# MSc projects 2024

UCL LASP

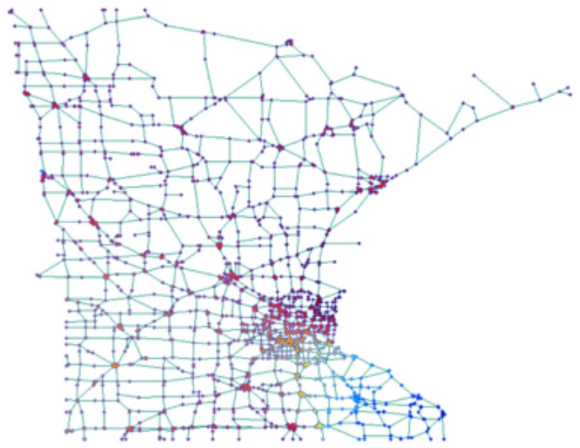
By Dr. Laura Toni

Presenter: Keyue Jiang

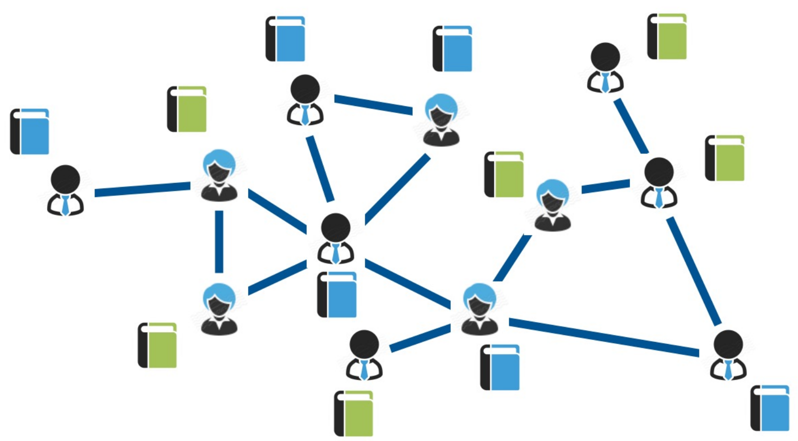
# Introduction

- **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



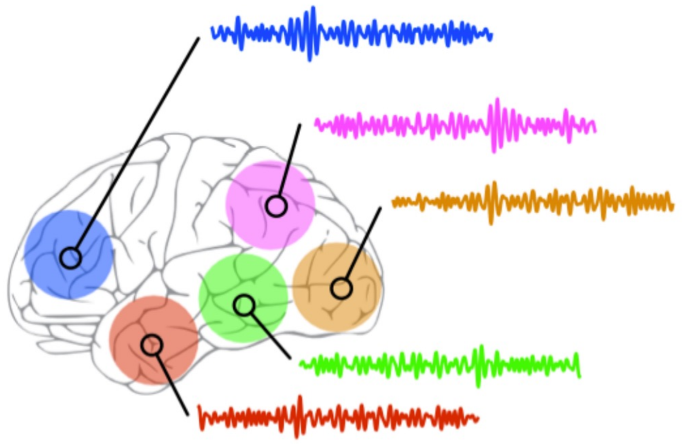
congestion in road junctions



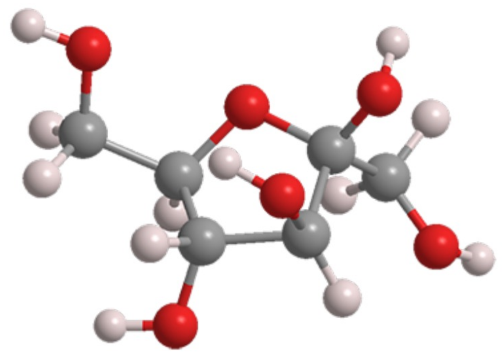
preferences of individuals

Social Networks

Brain



activities in brain regions



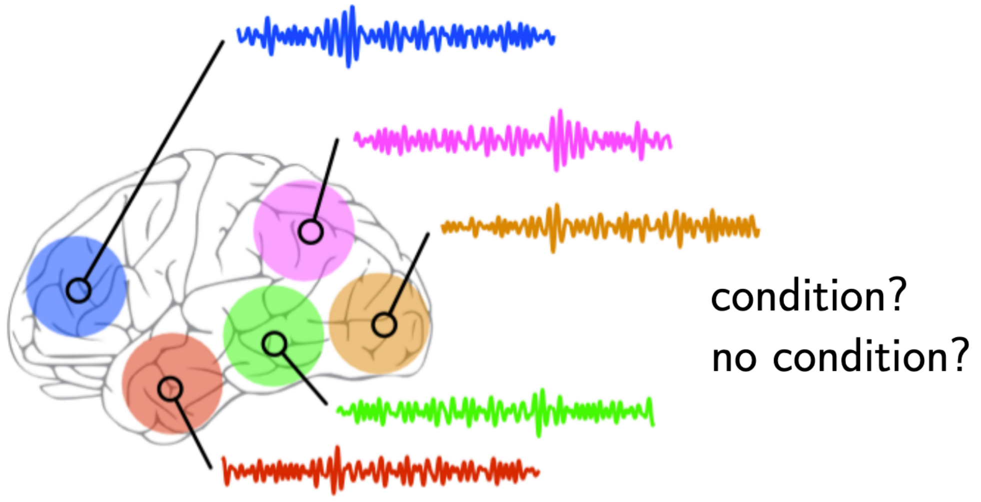
properties of atoms

Molecules

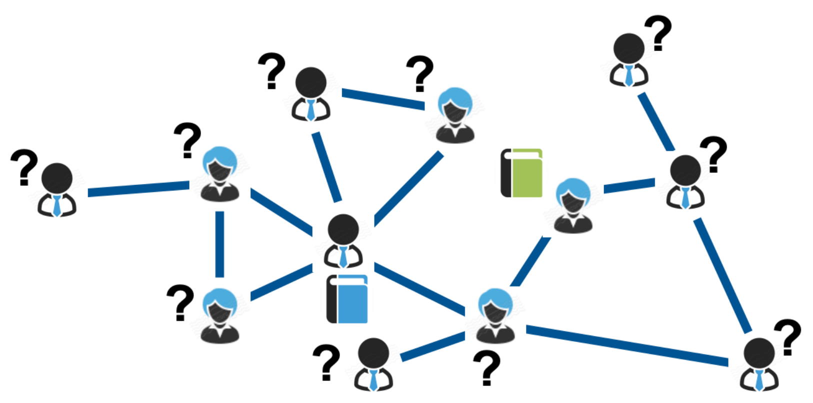
# Graph Machine Learning

UCL

- **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)**

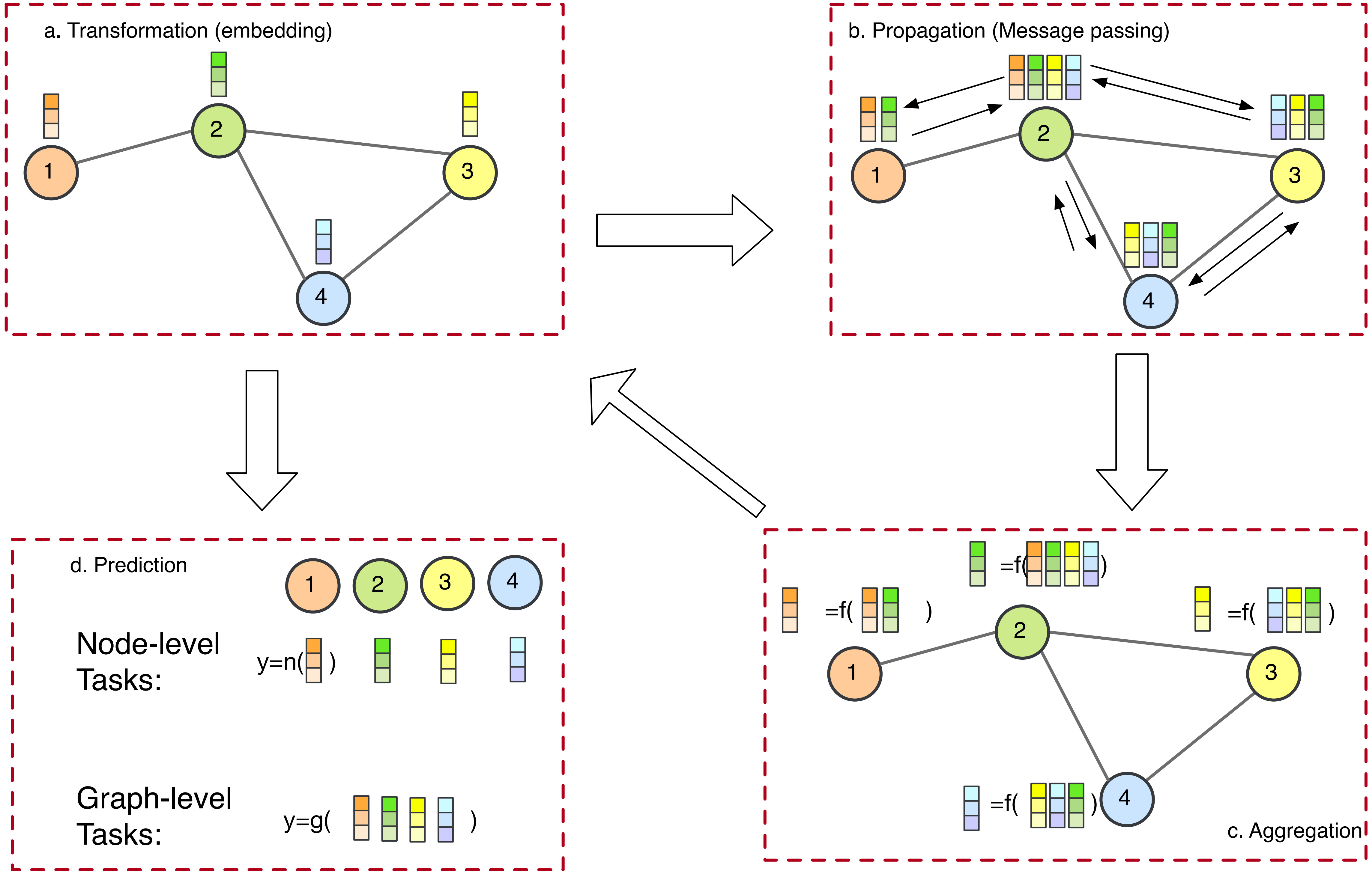



**node-level classification (semi-supervised)**

- **The models for GML - Graph Neural Networks**

# The Model

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



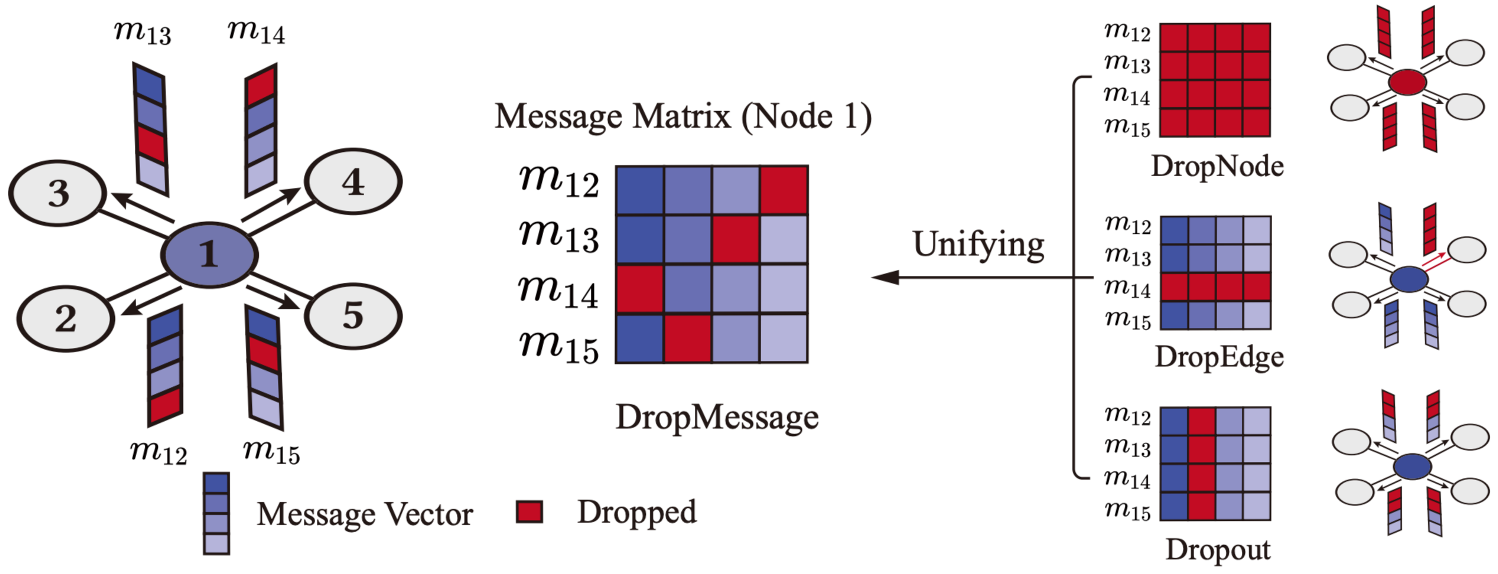
# Projects

❖ **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? (e.g. generalizability)

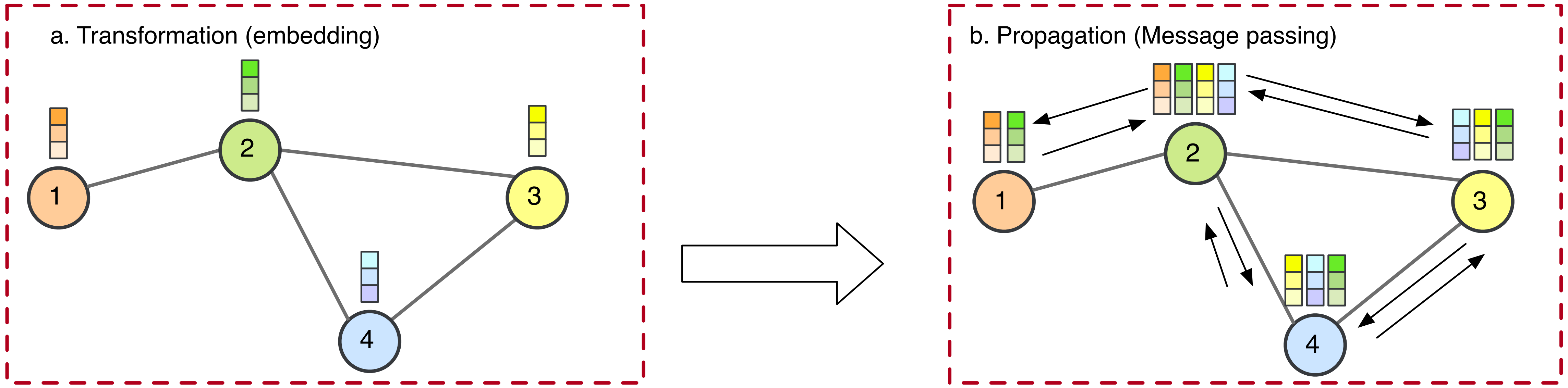


# Projects

## ❖ 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.



# Reinforcement Learning

- Direction 1: **Autocurricula and intrinsic rewards**
- Goals of the project:
    - Investigating the **effect of different intrinsic rewards** in **MiniMax** Baseline (Unsupervised environment design)
    - Understanding if **behavioural diversity** can help exploration in Amaze navigation benchmark

- Direction 2: **Learning diverse skills**
- Goals of the project:
    - Maximizing the diversity of skills by using **F-divergence** between skills instead of a discriminator
    - Investigating whether **incorporating LLMs** into an intrinsic reward can help distinguish various skills

# Multi-target conditional molecule generation

- Drugs that are active on **multiple target** genes have the potential to **treat complex diseases**.
- Many single-target generative models have been presented.
- A **gap** remains in the domain of multi-target generation.

- **Goals of the project:**
  - Explore the **literature** of multi-target conditioning
  - Construct a **graph-based molecule generative model** that can produce molecules **active on two or more targets**.

# 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.
[2] Chen, J., Ma, T., and Xiao, C. Fastgcn: Fast learning with graph convolutional networks via importance sampling. In ICLR (Poster) (2018),
[3] Hamilton, W. L., Ying, Z., and Leskovec, J. Inductive representation learning on large graphs. In Advances in Neural Information Processing Systems (2017)
[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.
[5] Papp, P. A., Martinkus, K., Faber, L., and Wattenhofer, R. Dropgnn: Random dropouts increase the expressiveness of graph neural networks. In In Advances in Neural Information Processing Systems (NeurIPS 2021), pp. 21997–22009.
[6] Fang, T., Xiao, Z., 0001, C. W., Xu, J., Yang, X., and 0009, Y. Y. Dropmessage: Unifying random dropping for graph neural networks. In Thirty-Seventh AAAI Conference on Artificial Intelligence, AAAI 2023.
[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 (in the pdf)**
- **You are welcome to bring your own ideas.**
- **Contact**
  - Dr. Laura Toni (l.toni@ucl.ac.uk), Keyue Jiang (keyue.jiang.18@ucl.ac.uk)

# Other projects

UCL

- **Reinforcement Learning**
  - The impact of different intrinsic rewards on the exploration behavior in MiniMax baseline for AutoCurricula:
  - Maximizing the divergence between skills in RL
  - The impact of time: lifetime as governing reward In RL
  - NAVIX: Accelerated minigrid environments with JAX
- **Drug Discovery**
  - Multi-target conditional molecule generation