AI For Science and Engineering(CS286)

Tutorial 5: Graph Neural Network (GNN)

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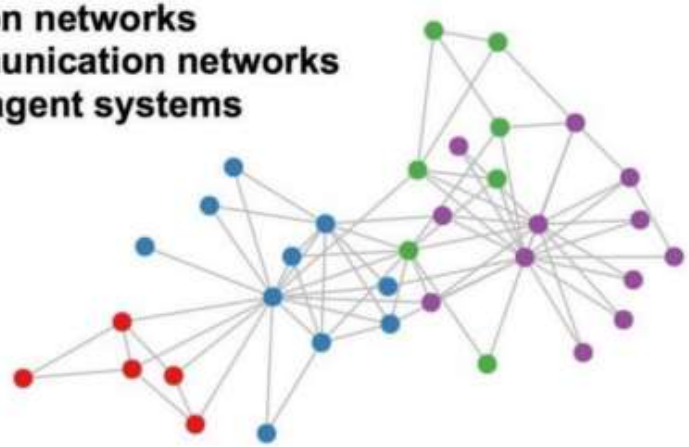
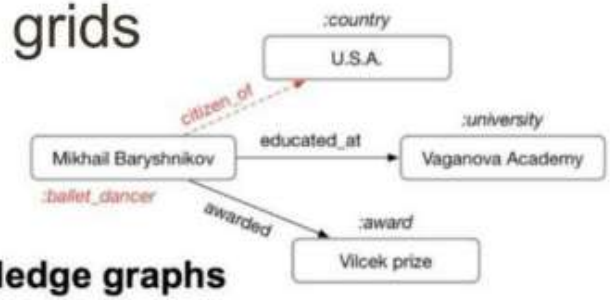
Why we need Graph Neural Networks?

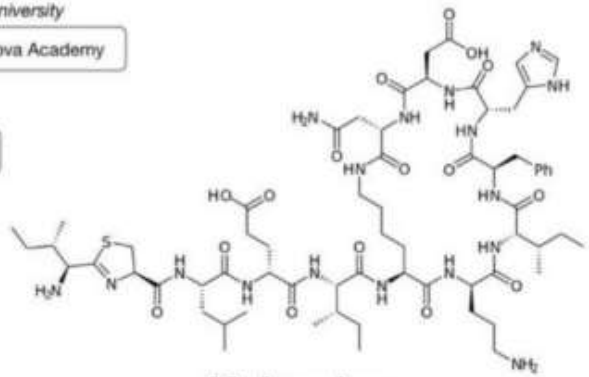
A lot of real-world data does not “live” on grids

Social networks
Citation networks
Communication networks
Multi-agent systems

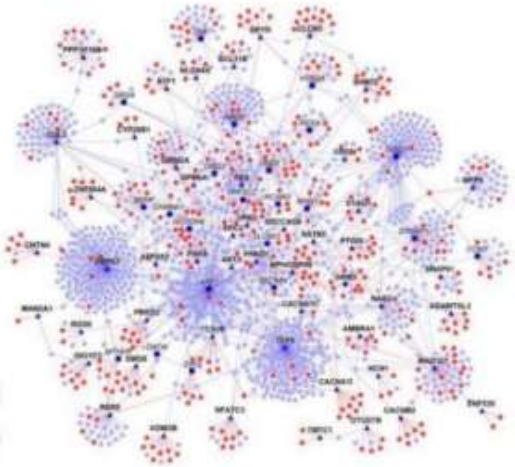




Knowledge graphs



Molecules



Protein interaction networks

Road maps

Standard **CNN** and **RNN** architectures don’t work on this data

Graph Neural Networks (GNN)

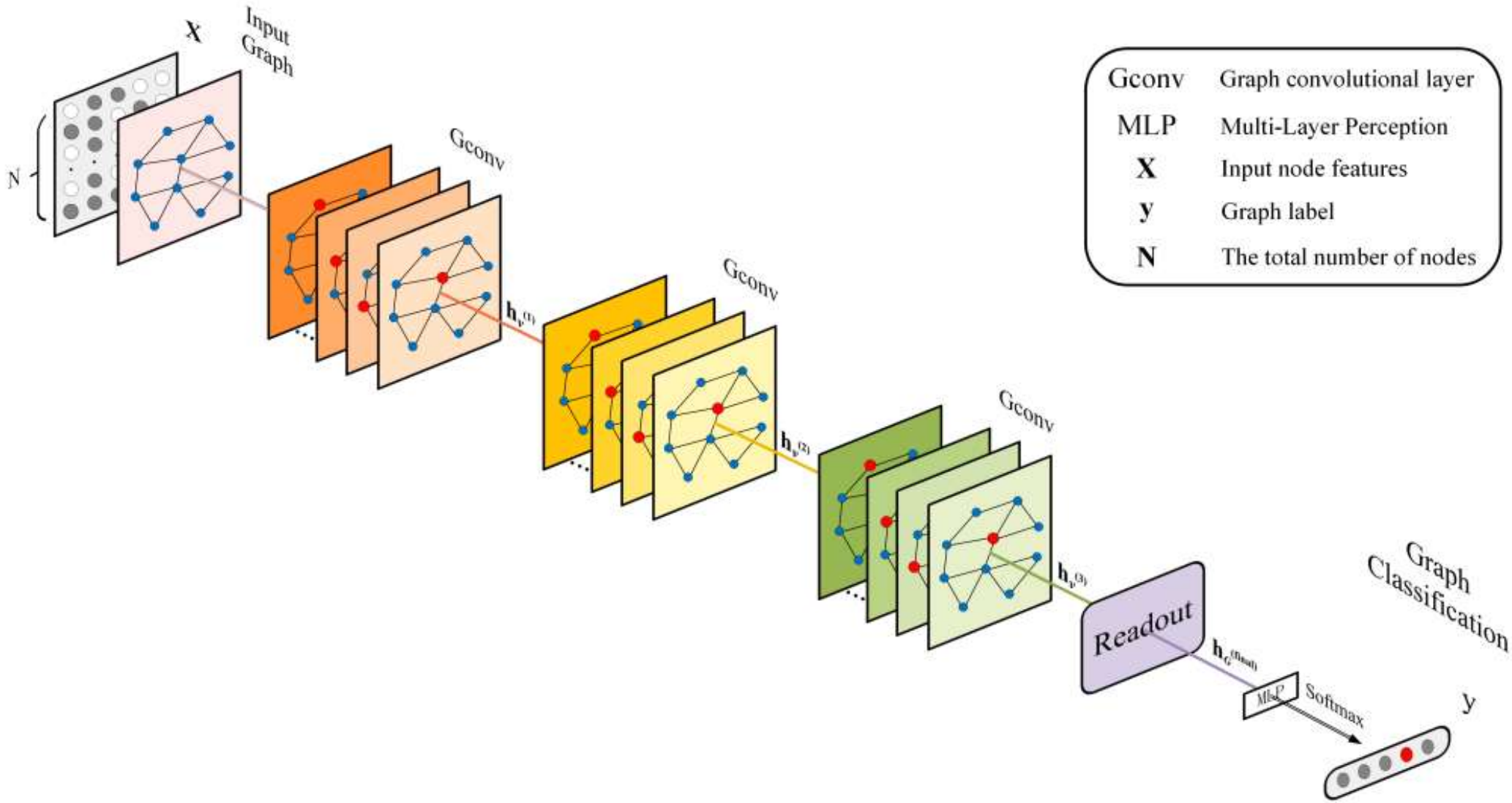
- *Node-level tasks*
  - *Node classification (node type, node properties)*

- *Edge-level tasks*
  - *Link prediction*

  (recommendation system, biomedical interactions)

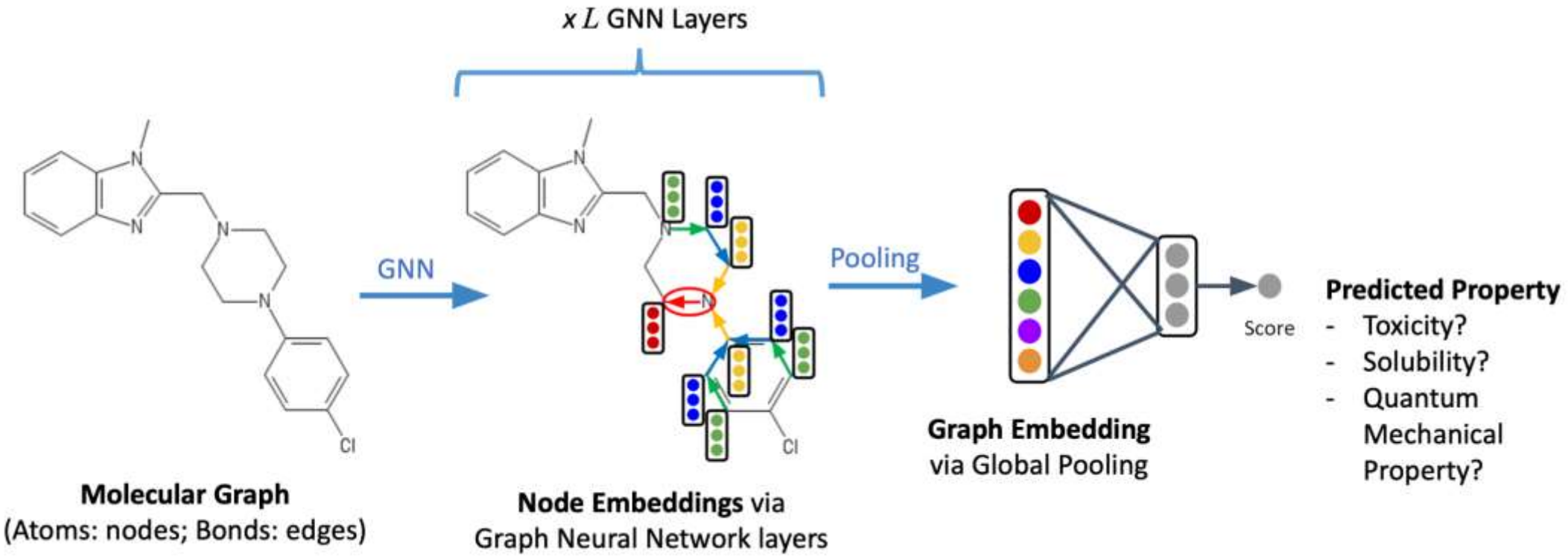
- *Graph-level tasks*
  - *Graph classification (Molecular property prediction)*

Graph Classification



Molecular property prediction

- ***Predicting the properties of a molecule from its structure***



Pytorch Geometric

- *Installation*
  - *conda install pyg -c pyg*
  - *https://pytorch-geometric.readthedocs.io/en/latest/*