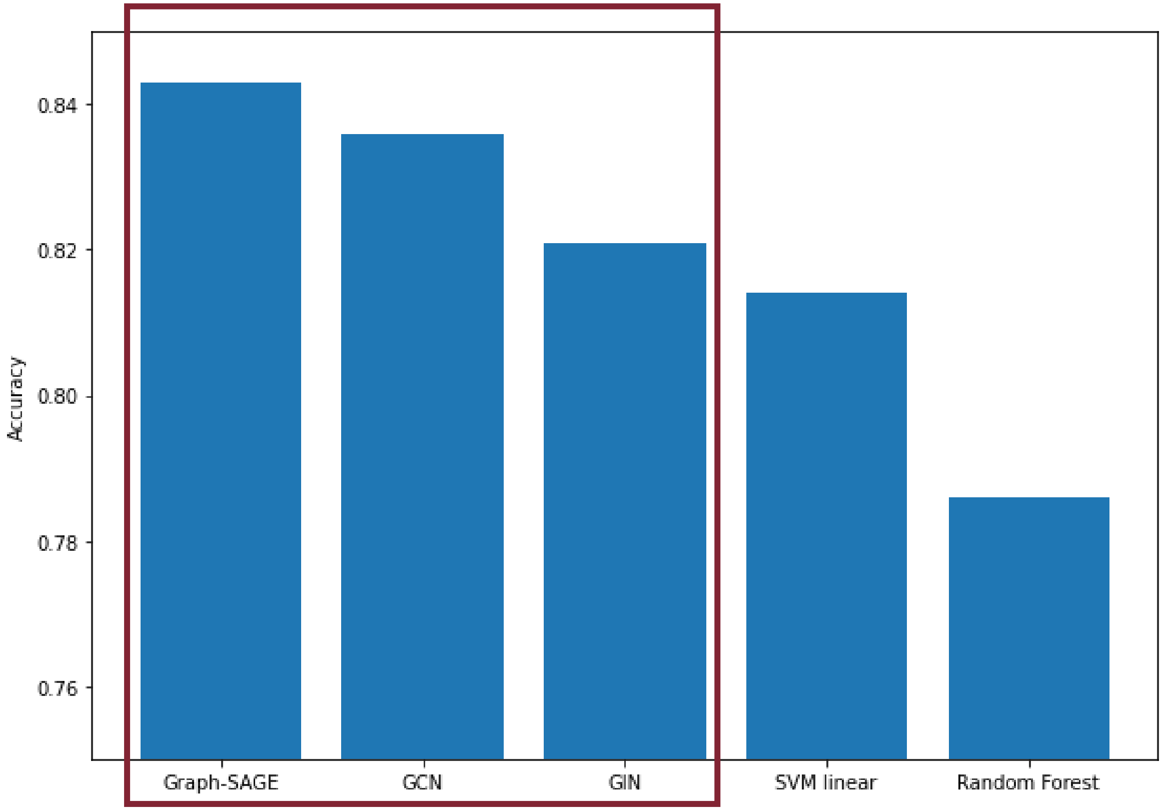
Results – Machine learning baselines features comparison



Results – Graph neural networks



Comparison between GNNs



GNNs compared with the baselines

2nd study

Development of an automatic mechanism for

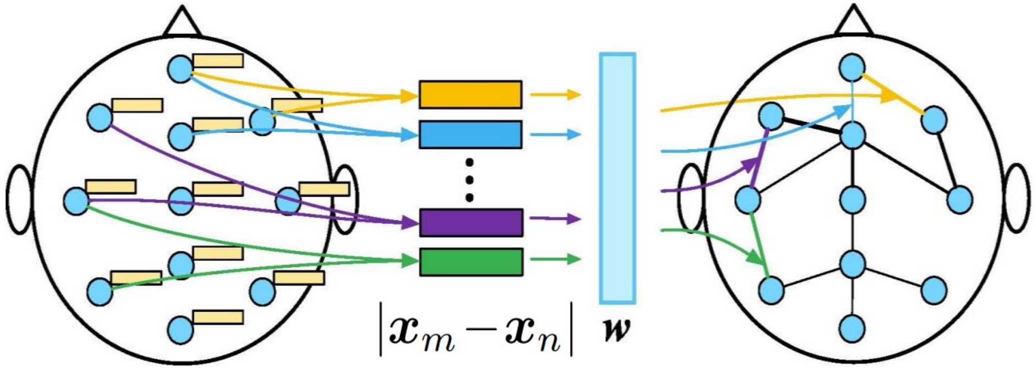
graph structure learning:

allowing the model itself to learn the graph topology.

Automatic graph-structure learning mechanism - Motivations

- Improve interpretability
- Avoid arbitrary decisions about edge determination
- Allow quantitative and statistical tests on the connectivity maps learned by the algorithm

Automatic graph-structure learning mechanism - Explanation



Node connections formula:

$$A_{mn} = g(\boldsymbol{x}_m, \boldsymbol{x}_n) = \frac{\exp(\mathrm{ReLU}(\boldsymbol{w}^T |\boldsymbol{x}_m - \boldsymbol{x}_n|))}{\sum_{n=1}^{N} \exp\left(\mathrm{ReLU}\left(\boldsymbol{w}^T \left|\boldsymbol{x}_m - \boldsymbol{x}_n\right|\right)\right)}$$

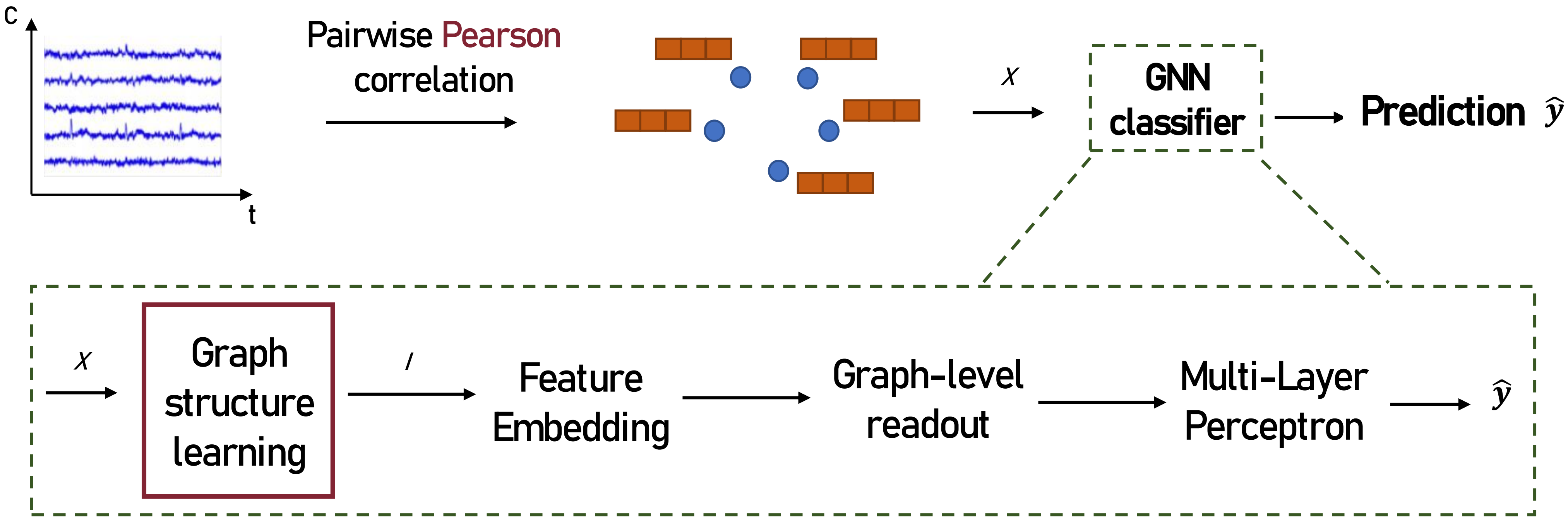
Loss function to be minimized:

$$\mathcal{L}_{\text{graph\_learning}} = \sum_{m,n=1}^{N} \|\boldsymbol{x}_m - \boldsymbol{x}_n\|_2^2 A_{mn} + \lambda \|\boldsymbol{A}\|_F^2$$

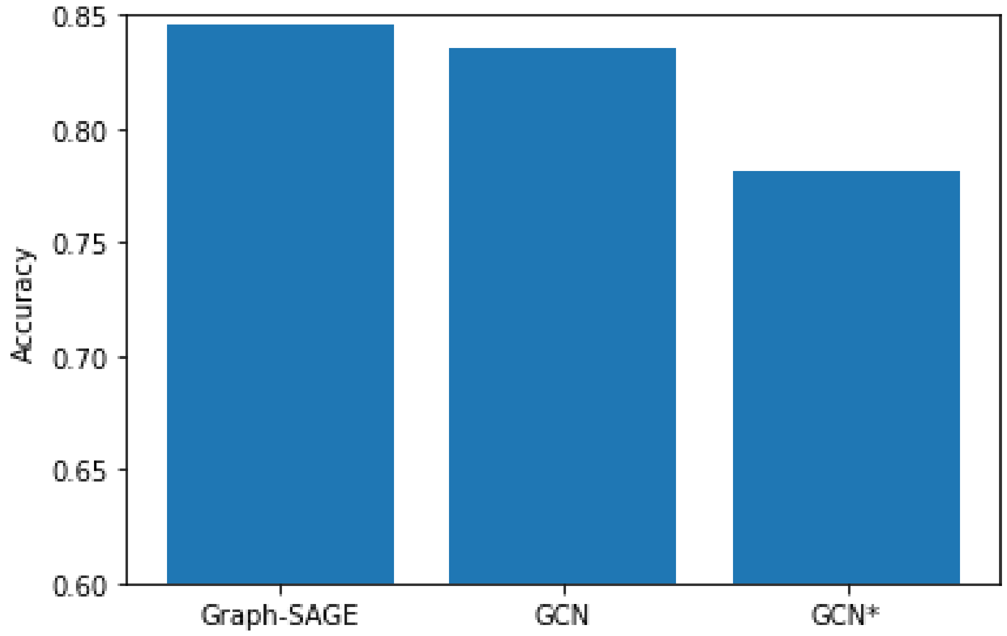
Automatic graph-structure learning mechanism – Adaptation

- Insertion in a new classification pipeline: new input features and new network architecture
- New normalization strategy to avoid artefactual asymmetry

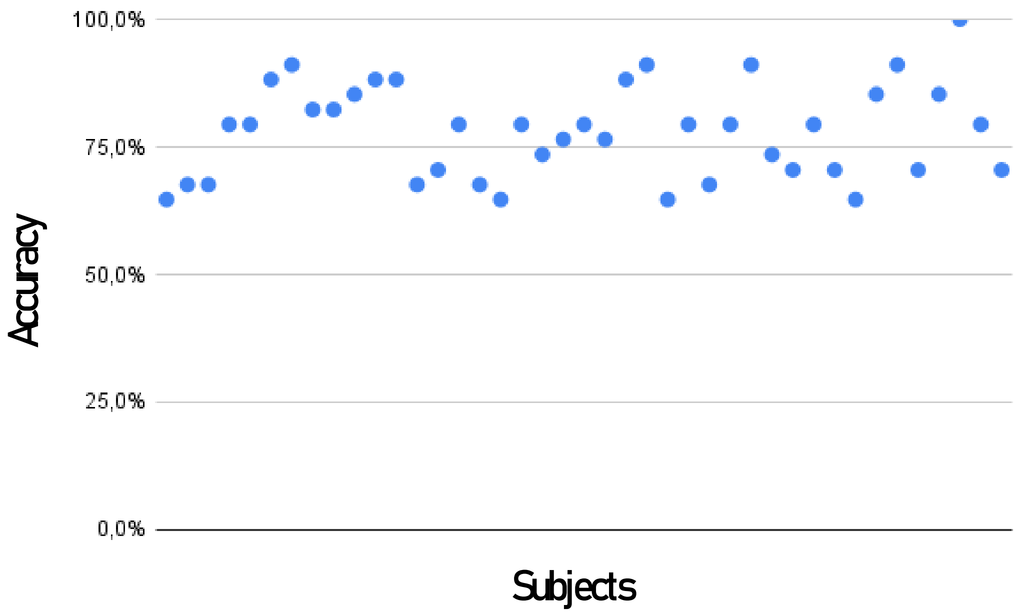
Graph neural networks - Modified classification pipeline



Results – Adaptive graph-structure learning mechanism

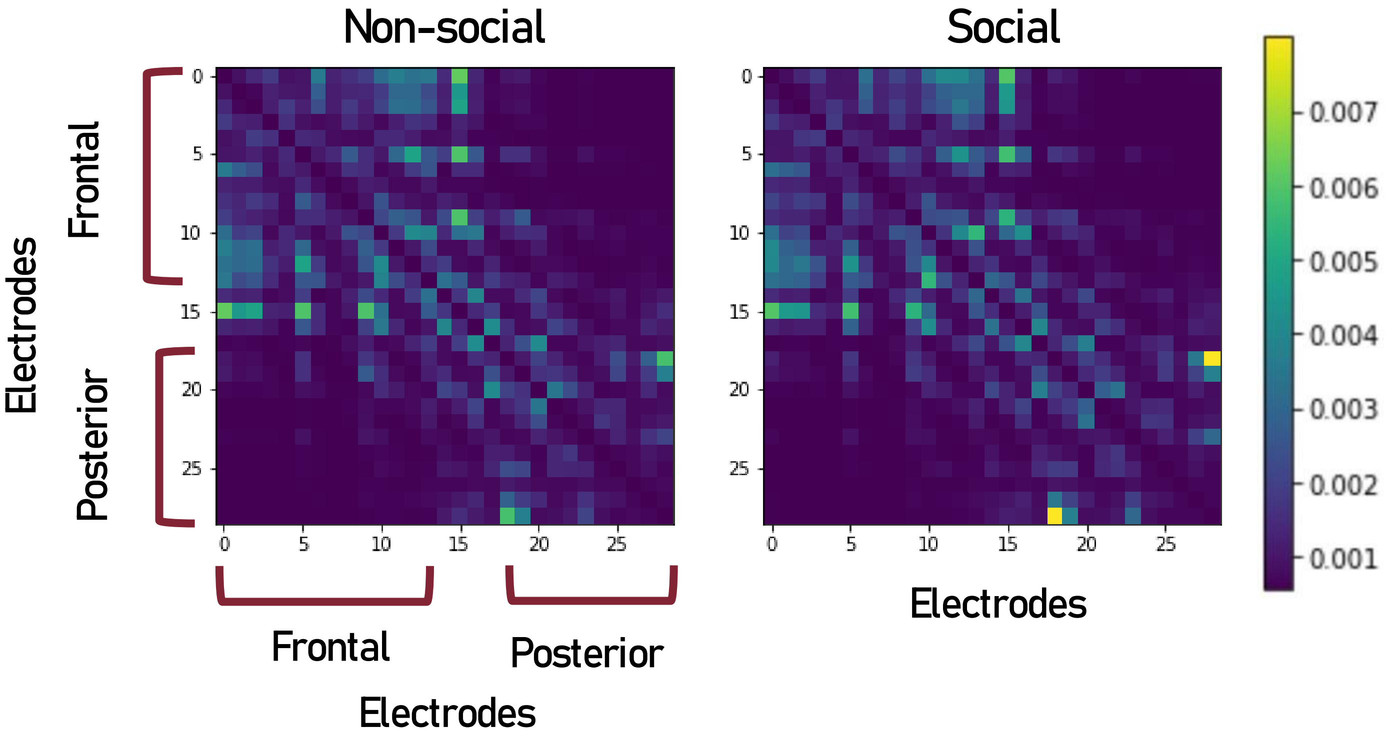


Graph-structure learning based classifier compared with 'standard' ones

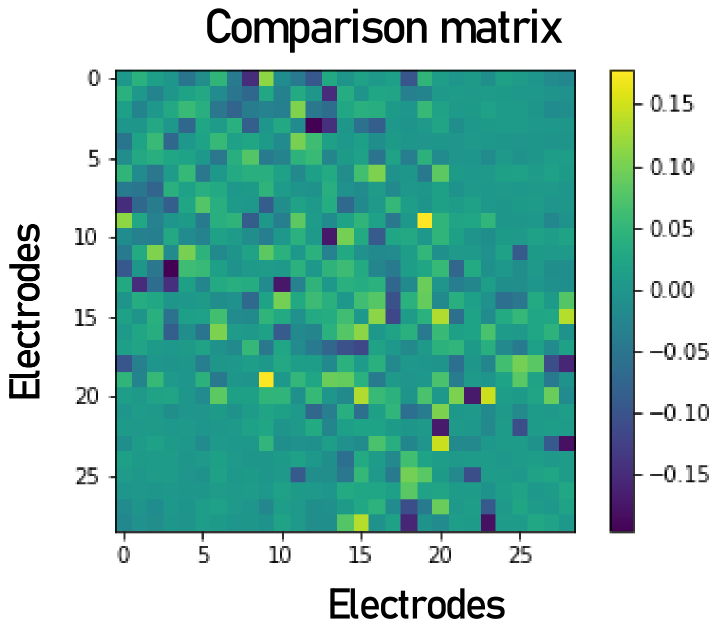


Graph-structure learning based classifier accuracies over subjects

Results – Learned Adjacency Matrices



Average matrices across all subjects

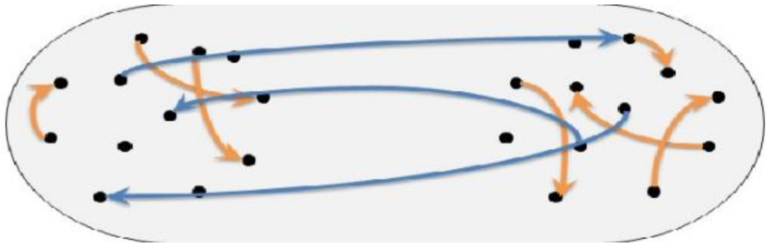


Normalized difference matrix

Results – Quantitative analysis of the learned matrices

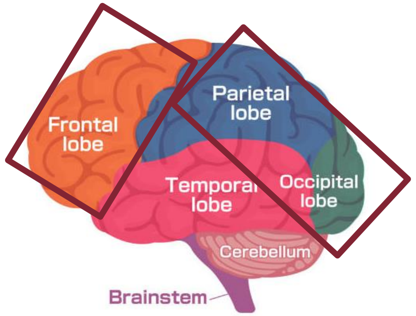
- Integration and segregation test on learned subject-specific matrices
- Computation of three graph indices on the matrices of the two conditions and on their difference matrix:
  - Modularity
  - Divisibility
  - Weights of intra- and inter-connections between submatrices (classes)

Intra-classes and inter-classes links



Chosen classes:

Right and left hemispheres

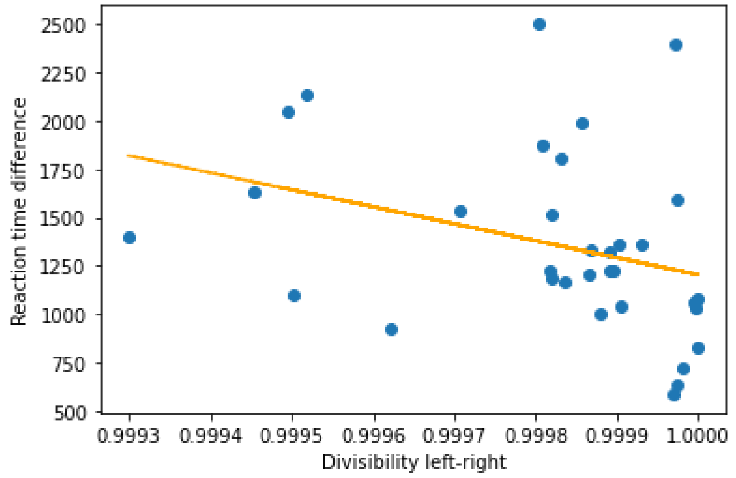


Frontal and parietal-occipital lobes

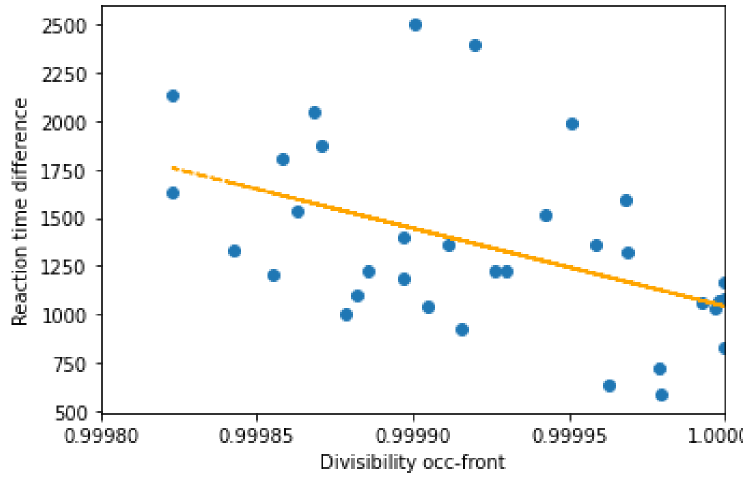
Results – Statistical tests on behavioral data

Two significant correlation results:

- absolute value of the difference between reaction times and the divisibility computed on the difference matrices, considering the two hemispheres as classes (r = -0.338; p=0.05)



- absolute value of the difference between reaction times and the divisibility computed on the difference matrices, considering the the frontal and parietal-occipital lobes as classes (r =-0.473; **p=0.004**)



Conclusion

1. I proposed a classification pipeline based on GNNs and meaningful features that shows better classification accuracies than the baseline, effectively classifying some challenging human EEG data that only differ for the social component of the stimulus

2. I developed an automatic mechanism for graph structure learning to avoid any arbitrariness in the choice of graph edges. This also improves the interpretability of the results, as shown by the physiologically meaningful results in terms of learned matrices and by the significant correlations between graph indices and behavioral data

Novelty

1. The choice of expressive and meaningful node features, never used before in the literature, leading to better classification accuracies

2. The development of an automatic graph-structure learning mechanism to improve the interpretability of the results

3. The application to a particularly challenging dataset, significantly different from the previous literature targets, and the quantitative (statistical) analysis which returned results physiologically meaningful.

Thank you for your kind attention!

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