MSc projects 2024

UCL LASP

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Introduction

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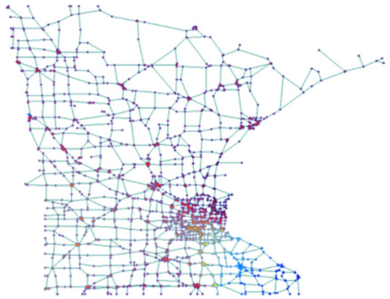
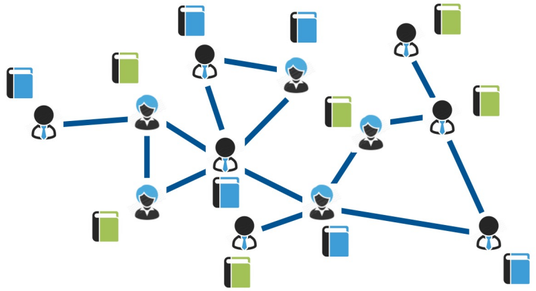
- **Our Research - Graph**
  - A powerful and ubiquitous representation of complex data in many network systems
  - A graph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$ consists of a set of nodes $\mathcal{V} = \{v_i\}_{i\in[N]}$, a set of edges $\mathcal{E} = \{e_{ij}\}$
- **Graph-structured Data are Pervasive**

Traffic Networks



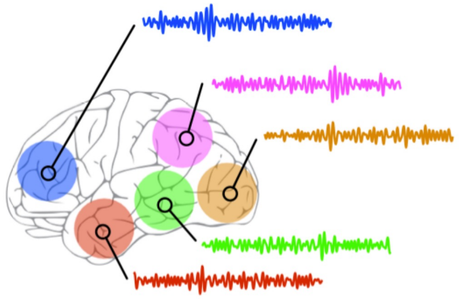
congestion in road junctions



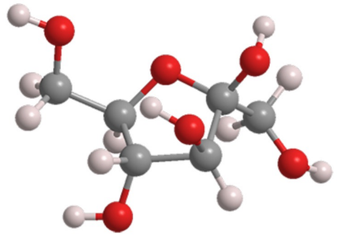
preferences of individuals

Social Networks

Brain



activities in brain regions



properties of atoms

Molecules

Graph Machine Learning

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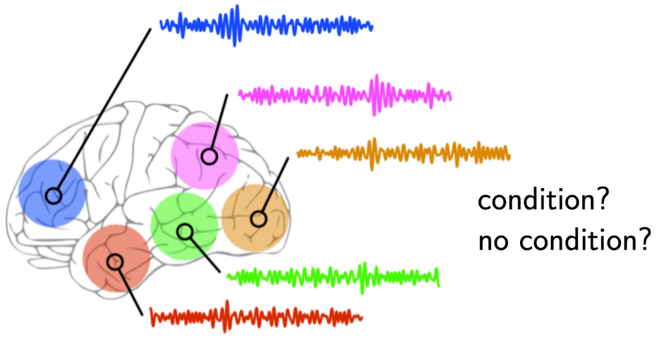
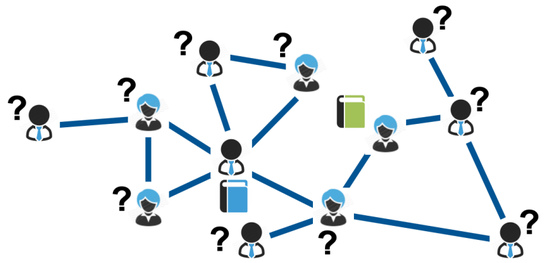
❖ Machine Learning on Graphs

- Graph-level tasks: predict a label $y_{\mathcal{G}}$, given Graph $\mathcal{G}$ and Node Features $\{X_i\}_{i\in[N]}$
- Node-level tasks: predict a label y_i for node v_i, given graph $\mathcal{G}$ and $\{X_i\}_{i\in[N]}$



graph-level classification (supervised)

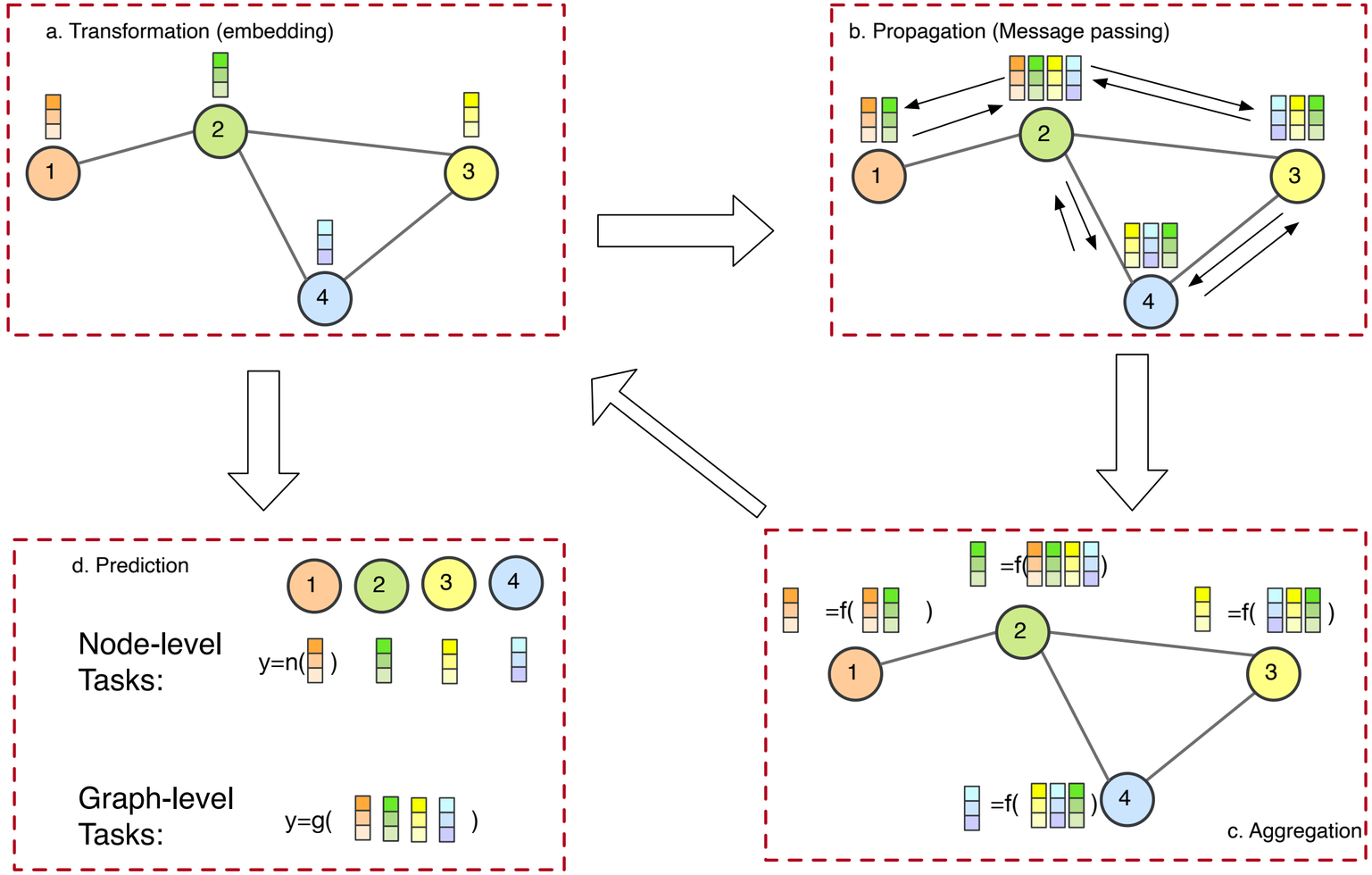


node-level classification (semi-supervised)

❖ The models for GML - Graph Neural Networks

The Model

- **Graph Neural Networks (GNNs)**
  - a. Transformation
  - b. Propagation
  - c. Aggregation
  - d. Prediction



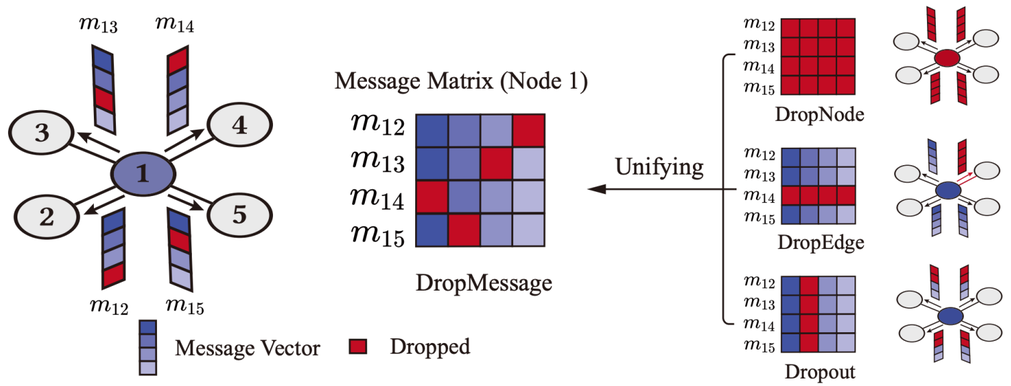
Projects

❖ Understanding Dropout in GNNs from a Bayesian Approach

- Analogous to dropout in Neural networks [1], randomly deactivating nodes/edges in the training graph can improve the generalization ability of GNNs.
- Complex structure of graphs gives different variants of dropping, such as dropout on nodes [2,3,4], edges [5], message [6], but most of them are empirical studies.
- The project wishes to answer:

  - What is the statistical framework unifying those variants?

  - How will model behavior be influenced by these methods?

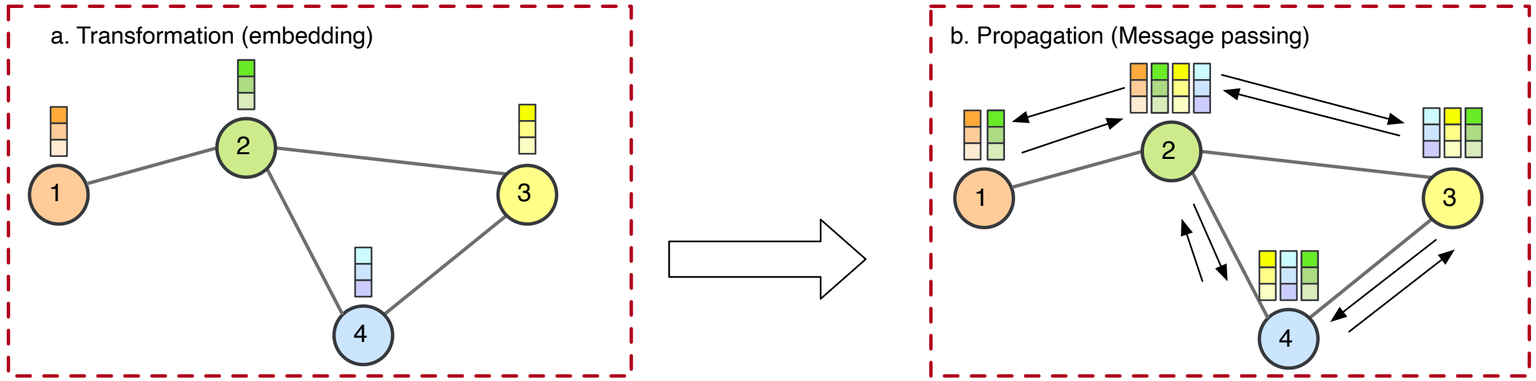


Projects

❖ Graph Neural Networks with Adaptive Architecture

- The requirement of Feature Transformations (T) and Message Propagation (P) depends both on the tasks and data properties of graphs [7],
- We do not have prior information about data properties, and in large-scale graphs, different subgraphs could even exhibit different data patterns [8].
- GNN models with fixed T-P architecture cannot achieve satisfactory performance
- This project aims at making GNN adaptive by:

  - Utilizing the prompt learning and in-context learning in large language models.



References

[1] Srivastava, N., Hinton, G. E., Krizhevsky, A., Sutskever, I., and Salakhutdinov, R. Dropout: a simple way to prevent neural networks from overfitting. J. Mach. Learn. Res. 15, 1 (2014), 1929–1958.

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[4] Huang, W., Zhang, T., Rong, Y., and Huang, J. Adaptive sampling towards fast graph representation learning. In Advances in Neural Information Processing Systems (NeurIPS 2018), pp. 4563–4572.

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[7] Mao, H., Chen, Z., Jin, W., Han, H., Ma, Y., Zhao, T., Shah, N., and Tang, J. Demystifying structural disparity in graph neural networks: Can one size fit all? In Advances in Neural Information Processing Systems (NeurIPS 2023).

[8] Mao, H., Li, J., Shomer, H., Li, B., Fan, W., Ma, Y., Zhao, T., Shah, N., and Tang, J. Revisiting link prediction: A data perspective. CoRR abs/2310.00793 (2023).

Interested?

- **We also have other projects related to reinforcement learning**
- **You are welcome to bring your own ideas.**
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