BrainGNN: Interpretable Brain Graph Neural Network for fMRI Analysis

(Li et al., Medical Image Analysis, 2021)

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Seminar **Deep Learning for Biomedical Image Analysis**
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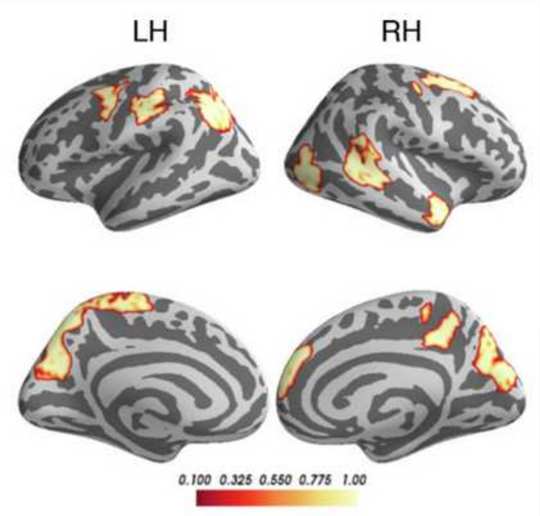
Agenda

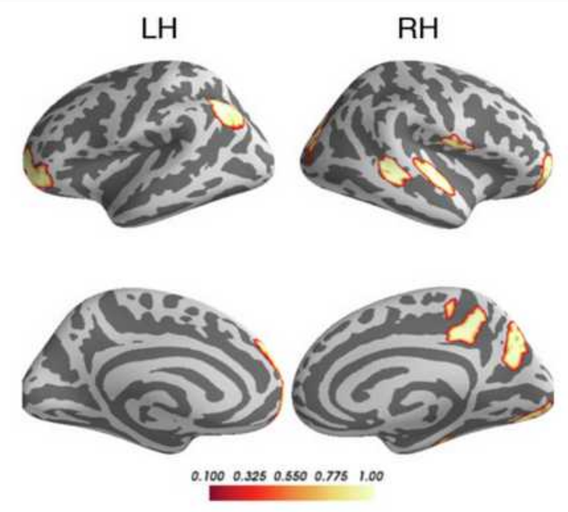
1. Introduction
2. Approach
3. Experiments and results
4. Discussion
5. Conclusion

1. Introduction

- Brain = complex system
- Modern neuroscience: understanding the brain
- Especially: Connection of brain regions to
  - neurological disorders
  - cognitive stimuli



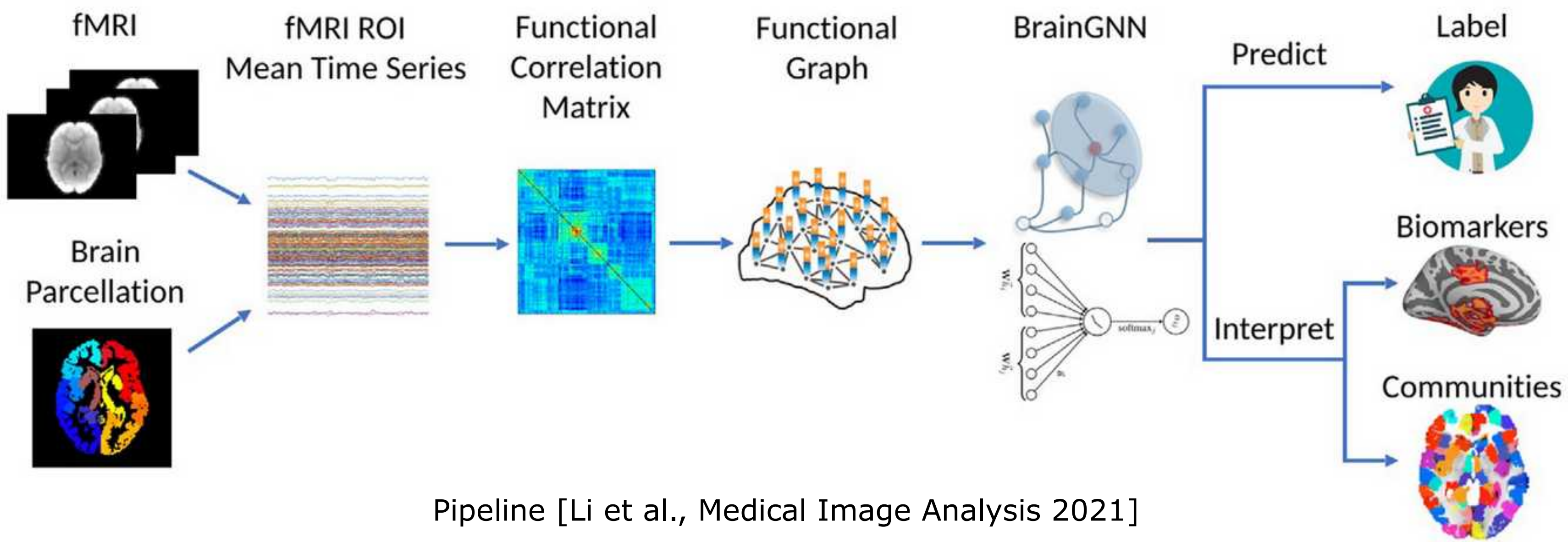
(b) Language



(c) Motor

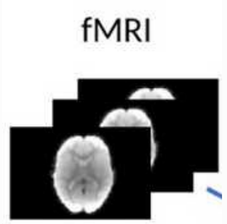
[Li et al., Medical Image Analysis 2021]

2. Approach
2.1. Pipeline



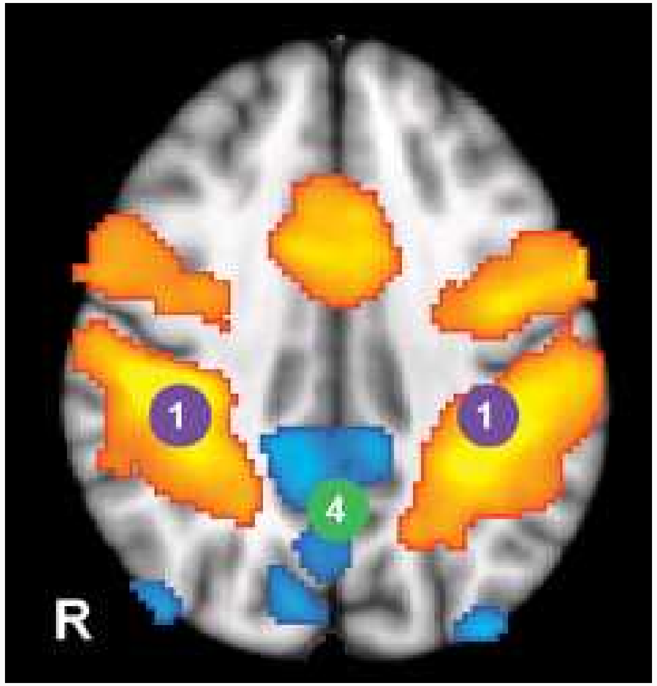
Pipeline [Li et al., Medical Image Analysis 2021]

2. Approach
2.2. fMRI



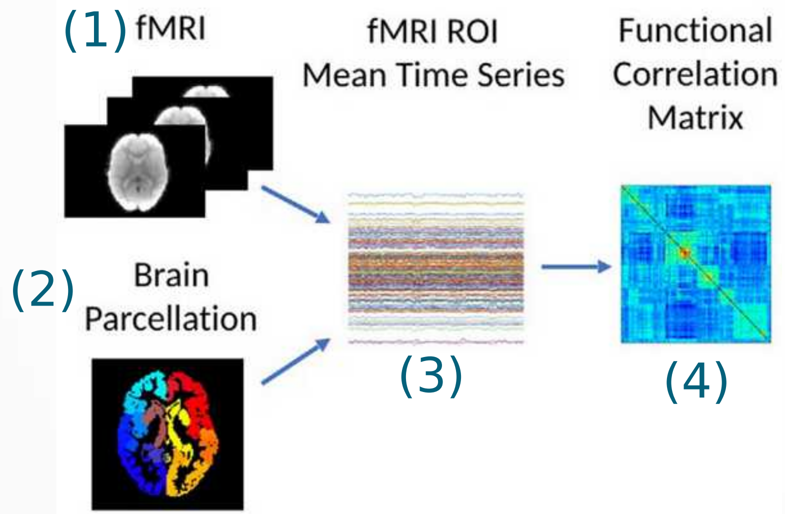
- Functional magnetic resonance imaging (fMRI)
- Measures blood flow changes
- Blood flow and neural activity are coupled
  - Brain region in use → blood flow increases

→ fMRI measures activity of different brain regions



fMRI image: color indicates activity [Hellyer et al., The Journal of neuroscience 2014]

2. Approach
2.3. Preprocessing



(1) Series of consecutive fMRI images

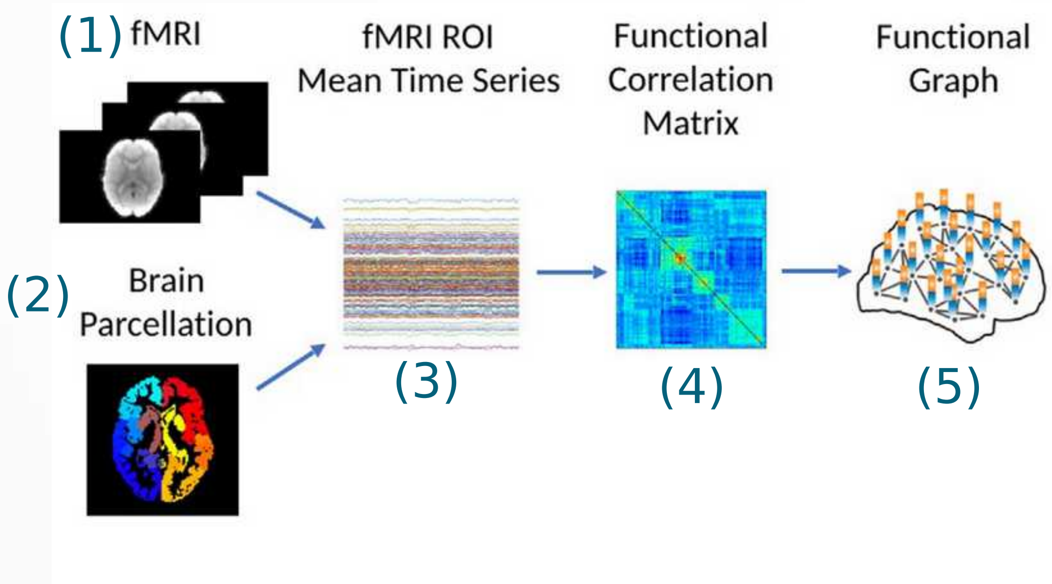
(2) Which brain areas (voxels) should be grouped?

- Brain parcellation by an atlas → Clustered voxels
- Each cluster = one region of interest (ROI)

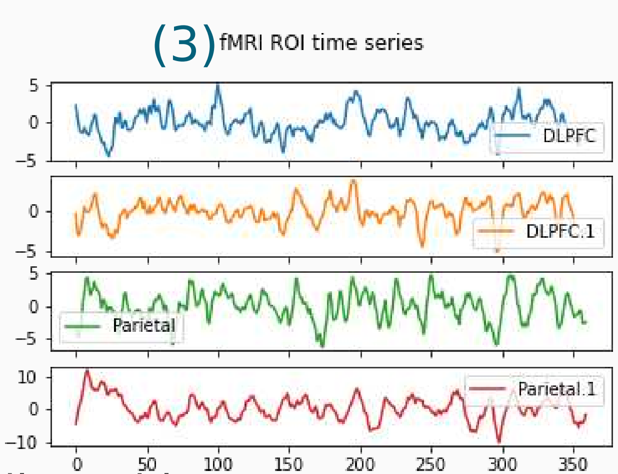
(3) Each ROI is represented by one time series

(4) Pairwise correlations between all time series

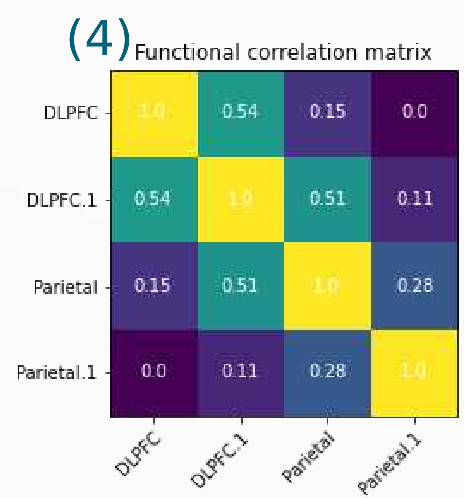
2.4. Graph construction



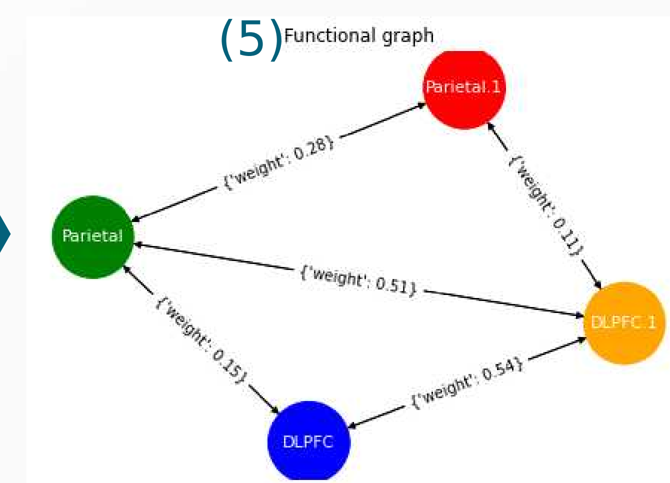
Toy example steps (3) – (5):



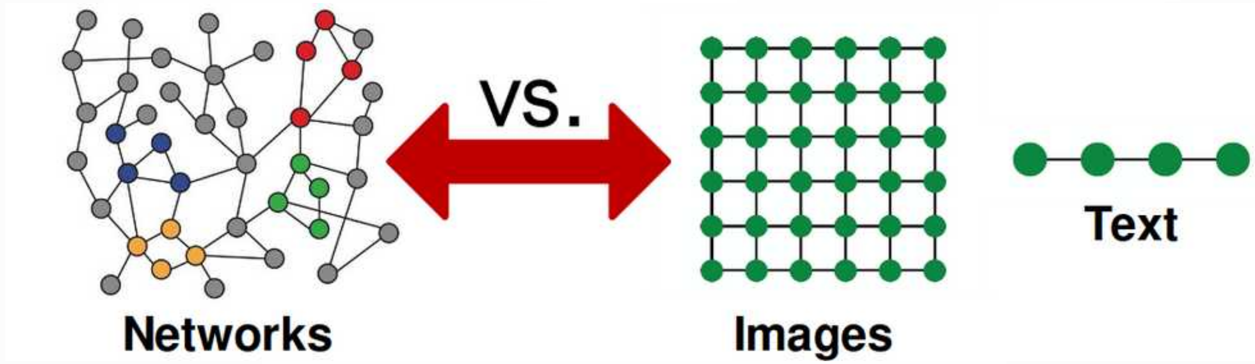
Correlations between time series

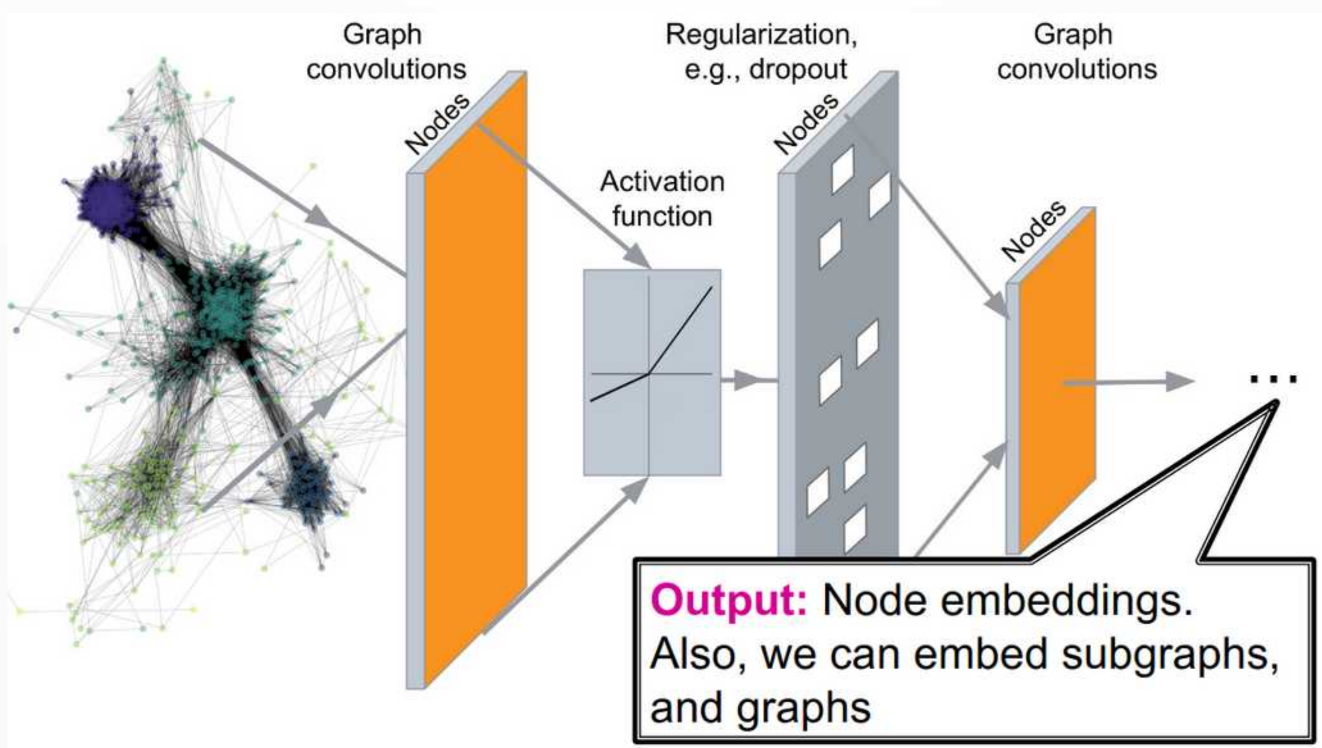


Adjacency matrix → Graph



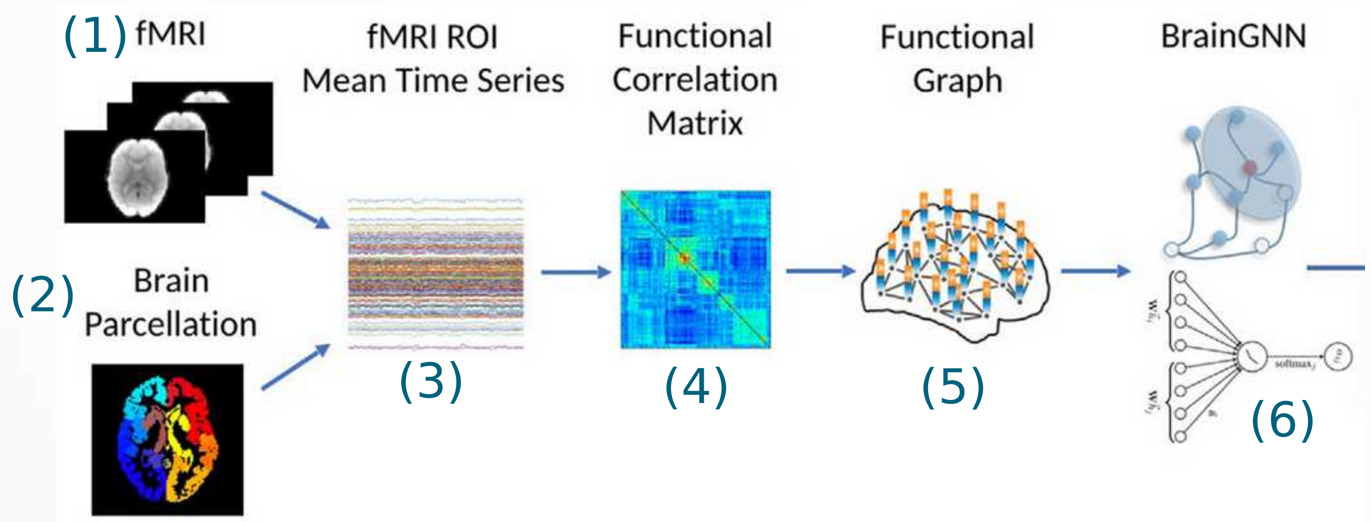
2.5. Graph Neural Networks



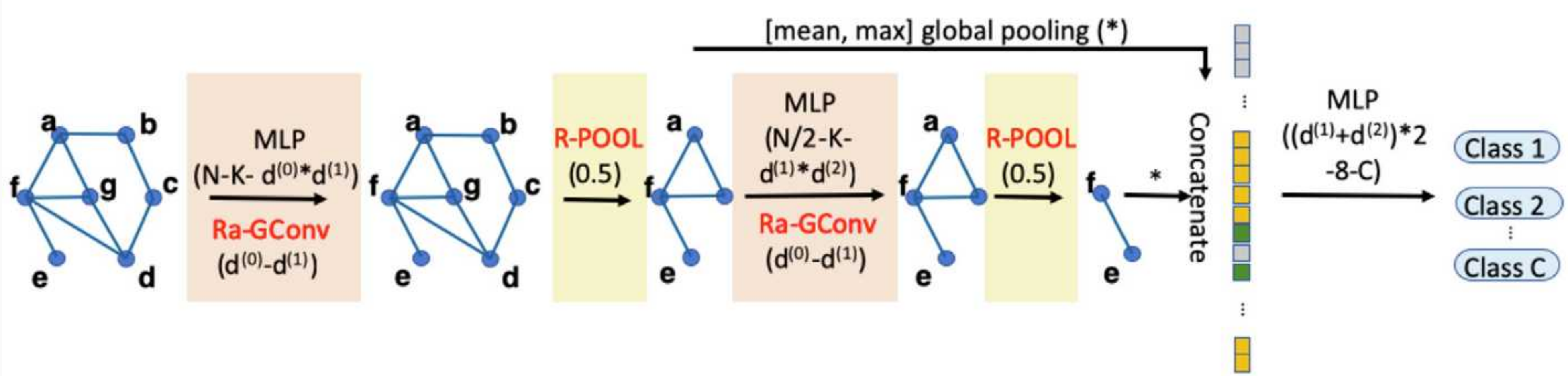


[Leskovec, Machine Learning with Graphs 2021]

2. Approach
2.6. Brain GNN architecture



(6) Brain GNN Architecture:

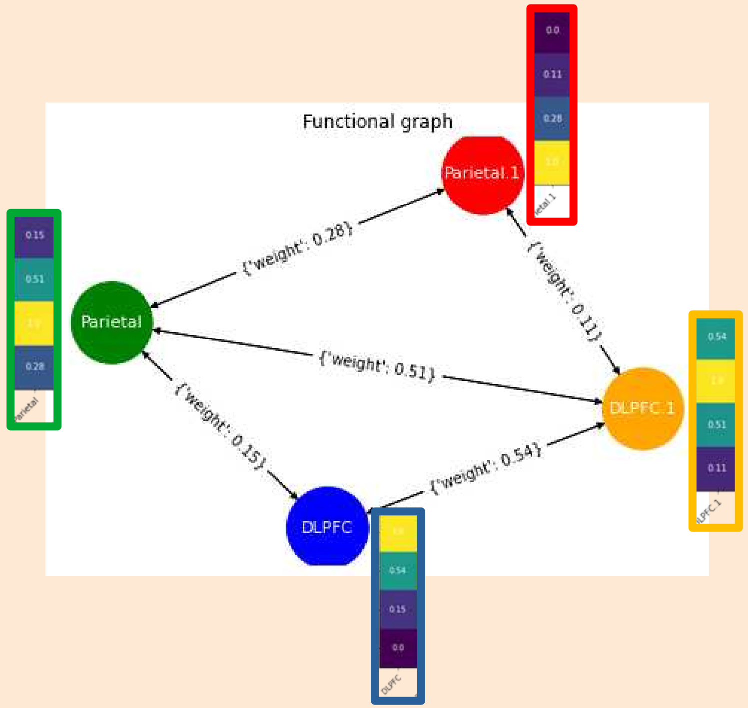


[Li et al., Medical Image Analysis 2021]

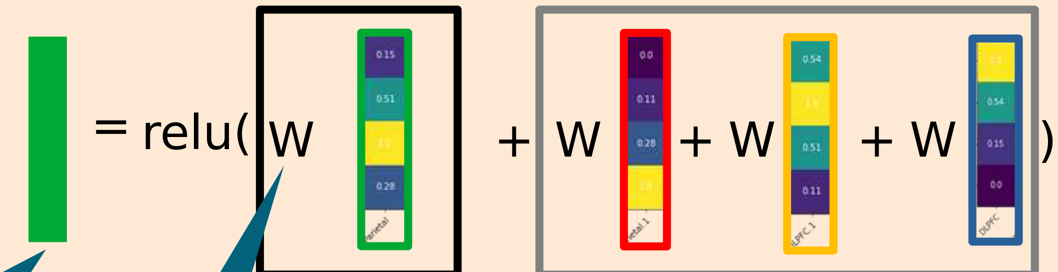
2. Approach
2.7. Brain GNN: convolutional layer

Layers in detail: **Ra-GConv**

- Basis: One feature vector describes each node
- Goal: Learn new feature vectors (encoding the relationship between different ROIs)
- Intuition:



e.g. new feature vector for node „Parietal“:



New node feature vector

Learned model weights

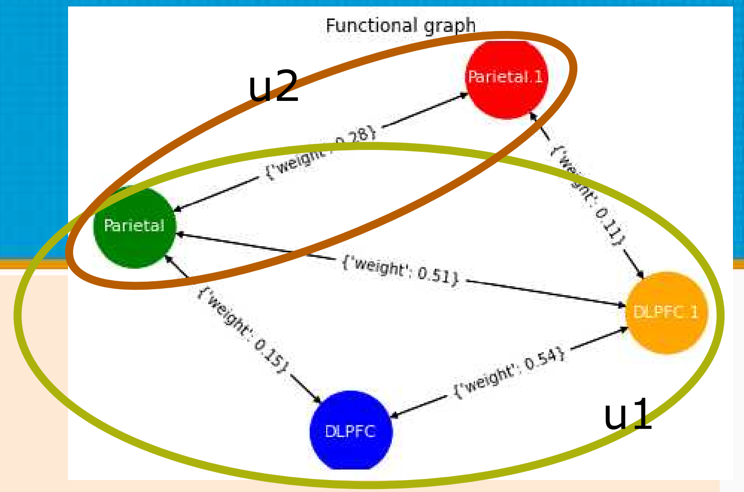
Previous node feature vector

Sum feature vectors of neighbors

- Forward pass node feature vector update (Schlichtkrull et al. (2018))

$$\tilde{\mathbf{h}}_i^{(l+1)} = \mathrm{relu}\left(\boxed{W_i^{(l)}\mathbf{h}_i^{(l)}} + \boxed{\sum_{j\in\mathcal{N}^{(l)}(i)} e_{ij}^{(l)} W_j^{(l)} \mathbf{h}_j^{(l)}}\right)$$

2. Approach
2.7. Brain GNN: convolutional layer



Layers in detail: **Ra-GConv**

- Improvements of Brain GNN:
  1) Different embedding weights for each ROI
     - Weights = encode community membership for each node

$$\mathrm{vec}(W_i^{(l)}) = \sum_{u=1}^{K^{(l)}} \boxed{(\alpha_{iu}^{(l)})}\boxed{\boldsymbol{\beta}_u^{(l)}} + \boldsymbol{b}^{(l)}$$

α =

	u1	u2
DLPFC	1	0
DLPFC.1	1	0
Parietal	1	1
Parietal.1	0	1

β =

u1	u2
0	4
1	5
2	6
3	7

       – α = Is ROI i member of community u?
       – β = Community Basis vector

e.g. weight vector for node „Parietal.1“: $\alpha_{i=Parietal.1,u=u1} * \beta_{u=u1} + \alpha_{i=Parietal.1,u=u2} * \beta_{u=u2}$

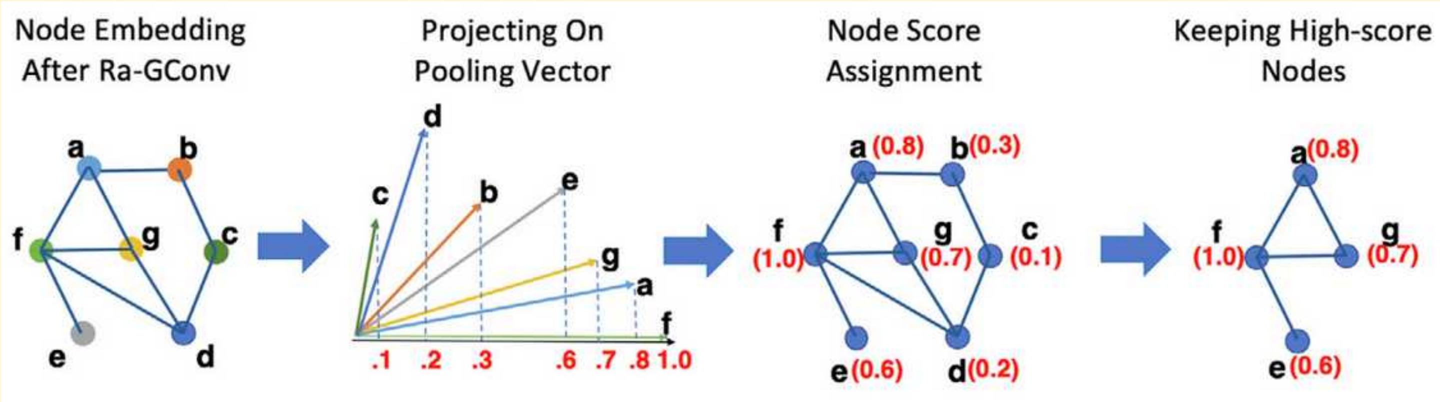
$0 * \beta_{u=u1} + 1 * \beta_{u=u2}$

  2) Include edge weight: node feature vector * edge weight → strongly coupled neighbors have stronger influence

2. Approach
2.8. Brain GNN: pooling layer

Layers in detail: **R-Pool**

- Goal: Dimensionality reduction of the graph
- some ROIs more indicative for predicting neurological disorders (Kaiser et al., 2010; Baker et al., 2014)
- Dimensionality reduction: keep indicative ROIs; remove other ROIs
- Approach from Cangea et al. (2018), Gao and Ji (2019)
- Intuition:



[Li et al., Medical Image Analysis 2021]

2. Approach
2.9. Brain GNN: loss functions

Loss functions:

- **Cross entropy loss**: classification loss

$$L_{ce} = -\frac{1}{M}\sum_{m=1}^{M}\sum_{c=1}^{C} y_{m,c}\log(\hat{y}_{m,c})$$

Sum over all instances M

Sum over all classes C

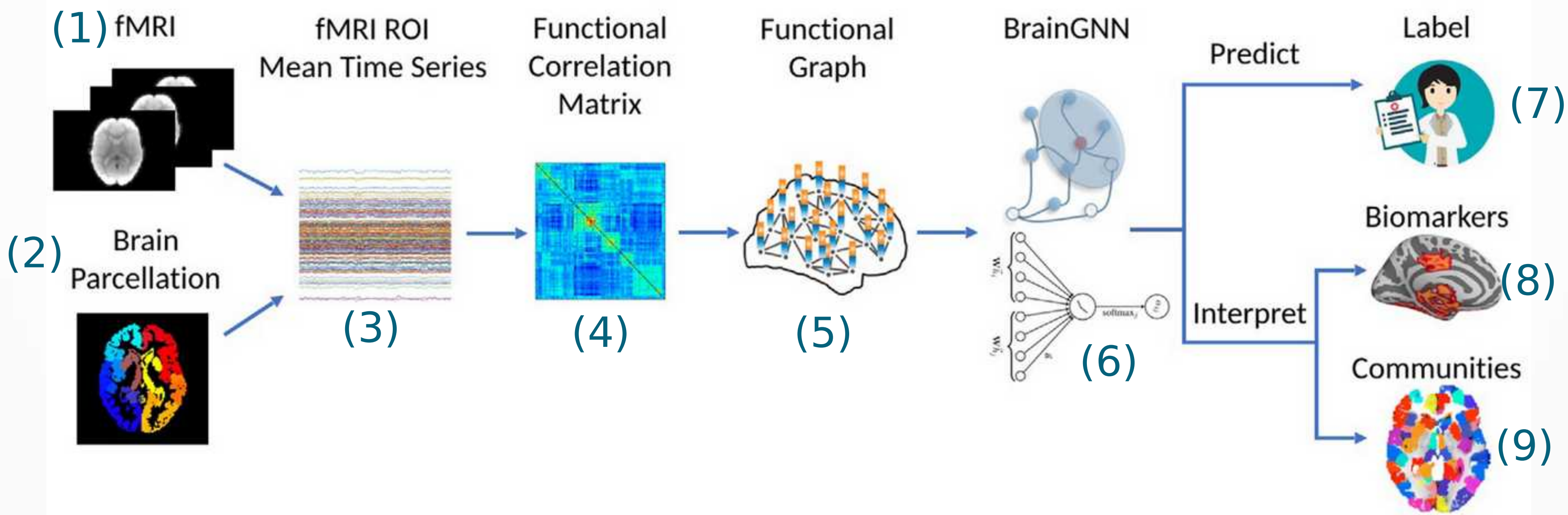
Ground truth label

Model prediction

- **Unit loss**: learned pooling vector is unique
- **Group-level consistency loss**: select similar ROIs in R-Pool layer for different input instances
- **TopK pooling loss**: improve node selection in R-Pool layer (indicative and unselected ROIs should have significantly different scores)
- **Final combined loss**:

$$L_{total} = L_{ce} + \sum_{l=1}^{L} L_{unit}^{(l)} + \lambda_1 \sum_{l=1}^{L} L_{TPK}^{(l)} + \lambda_2 L_{GLC}$$

2. Approach
2.10. Results



Brain GNN results:

(7) Prediction: e.g. healthy vs. disease

(8) Biomarkers: Evaluation by adapting Group-level consistency loss

Level	Goal	Strenght of GLC
group-level biomarkers	characteristic patterns of a disease	+
individual-level biomarkers	individual-level biomarkers needed for precision medicine	-

(9) Communities: detected as part of the graph convolutional layers

3. Experiments and results (1/3)

Datasets

(a) Biopoint Autism Study Dataset (Biopoint)

- Binary classification: Autism vs. healthy

(b) Human Connectome Project (HCP)

- Multi class classification: gambling, language, motor, relational, social, working memory (WM), emotion

Prediction

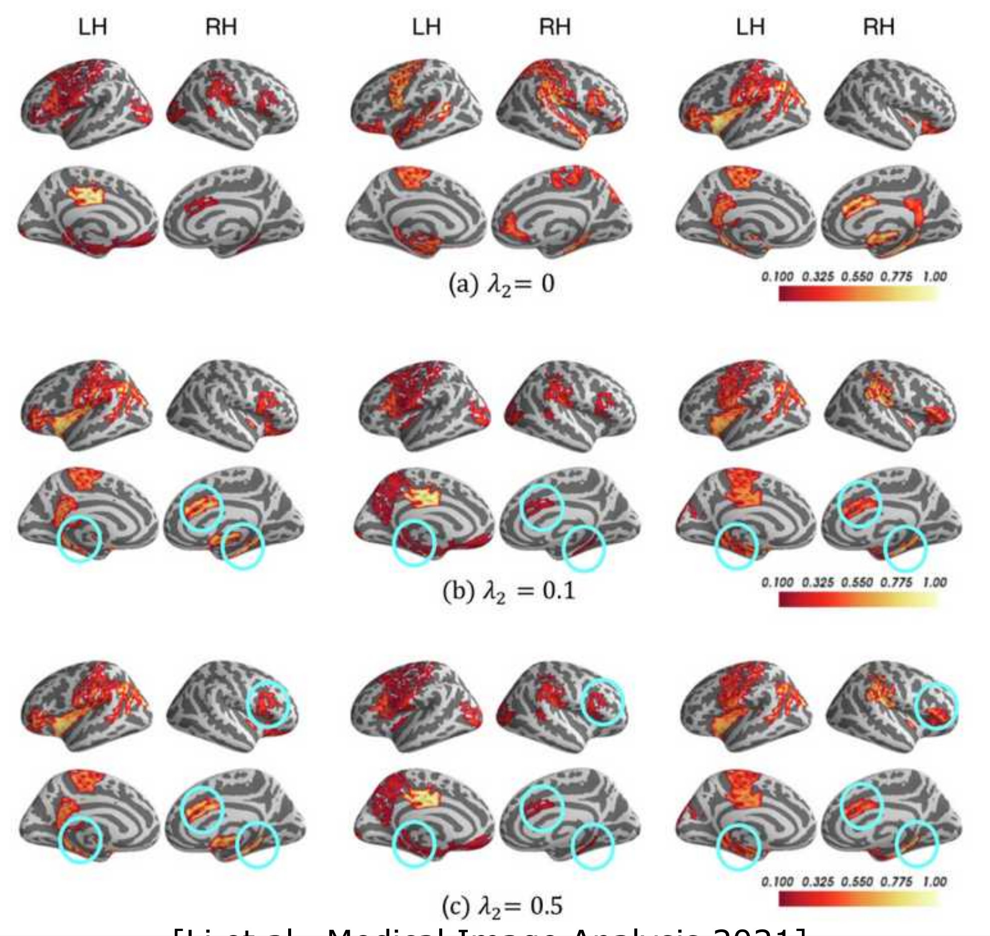
		SVM	Random Forest	MLP	BrainNetCNN	GAT	GraphSAGE	PR-GNN	BrainGNN
Biopoint	Accuracy (%)	62.80(4.92) [a]	68.60(3.58)	58.80(1.79)	75.20(3.49)	77.40(3.51)	78.60(5.90)	77.10(8.71)	**79.80(3.63)** [c]
	F1 (%)	60.08(3.91)	63.97(4.95)	55.25(9.49)	65.58(14.48)	75.08(5.19)	75.55(7.03)	75.20(7.01)	**75.80(6.03)**
	Recall (%)	60.20(4.49)	71.11(8.12)	61.00(4.85)	66.20(10.85)	71.60(6.07)	75.20(6.46)	78.26(10.28)	**72.60(5.64)**
	Precision (%)	60.00(3.81)	67.80(5.36)	53.40(12.52)	65.60(17.95)	79.40(8.02)	76.20(8.11)	76.50(14.32)	**79.60(8.59)**
	Parameter (k) [b]	3	3	138	1438	16	6	6	41
HCP	Accuracy (%)	90.00(8.20)	90.20(4.15)	67.20(34.40)	90.60(4.04)	78.60(10.45)	89.80(12.51)	91.20(8.28)	**94.40(4.04)*** [d]
	F1 (%)	90.20(5.81)	90.14(5.55)	63.49(41.80)	90.96(3.50)	77.00(11.58)	88.60(13.19)	91.09(8.35)	**94.34(3.27)***
	Recall (%)	89.57(8.04)	90.06(7.35)	67.97(41.66)	91.12(4.13)	78.60(10.45)	89.43(12.43)	91.00(8.95)	**94.29(3.73)***
	Precision (%)	90.85(9.35)	90.22(4.77)	62.97(42.47)	90.81(3.27)	91.20(3.32)	87.80(14.02)	91.14(8.52)	**94.40(3.59)***
	Parameter (k)	36	36	713	4547	34	12	12	96

[Li et al., Medical Image Analysis 2021]

3. Experiments and results (2/3)

Interpretability of BrainGNN

(1) Biomarkers: Which brain regions are relevant for the prediction task?



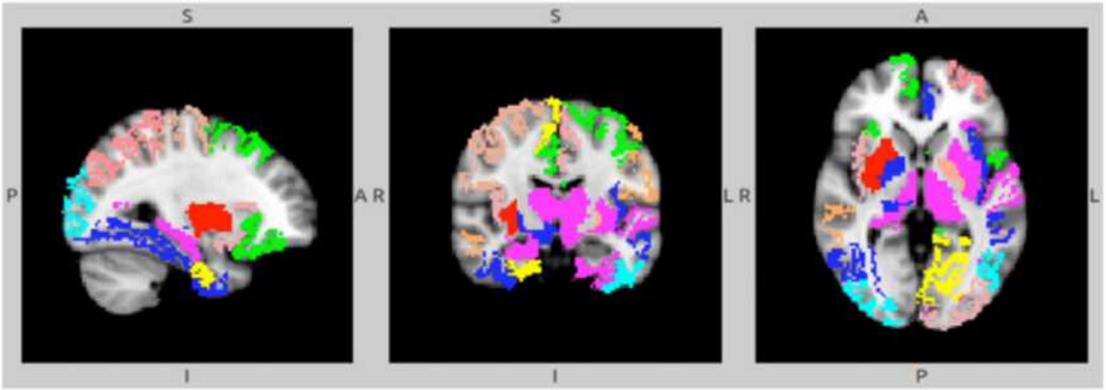
[Li et al., Medical Image Analysis 2021]

→ suitable Biomarkers for Autists found

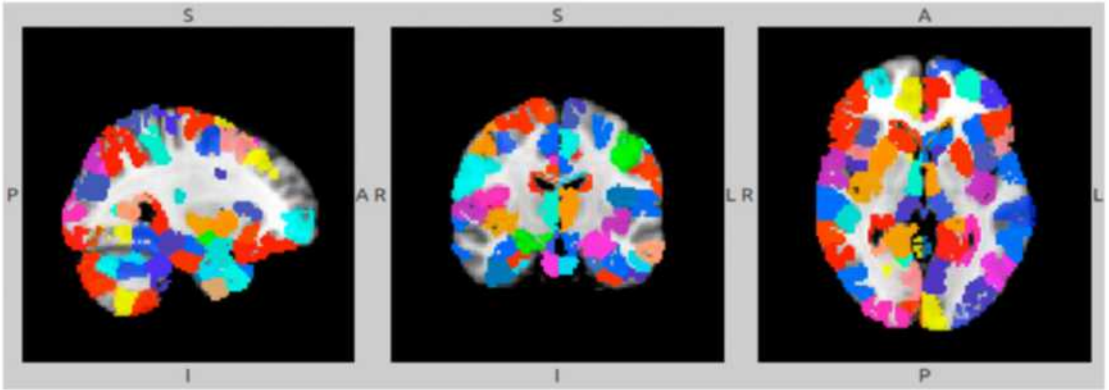
3. Experiments and results (3/3)

Interpretability of BrainGNN

(2) Communities: Which brain regions form communities?



(a) Biopoint



(b) HCP

- Based on Ra-GConv layer
- Number of communities = 8
- Not the same communities for (a) & (b)

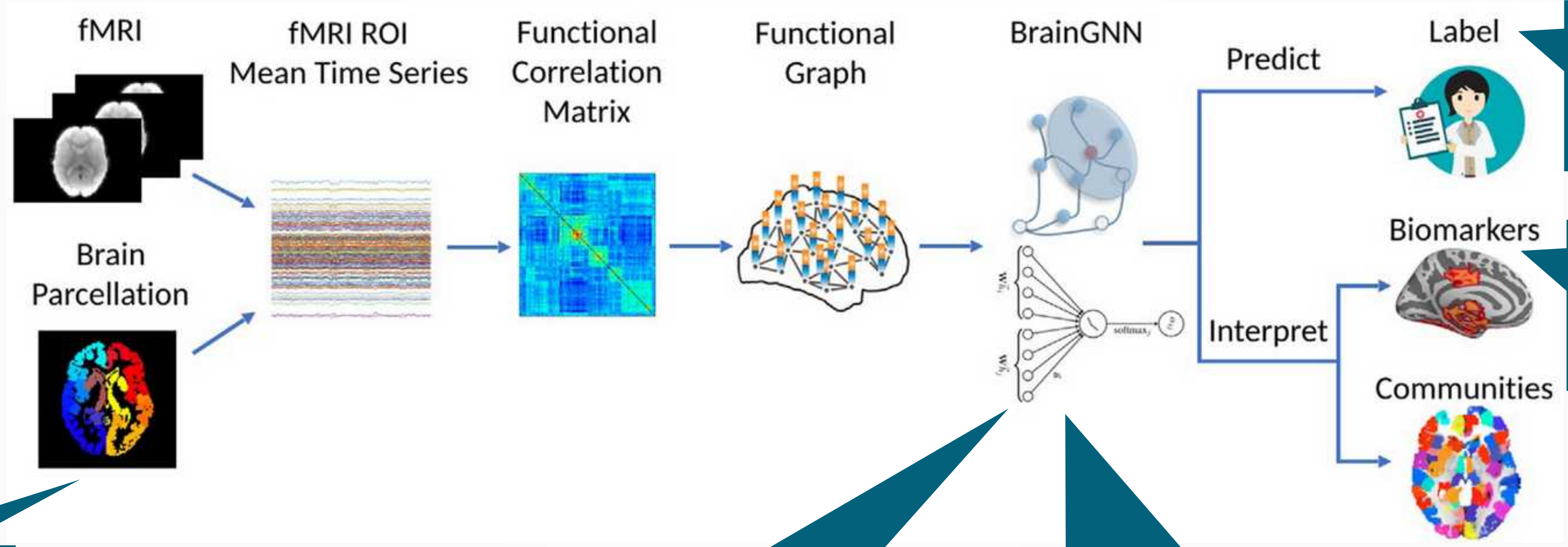
  → Communities are task specific

 [Li et al., Medical Image Analysis 2021]

4. Discussion

Limitations and future work

Different **Pre-processing** strategies:
e.g. End-to-end training procedure



Explore
failure cases

Application for
different tasks

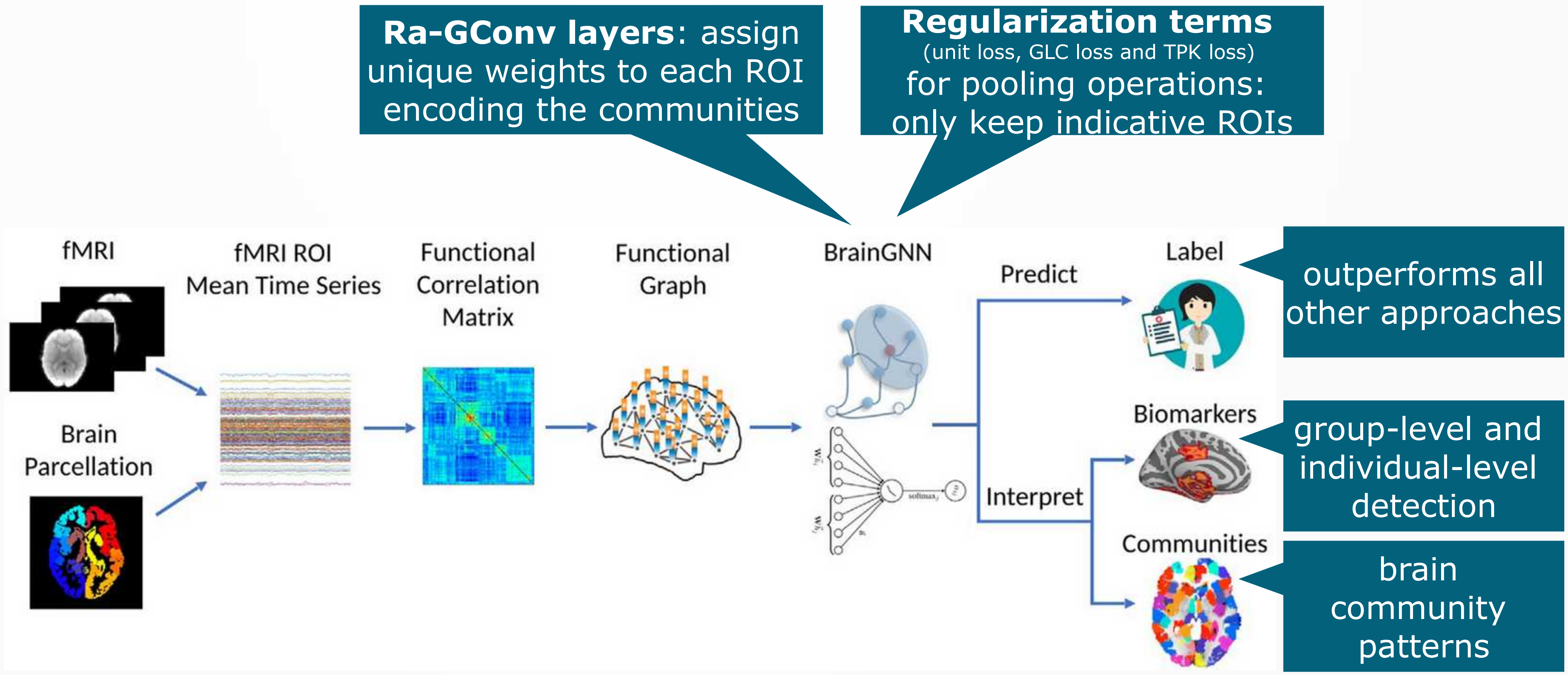
Different Brain
parcellation
atlases

Different **Hyperparameters**:
e.g. number of
convolutional layers,
number of communities

Understand **Ra-GConv layer**:
quantitative evaluations
and theoretical studies

Pipeline [Li et al., Medical Image Analysis 2021]

5. Conclusion



Pipeline [Li et al., Medical Image Analysis 2021]

Thanks for your attention!

Questions?