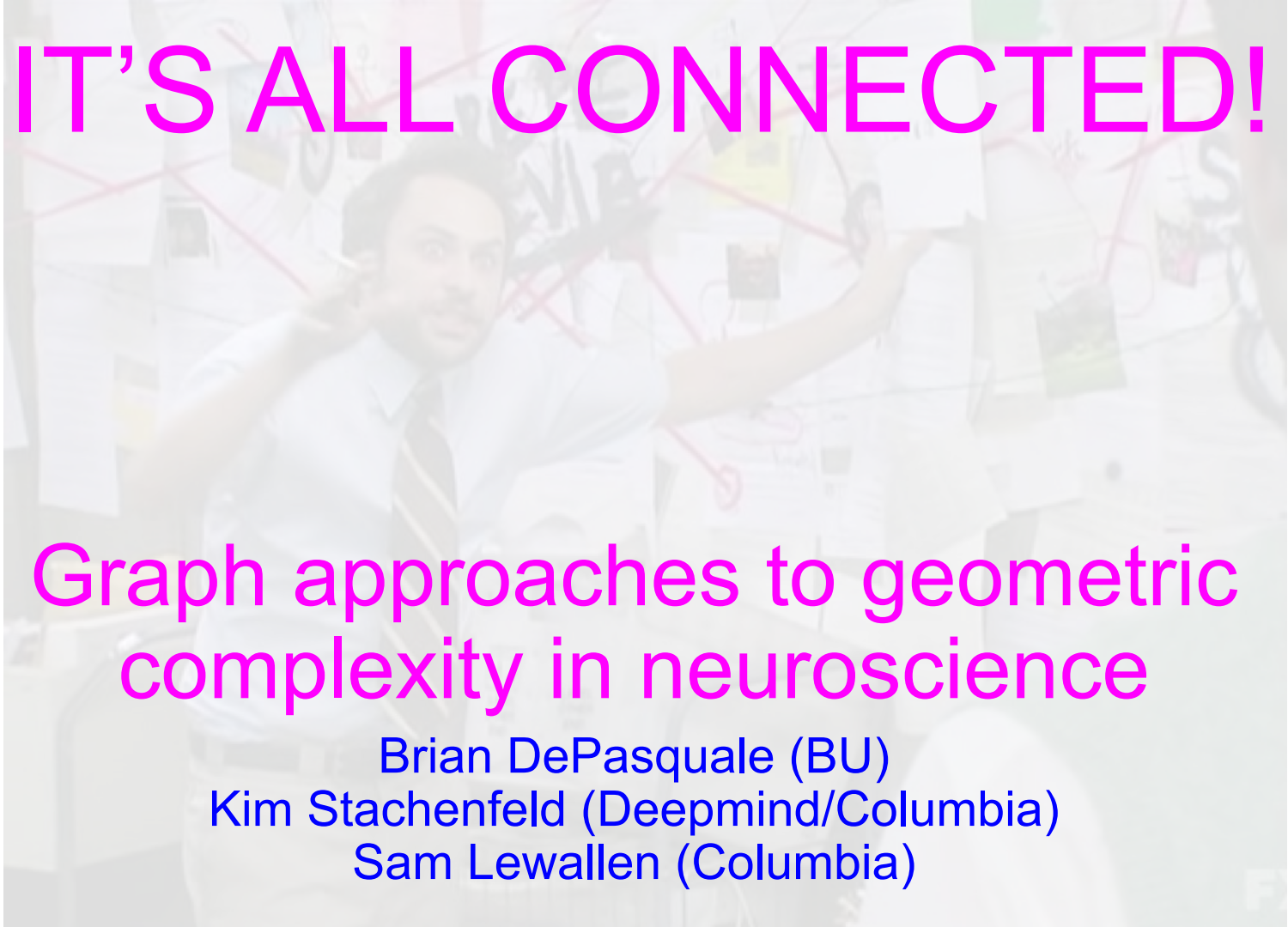


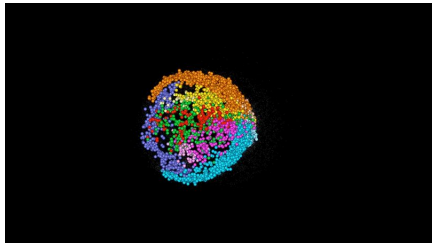
IT'S ALL CONNECTED!

Graph approaches to geometric complexity in neuroscience

Brian DePasquale (BU)
Kim Stachenfeld (Deepmind/Columbia)
Sam Lewallen (Columbia)

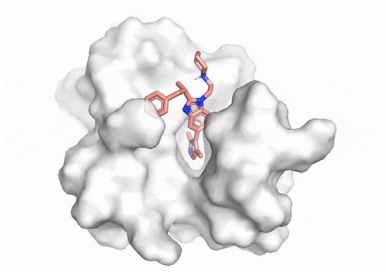
Geometrically complex data are *everywhere* in biology

Development



McDole et al 2018

Biochemistry



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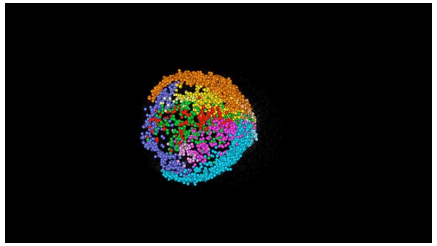
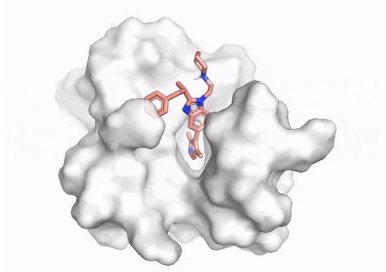


McDole et al 2018

Neural Dynamics

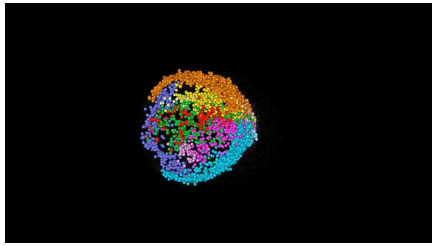
Biochemistry



Connectomics

Geometrically complex data are *everywhere* in biology

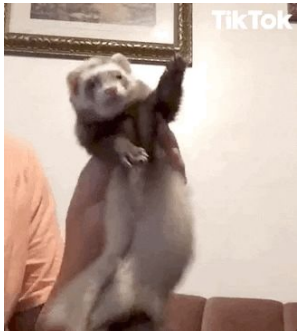
Development



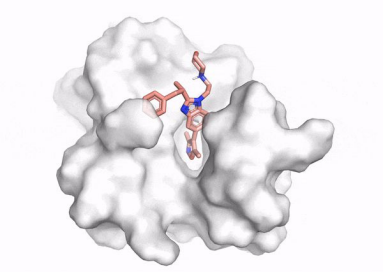
McDole et al 2018

Neural Dynamics

Biomechanics

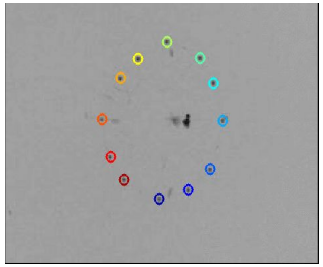


Biochemistry



Connectomics

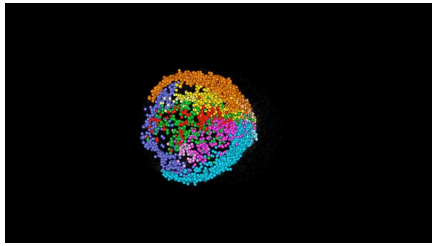
Behavior keypoints



Courtesy of Brady Weissbourd (MIT)

Geometrically complex data are *everywhere* in biology

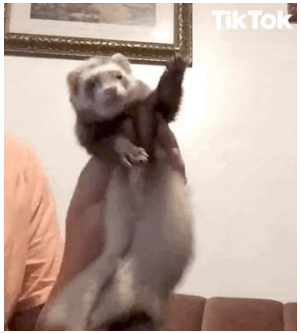
Development



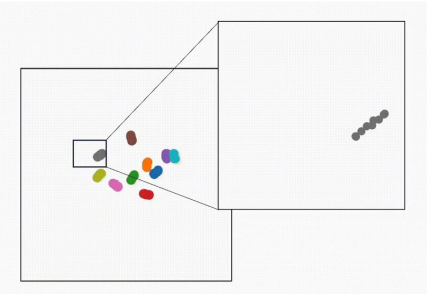
McDole et al 2018

Neural Dynamics

Biomechanics

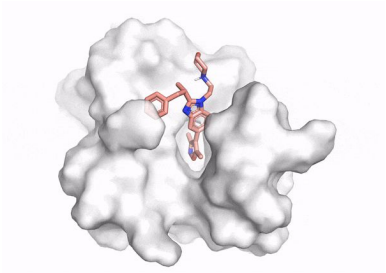


Multiagent behavior



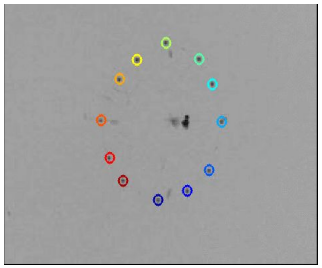
Courtesy of Matt Lovett-Barron (UCSD) and Grant McConachie (BU)

Biochemistry



Connectomics

Behavior keypoints



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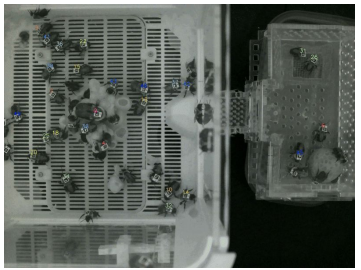
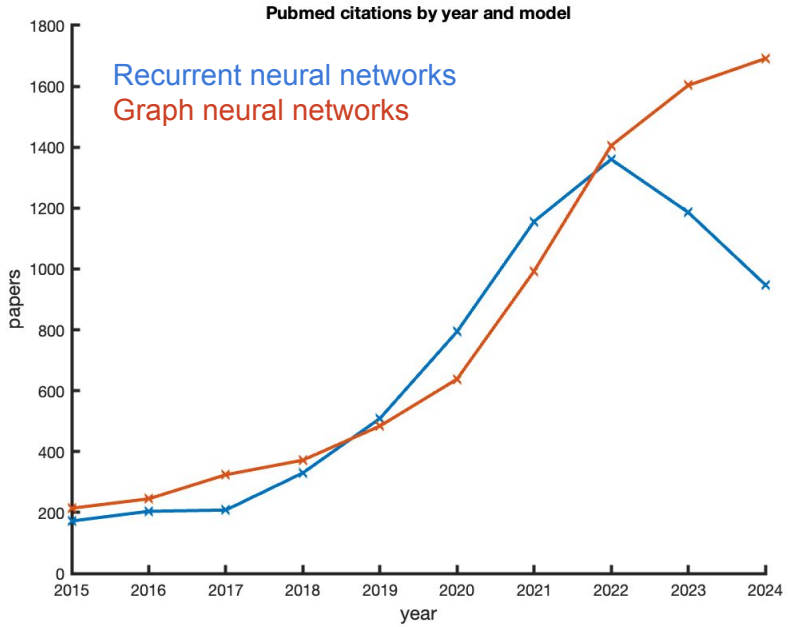
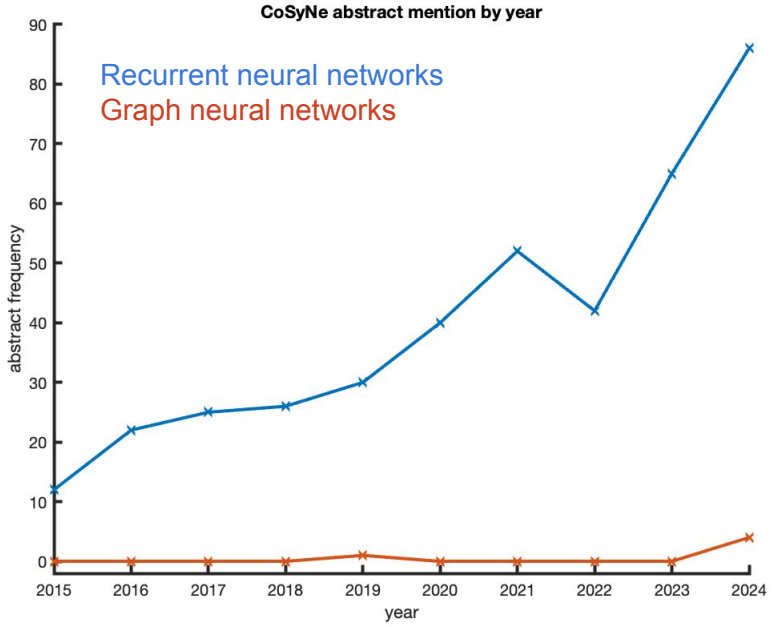


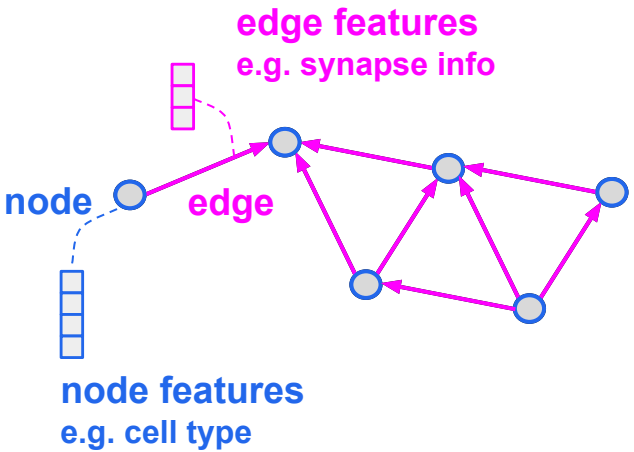
Courtesy of James Crall (Wisc-Mad)

Something is rotten in the state of CoSyNe





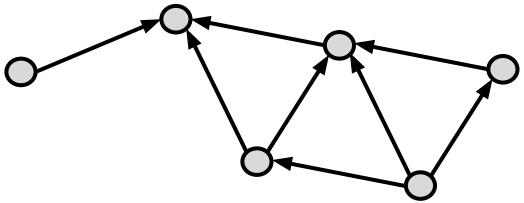
What are Graph Neural Networks?



“Neural networks that operate over graph structured data”

What are Graph Neural Networks?

Graph Neural Network



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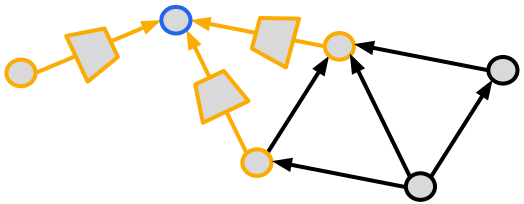
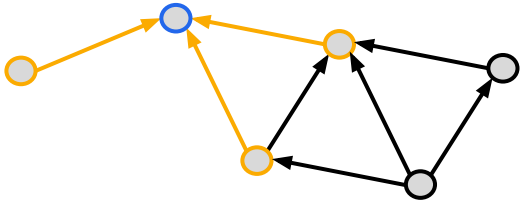


Local, Equivariant, Relational

“Neural networks that operate over graph structured data”

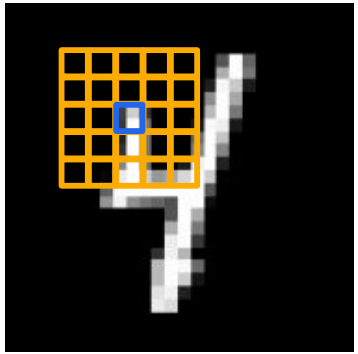
What are Graph Neural Networks?

Graph Neural Network



Local, Equivariant, Relational

Convolutional Neural Network

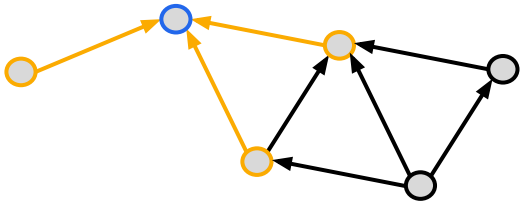


Local, Equivariant, ~~Relational~~

GNNs v. CNNs

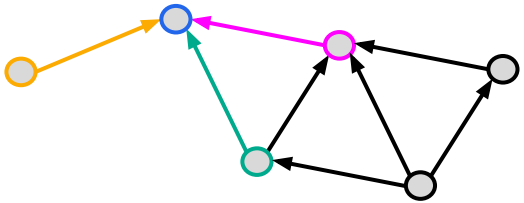
What are Graph Neural Networks?

Graph Neural Network



Local, Equivariant, Relational

RNNs

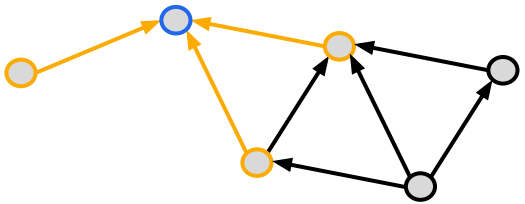


Local, ~~Equivariant,~~ Relational

GNNs v. RNNs

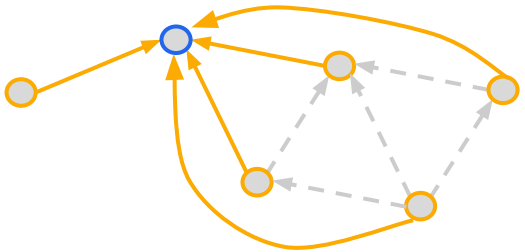
What are Graph Neural Networks?

Graph Neural Network



Local, Equivariant, Relational

Transformer

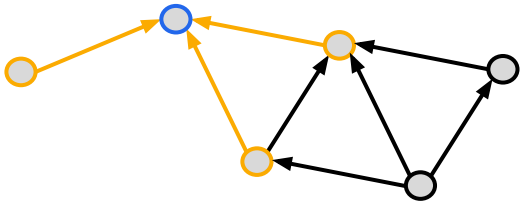


~~Local~~, Equivariant, Relational

GNNs v. transformers

What are Graph Neural Networks?

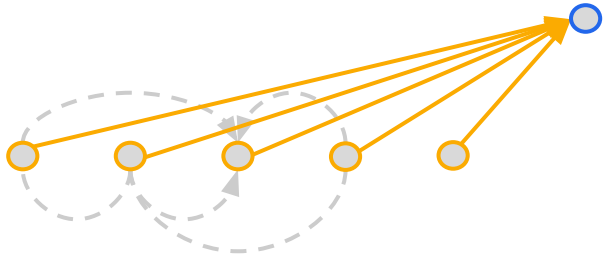
Graph Neural Network



Local, Equivariant, Relational

Transformer

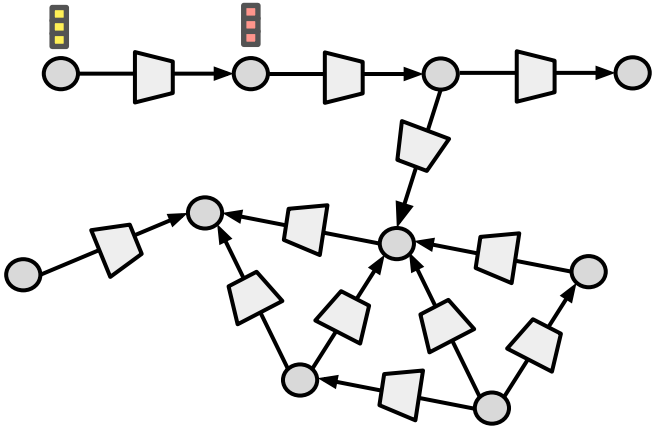
In sequence form



~~Local~~, Equivariant, Relational

GNNs v. transformers

Variable connectivity and size



Can apply the same model to data with variety of structures and sizes

“Local rules applied globally”

“Infinite use of finite means”

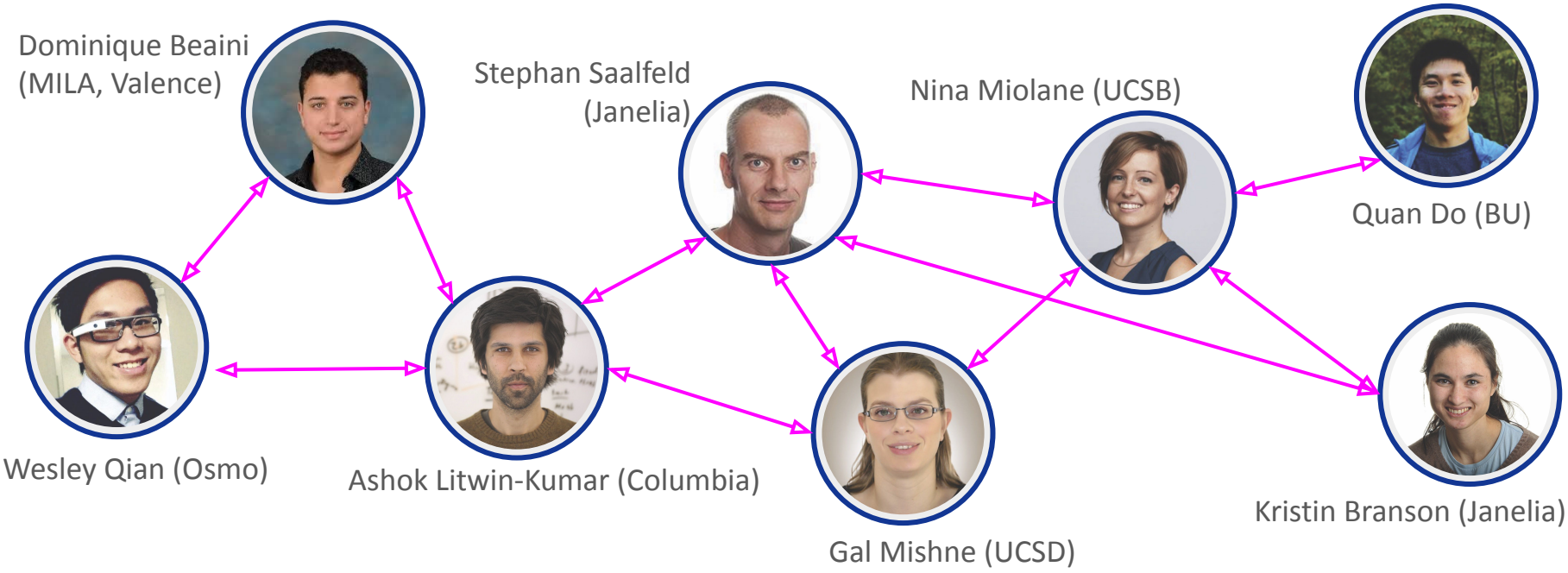
Relate structure to computation

Speakers from all walks of biology

Tiny – connectomes and chemicals

Midsize – neural activity and functional connectivity

Macro – human behavior and collective behavior



Schedule

Morning session

- 9:30 - 9:40: Welcome by Brian, Kim, and Sam
- 9:40 - 10:05: Ashok Litwin-Kumar
- 10:10 - 10:35: Gal Mishne
- 10:40 - 11:05: Quan Do
- 11:10 - 11:30: Coffee break
- 11:30 - 11:55: Wesley Qian
- 12:00 - 12:25: Stephan Saalfeld

Afternoon session

- 3:30 - 4:15: GNN Tutorial in PyTorch Geometric
- 4:15 - 4:40: Nina Miolane (virtual)
- 4:40 - 5:00: Coffee break
- 5:00 - 5:25: Dominique Beaini
- 5:30 - 5:55: Kristin Branson
- 6:00 - 6:30: Discussion (w/ wine!)

WEBSITE: https://sites.google.com/bu.edu/gnnworkshop-cosyne2025/home

ADD DISCUSSION TOPICS TO
THESE SLIDES: https://tinyurl.com/cosyne-gnn-2025-slides

Discussion Topics (please add!)

https://tinyurl.com/cosyne-gnn-2025-slides

Tutorial Time!

https://tinyurl.com/cosyne-gnn-2025

Tutorial Time! (https://tinyurl.com/cosyne-gnn-2025)

- Node classification task – predict the missing labels using knowledge about their neighbors!
- Using FlyWire connectome data, predict the cell labels (central, motor, vision, etc.) using the connectivity
- Get familiar with PyTorch Geometric data
- Visualize graphs with NetworkX
- Understand message passing operation
- Learn a few graph analysis techniques not specific to GNNs
- Try to go further – can neurotransmitter info improve prediction?

Discussion Topics (please add!)

- What neuroscience datasets are most ripe for this analysis?
- Should we build a graph foundation model for collective behavior?
- Are transformers just fully connected Graph Attention Networks? If so, are there appropriate instances where we should not fully connect a graph?

https://tinyurl.com/cosyne-gnn-2025-slides

Discussion Topics (cont.)

- For those with graph data, why aren't you using these methods?
- Related to the question above, when would a GNN be an overkill?
- What barriers exist to getting started?
- If you are a recent convert, what got you excited about these methods?
- An answer to the question above, GNNs are said to be transferable across scales, similar to the odor map talk. Is transferability a forefront consideration for you?
- Let's talk about scaling, bay-bee.
- (re:Ashok's talk): What other symmetries might we want to look for in graphs to tell us something about computation?

Discussion Topics (cont.)

- Anyone looked at similarities/differences in connectomes at different scales (synaptic level, mesoscale, macroscale - MRI ROIs)?
- For those considering GNN for human neuroimage, what are your approaches for defining your nodes?
- A few speakers have mentioned small incomplete datasets. How can the community address this for the most pressing use applications?
- If you read a paper using GNN, what information would you like to see (e.g., how the graph is constructed, how the training is evaluated, which “architectures” are considered, etc.)?