Proposed schedule

GNN foundation:

Groups for the GNN foundation should mainly focus on laying down the basic knowledge and theories of GNN. Require people to prepare with details and thorough understanding of their materials. In this category, the content from different groups might overlap and each group might have more sessions to present.

- 1. Give the background
- 2. Highlight the problems the authors are trying to solve
- 3. Explain the methods / algorithms of the solution including
 - a. math formulas explanation
 - b. Method visualization
 - c. code explanation (if available)
- 4. Conclude presentation with structured key points
- Will select one material for this category and each group will present one section of selected material
- After all sessions, people in the study group should have a deep understanding of the basic knowledge and theories of GNN.

Application: Other Graph Approaches:

Groups for Graph deep learning models should provide an overview of selected GNN approaches with following key points:

- 1. Reason the origin and background of model
- 2. Explain the core/novel algorithms
 - a. Necessary math formulas explanation
 - b. Novel algorithms vitalization
- 3. Illustrate applications of the models, highlighting pros/cons with examples
- After all sessions, people in the group should have an overall picture of various GNN approaches and their properties for application.
- People should pick up their interested model and collect their own materials.

Suggested material for Foundation (Important!):

1. Bronstein (2017)

This is a long paper with lots of math. It's gonna take some time. Everyone should study it and we assign one section per group. The main sections are 3 -> 8. Sections **III** and **IV** are the theoretical foundations, and would require somebody more experienced.

- a. III. DEEP LEARNING ON EUCLIDEAN DOMAINS
- b. IV. THE GEOMETRY OF MANIFOLDS AND GRAPHS
- c. V. SPECTRAL METHODS
- d. VI. SPECTRUM-FREE METHODS
- e. VII. CHARTING-BASED METHODS [not sure if we'll need this]
- f. VIII. COMBINED SPATIAL/SPECTRAL METHODS [not sure if we'll need this]

2. Relational inductive biases, deep learning, and graph networks (2018)

This paper describes key design principles for building powerful graph architectures using graph networks framework as example with entity- and relation-based reasoning. This paper contains open-source library for building graph networks.

- Relational inductive biases (Fully connected layers / convolutional layers / recurrent layers)
- b. Graph networks block (graph basis / internal structure / computational steps / Relational inductive biases in GN)
- c. Design principles for GN (attributes / graph structure)

3. Chami (2020)

This paper uses Graph Encoder Decoder Model as entry to go through Unsupervised and surprised Graph embedding schemes with comprehensive taxonomy. It might cover too much content and might need to be subsetted.

- a. Intro & preliminaries
- b. The GRAPHEDM framework (objective function / Encoders)
- c. Unsupervised embedding (auto encoder / Graph neural networks)
- d. Supervised embedding (graph regularization / graph convolution framework / spectral / spatial convolutions)

Suggested material for Application:

- 1. Graph convolutional networks: a comprehensive review by Zhang S (2019)
- 2. <u>deep convolutional networks on graph-structured data</u>
- Original GNN model <u>https://persagen.com/files/misc/scarselli2009graph.pdf</u>
- 4. Methods preceding modern GNN models:

https://arxiv.org/abs/1403.6652 https://cs.stanford.edu/~jure/pubs/node2vec-kdd16.pdf

Initial spectral approaches: https://arxiv.org/pdf/1606.09375.pdf

Graph Convolutinal Network: https://arxiv.org/abs/1609.02907

7. Graph Attention Network: https://arxiv.org/abs/1710.10903

8. WL-test and isomorphism approaches: https://arxiv.org/abs/1810.00826

 Benchmarkin, which also gives a good overview of SOTA: https://arxiv.org/abs/2003.00982

10. For different approaches I found this to be an interesting analogy: https://twitter.com/dom_beaini/status/1499019741234704385

Collected Materials