Data-centric Graph Machine Learning

By Dr. Laura Toni

Presenter: Keyue Jiang

Introduction

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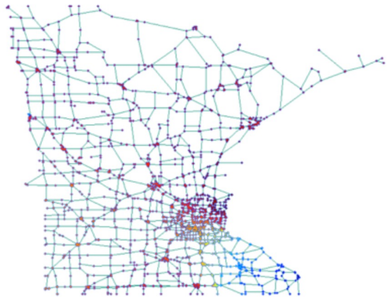
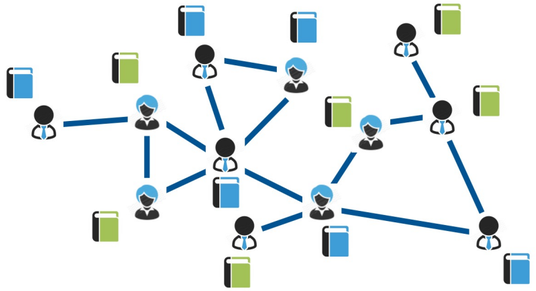
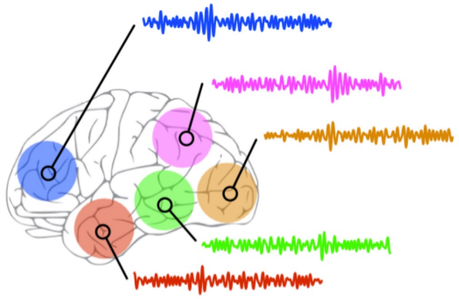
- **Graph**
  - A powerful and ubiquitous representation of complex data in many network systems
  - A graph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$ consists of a set of nodes $\mathcal{V} = \{v_i\}_{i\in[N]}$, a set of edges $\mathcal{E} = \{e_{ij}\}$
- **Graph-structured Data are Pervasive**



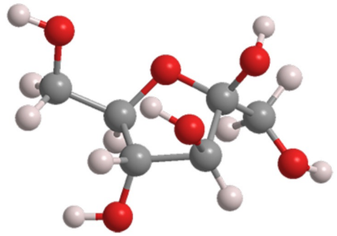
congestion in road junctions



preferences of individuals



activities in brain regions



properties of atoms

Graph Machine Learning

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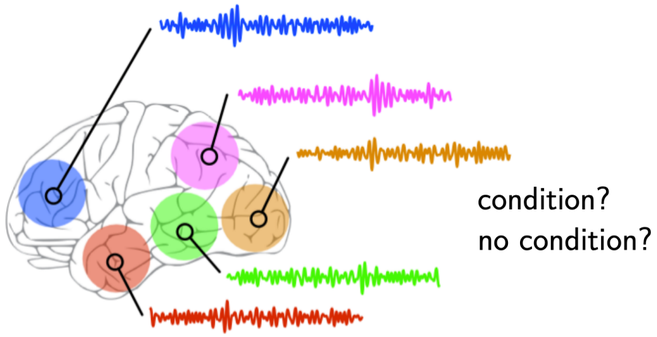
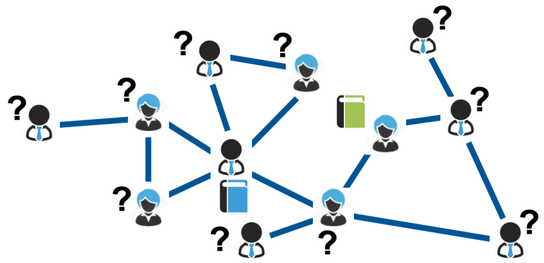
❖ Machine Learning on Graphs

- 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

Graph Neural Networks

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❖ Machine Learning on Graphs

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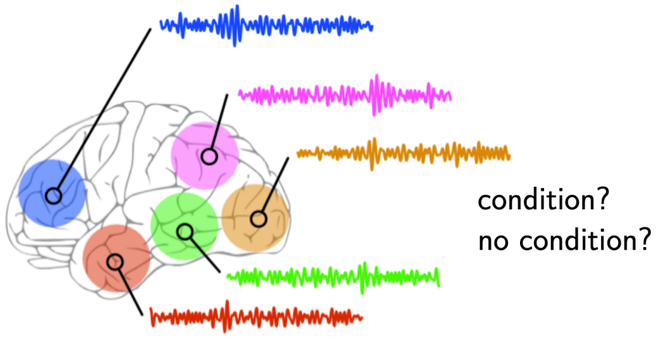
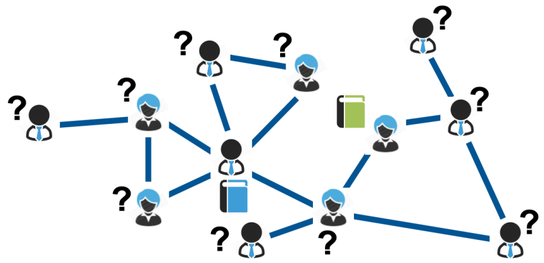


graph-level classification (supervised)



node-level classification (semi-supervised)

Projects

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- **Understanding Dropout in Graphs Neural Networks from a Bayesian Approach**
  - Graph-level tasks: predict a label $y_{\mathcal{G}}$, given Graph $\mathcal{G}$ and Node Features $\{X_i\}_{i\in[N]}$

Projects

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- **Graph Neural Networks with Adaptive Architecture**
  - Graph-level tasks: predict a label $y_{\mathcal{G}}$, given Graph $\mathcal{G}$ and Node Features $\{X_i\}_{i \in [N]}$

Graph Machine Learning

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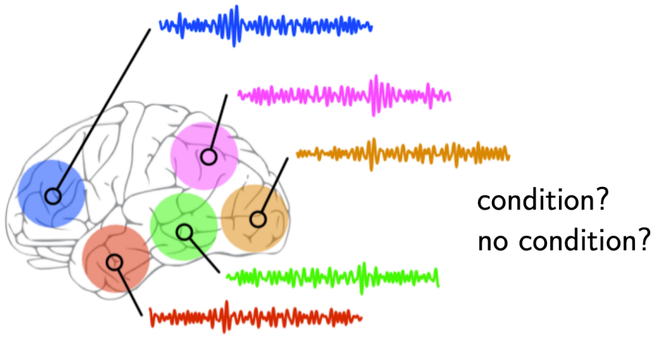
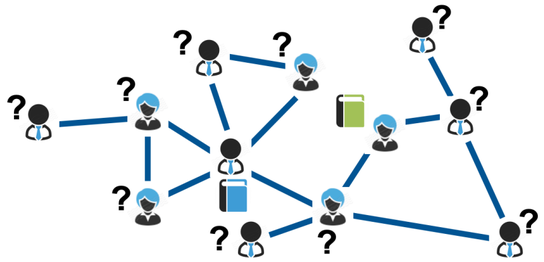
- **Graph**
  - A graph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$ consists of a set of nodes $\mathcal{V} = \{v_i\}_{i\in[N]}$, a set of edges $\mathcal{E} = \{e_{ij}\}$
  - Usually, each node v_i is associated with a feature X_i.
- **Machine Learning on Graphs**
  - Graph-level tasks: predict a label $y_{\mathcal{G}}$, given $\mathcal{G}$ and $\{X_i\}_{i\in[N]}$
  - 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)