Institute for Software Integrated Systems

neurdy lab

NeuroGraph: Benchmarks for Graph Machine Learning in Brain Connectomics

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NeurIPS2023 Datasets and Benchmarks Track

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NeuroGraph

- Provides a collection of 10 novel graph-based **neuroimaging benchmarks**
- **Python** package offering a suite of tools

Dataset	Type	Task
HCP-Task	Static	Graph Classification
HCP-Gender	Static	Graph Classification
HCP-Age	Static	Graph Classification
HCP-Fluid Intelligence	Static	Graph Regression
HCP-Working Memory	Static	Graph Regression
DynHCP-Task	Dynamic	Graph Classification
DynHCP-Gender	Dynamic	Graph Classification
DynHCP-Age	Dynamic	Graph Classification
DynHCP-Fluid Intelligence	Dynamic	Graph Regression
DynHCP-Working Memory	Dynamic	Graph Regression

NeuroGraph Benchmarks

- fMRI data sourced from the **Human Connectome Project** database
- **HCP-Task Dataset**

Task classification

Social Cognition

Working Memory

- **Predicting Demographics**

Gender Classification

Age Classification

- **Estimating Cognitive Traits**

Fluid Intelligence

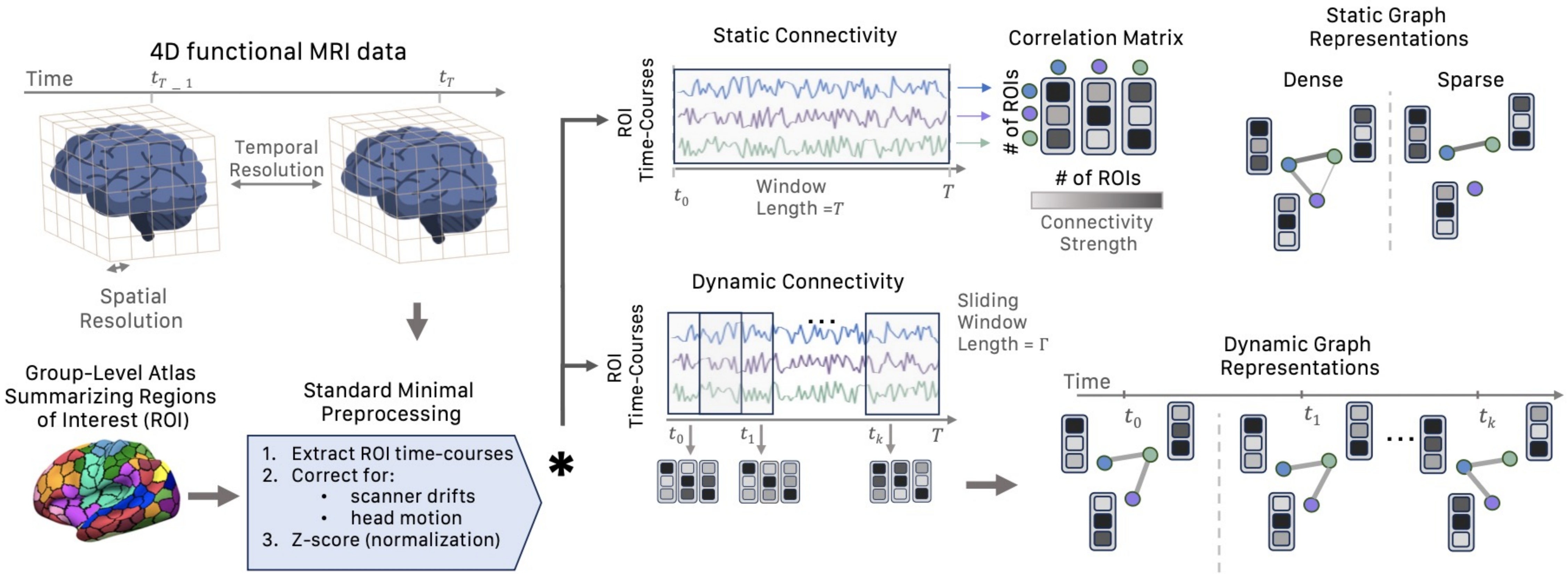
Working Memory

Benchmarks Statistics

NeuroGraph benchmarks statistics

Dataset		Statistics						Node Feat. (dim)	#Classes	Prediction Task
		$\|G\|$	$\|N\|_{avg}$	$\|E\|_{avg}$	d_{max}	d_{avg}	K_{avg}			
Static	HCP-Task	7443	400	7029.18	153	17.572	0.410	400	7	Graph Classification
	HCP-Gender	1078	1000	45578.61	413	45.579	0.466	1000	2	Graph Classification
	HCP-Age	1065	1000	45588.40	413	45.588	0.466	1000	3	Graph Classification
	HCP-FI	1071	1000	45573.67	413	45.574	0.466	1000	-	Graph Regression
	HCP-WM	1078	1000	45578.61	413	45.579	0.466	1000	-	Graph Regression
Dynamic	DynHCP-Task	7443	100	843.04	57	8.430	0.427	100	7	Graph Classification
	DynHCP-Gender	1080	100	874.88	53	8.749	0.439	100	2	Graph Classification
	DynHCP-Age	1067	100	875.42	53	8.754	0.439	100	3	Graph Classification
	DynHCP-FI	1073	100	874.82	53	8.748	0.438	100	-	Graph Regression
	DynHCP-WM	1080	100	874.88	53	8.749	0.439	100	-	Graph Regression

Preprocessing Pipeline



Large and Sparse Graphs yield the best performance

Analysis: Graph sizes, density, node features, and static/dynamic

Findings: Large ROIs, sparse graphs, and correlations as node features show the best performance.

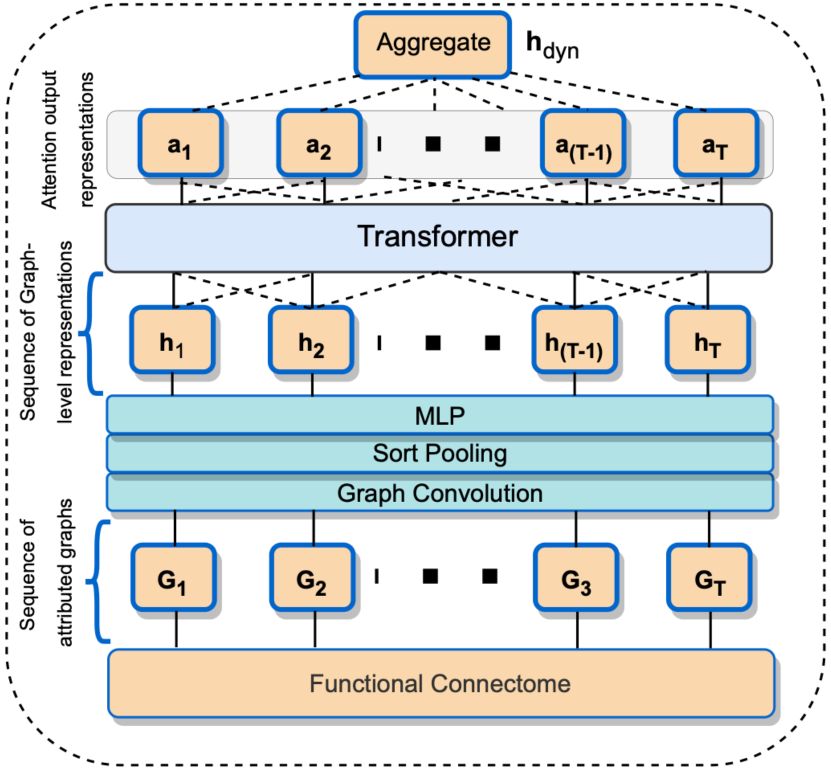
Dataset		k-GNN	GCN	SAGE	UniMP	ResGCN	GIN	Cheb	GAT	SGC	General	Avg.
100ROIs	CORR	65.65	68.98	68.70	68.33	66.06	68.24	63.94	69.49	68.43	64.95	**67.30**
	BOLD	49.58	50.97	51.67	51.30	51.34	55.09	53.19	49.95	51.90	51.11	51.11
	CORR+BOLD	52.78	51.02	50.28	50.79	50.60	54.91	49.44	50.37	51.57	51.30	51.36
400ROIs	CORR	72.21	74.10	61.66	68.57	70.09	71.89	58.94	69.35	**75.99**	**73.09**	**69.56**
	BOLD	51.16	51.62	53.94	51.39	52.31	55.09	49.07	50.46	53.24	53.94	52.22
	CORR+BOLD	51.53	51.90	52.96	51.57	52.36	55.56	50.63	52.13	52.08	52.61	53.33
1000ROIs	CORR	**78.80**	**75.19**	**71.71**	**75.14**	**78.75**	**77.22**	**64.77**	**71.34**	73.75	63.13	**72.98**
	BOLD	48.15	46.99	49.31	50.93	47.92	56.48	47.22	50.93	49.31	51.62	49.89
	CORR+BOLD	51.30	51.81	51.25	51.11	49.86	54.35	49.66	51.22	51.34	51.37	51.33

Dataset			$k-$GNN	GCN	SAGE	UniMP	ResGCN	GIN	Cheb	GAT	SGC	General
Gender Classification	100ROIs	Sparse	63.33	72.96	69.35	69.72	68.06	69.72	63.70	70.28	70.37	67.22
		Medium	65.65	68.98	68.70	68.33	66.06	68.24	63.94	69.49	68.43	64.95
		Dense	64.44	68.52	65.00	68.06	63.70	66.39	64.26	69.72	68.43	61.76
	400ROIs	Sparse	69.95	**77.14**	69.86	67.56	71.43	69.4	66.45	72.72	**78.25**	76.13
		Medium	65.65	68.98	68.70	68.33	66.06	68.24	63.94	69.49	68.43	64.95
		Dense	71.61	76.13	62.58	61.20	69.77	73.27	61.84	67.83	74.19	72.44
	1000ROIs	Sparse	**82.13**	75.46	77.69	**76.67**	78.33	75.56	59.07	**76.2**	76.48	**78.89**
		Medium	78.80	75.19	71.71	75.14	78.75	77.22	71.43	71.34	73.75	63.13
		Dense	61.57	73.80	**78.86**	72.50	**78.89**	**78.70**	**76.67**	71.67	75.25	72.69
Task Classification	100ROIs	Sparse	91.50	91.56	91.43	92.73	92.14	88.31	92.55	92.91	91.40	91.52
		Medium	90.91	90.80	91.81	92.75	92.25	88.01	93.06	93.15	91.40	91.22
		Dense	90.30	91.15	93.15	93.28	93.02	87.12	93.18	93.08	90.49	89.47
	400ROIs	Sparse	93.23	**94.21**	94.78	94.72	94.61	**89.79**	94.45	95.2	**94.17**	93.62
		Medium	92.26	93.93	93.89	95.02	94.33	89.44	79.03	94.67	93.39	93.58
		Dense	90.64	93.36	**95.76**	94.48	**94.64**	88.22	87.24	94.78	93.18	90.84
	1000ROIs	Sparse	93.50	93.80	94.09	93.59	94.23	85.14	93.82	94.66	93.2	**94.17**
		Medium	92.65	90.87	94.39	**95.79**	92.04	85.40	**94.88**	94.00	91.37	91.87
		Dense	**93.77**	93.12	94.12	94.54	93.59	81.59	92.92	**95.35**	93.76	93.76

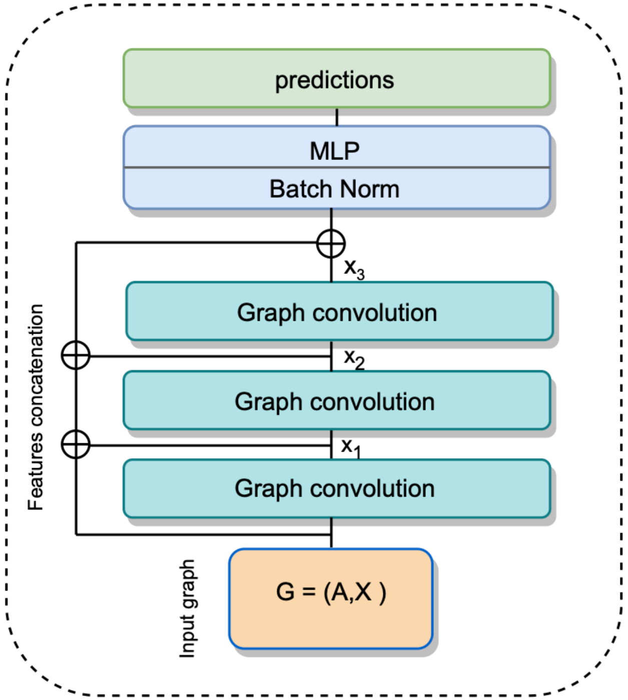
Benchmarking

- Consider 10 GNNs, three conventional ML methods and two simple newly implemented models as baselines for benchmarking

Dynamic GNNs



GNN*



Benchmarking results

Classification results in terms of accuracy on static benchmarks

Dataset	NN	CNN	RF	$k-$GNN	GCN	SAGE	UniMP	ResGCN	GIN	Cheb	GAT	SGC	General	GNN*
HCP-Task	97.78	95.88	88.98	93.23	94.21	94.78	94.72	94.61	89.79	94.45	95.2	94.17	93.62	**98.20**
HCP-Gender	86.67	76.39	69.9	82.13	75.46	77.69	76.67	78.33	75.56	59.07	76.20	76.48	78.89	**89.07**
HCP-Age	44.23	43.38	40.84	42.72	43.66	40.94	43.85	40.00	44.98	41.97	42.25	43.47	41.03	**50.23**

Regression results in terms of MAE on static benchmarks

Dataset	k-GNN	GCN	SAGE	UniMP	ResGCN	GIN	Cheb	GAT	SGC	General	GNN*
HCP-FI	0.284	0.288	0.283	0.287	0.281	6.548	0.278	0.290	0.282	0.283	**0.264**
HCP-WM	0.818	0.825	0.810	0.812	0.830	1.032	0.789	0.804	0.828	0.819	**0.751**

Models' performance in terms of Accuracy and MAE

Dataset	**Accuracy ↑**					**Dataset**	**MAE ↓**				
	UniMP	**$k-$GNN**	**GAT**	**SAGE**	**General**		**UniMP**	**$k-$GNN**	**GAT**	**SAGE**	**General**
DynHCP-Task	89.66	73.03	89.67	**90.93**	68.84	DynHCP-FI	**3.839**	3.841	3.861	3.842	3.862
DynHCP-Gender	**72.3**	68.45	67.13	66.20	62.04	DynHCP-WM	10.589	10.596	10.592	10.597	**10.571**
DynHCP-Age	**44.41**	44.25	44.39	40.65	42.99						

Easy to Download and Use Benchmarks

NeuroGraphDataset

`class NeuroGraphDataset(root: str, name: str, transform: Optional[Callable] = None, pre_transform: Optional[Callable] = None, pre_filter: Optional[Callable] = None)` [source]

Bases: `InMemoryDataset`

The NeuroGraph benchmark datasets from the "NeuroGraph: Benchmarks for Graph Machine Learning in Brain Connectomics" paper. `NeuroGraphDataset` holds a collection of five neuroimaging graph learning datasets that span multiple categories of demographics, mental states, and cognitive traits. See the documentation and the Github for more details.

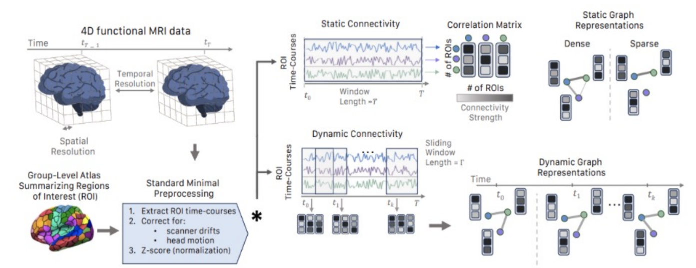
Dataset	#Graphs	Task
`HCPActivity`	7,443	Graph Classification
`HCPGender`	1,078	Graph Classification
`HCPAge`	1,065	Graph Classification
`HCPFI`	1,071	Graph Regression
`HCPWM`	1,078	Graph Regression

NeuroGraph

A Python package for fMRI preprocessing and a collection of graph-based Neuroimaging datasets for graph machine learning applications

Install: pip install NeuroGraph

NeuroGraph: Benchmarks for Graph Machine Learning in Brain Connectomics



Link to the documentation • Github Link • Link to the paper

NeuroGraph pipeline combined with CWL design studio

Dataset Downloads

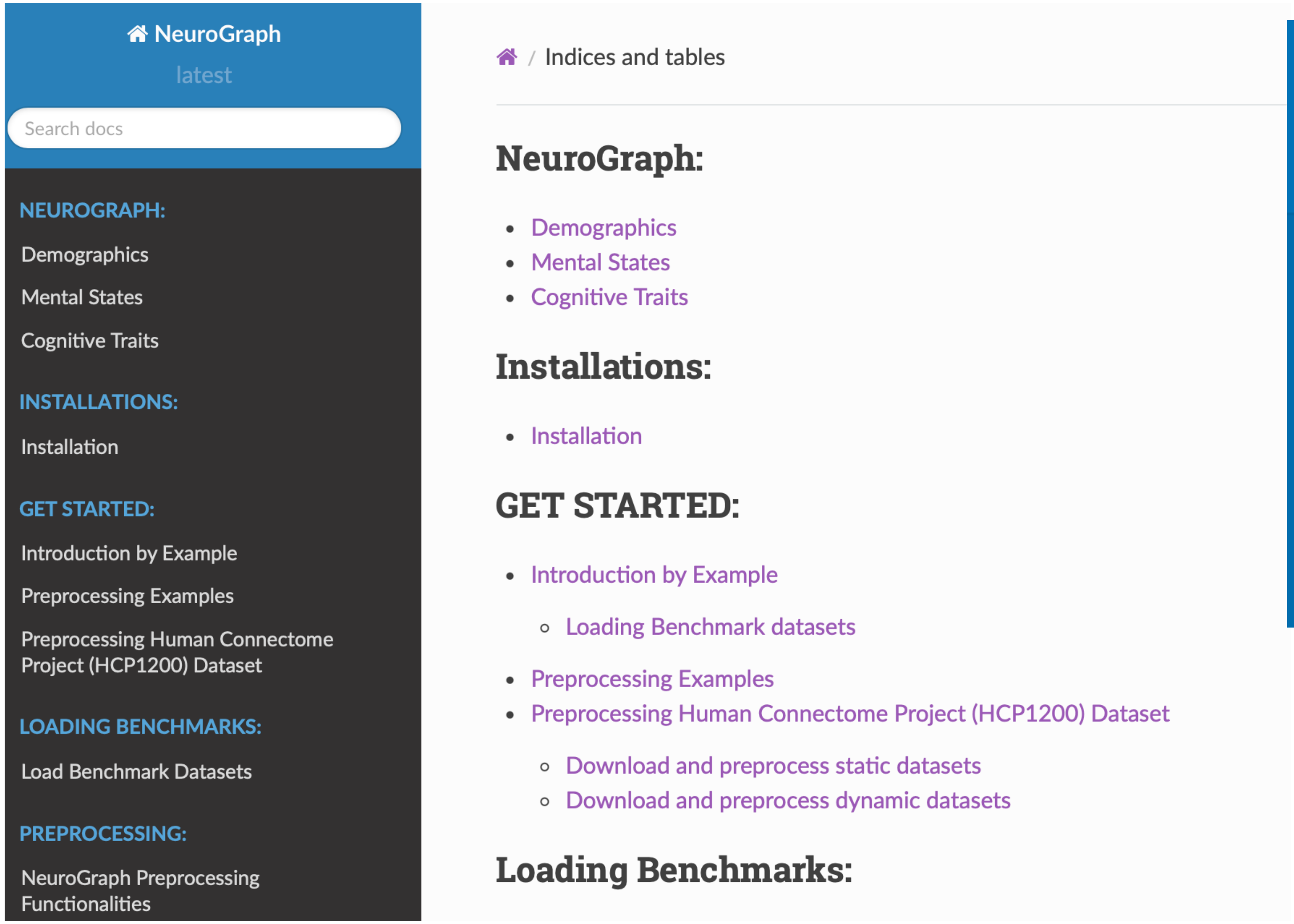
Static Datasets

- HCP-Task dataset
- HCP-Gender dataset
- HCP-Age dataset
- HCP-FI dataset
- HCP-WM dataset

Dynamic Datasets

- DynHCP-Task dataset
- DynHCP-Gender dataset
- DynHCP-Age dataset
- DynHCP-FI dataset
- DynHCP-WM dataset

Easy to Preprocess Neuroimaging Datasets



Documentation

Thank You!

Paper

GitHub

NeuroGraph: Benchmarks for Graph Machine Learning in Brain Connectomics

Paper: https://arxiv.org/abs/2306.06202
GitHub: https://github.com/Anwar-Said/NeuroGraph

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