IJCAI 2025 Tutorial

Towards Low-Distortion Graph Representation Learning

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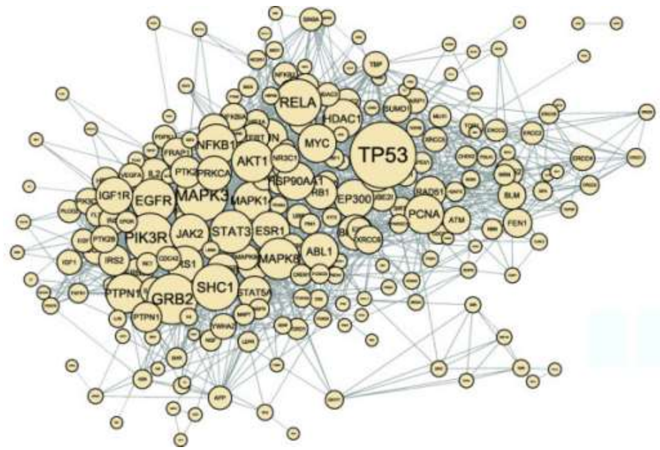
Outline

- Introduction (20min)
- Invariance-guided Graph Representation Learning (40min)
- Information-theoretic Graph Representation Learning (40min)
- Geometry-guided Graph Representation Learning (40min)
- Advanced Directions (30min)
- QA

Networks/Graphs

Social Network



Biology

Logistics

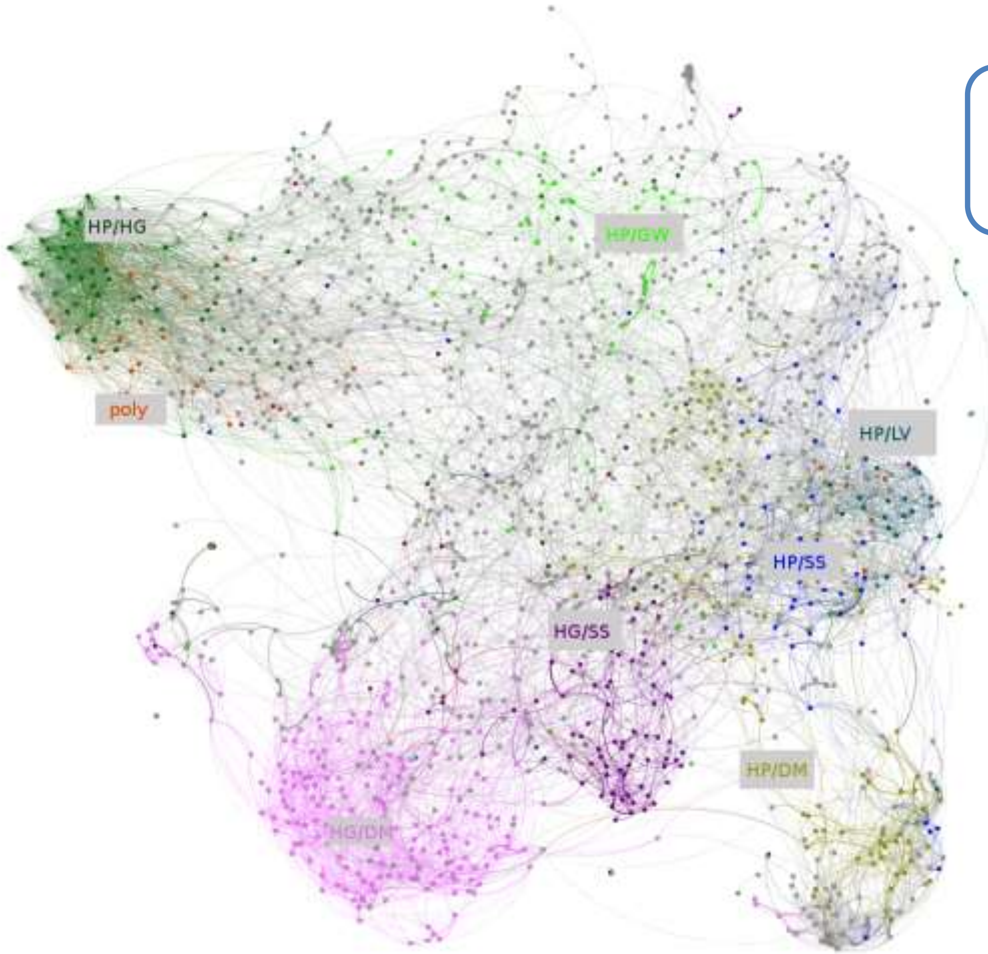
Internet of Things

Transaction

Knowledge Graphs

Picture credit: web search engines

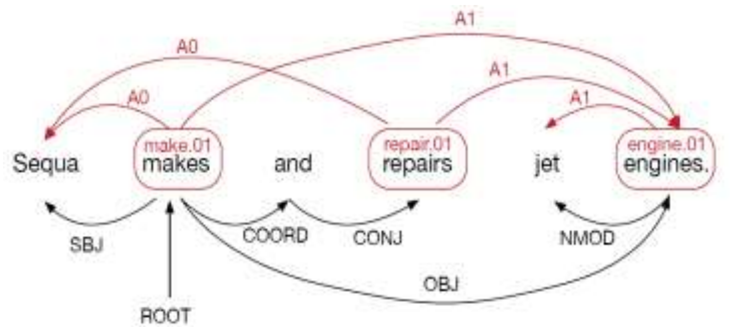
Graph Tasks



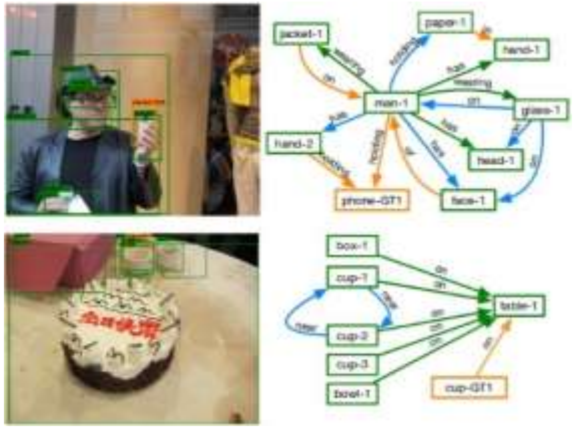
Descriptive and Predictive

- Node classification
- Link prediction
- Graph Classification
- Node importance
- Community detection
- Network distance
- Network evolution
- …

Graph Applications in Computer Science

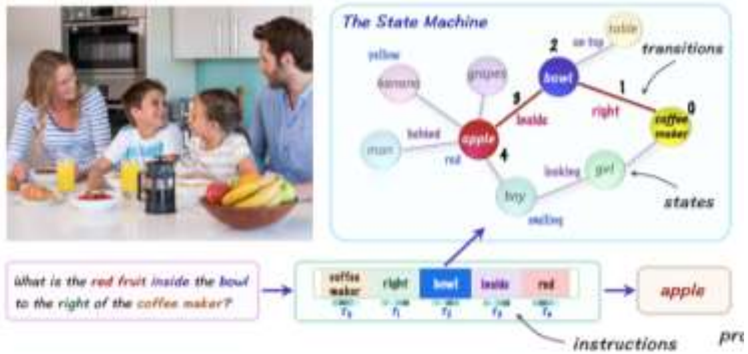


Natural Language Processing



Computer Vision

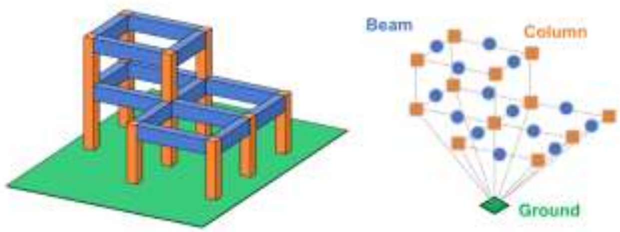
Data Mining



Multimedia

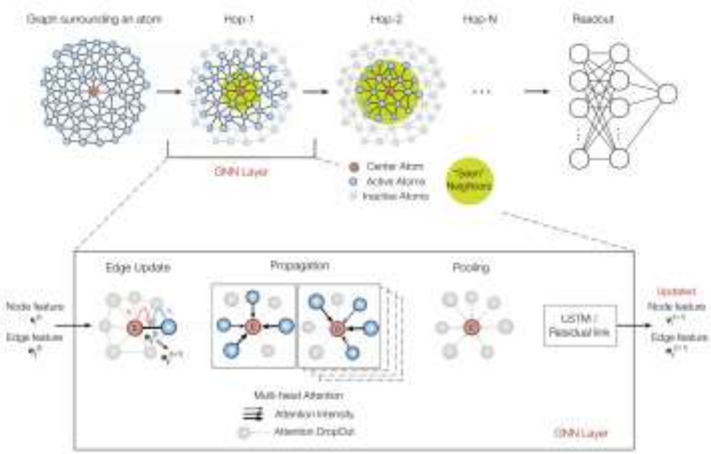
Encoding Sentences with Graph Convolutional Networks for Semantic Role Labeling, *EMNLP 2017*
Neural Motifs: Scene Graph Parsing with Global Context, *CVPR 2018*
Learning by Abstraction: The Neural State Machine. *NeurIPS 2019*

Graph Applications beyond Computer Science

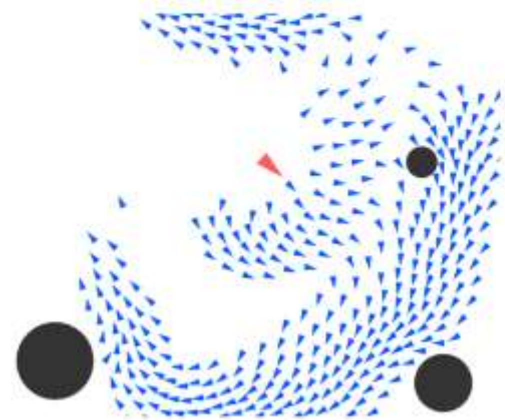


Structural Engineering

Drug repurposing for Covid-19



Material Science

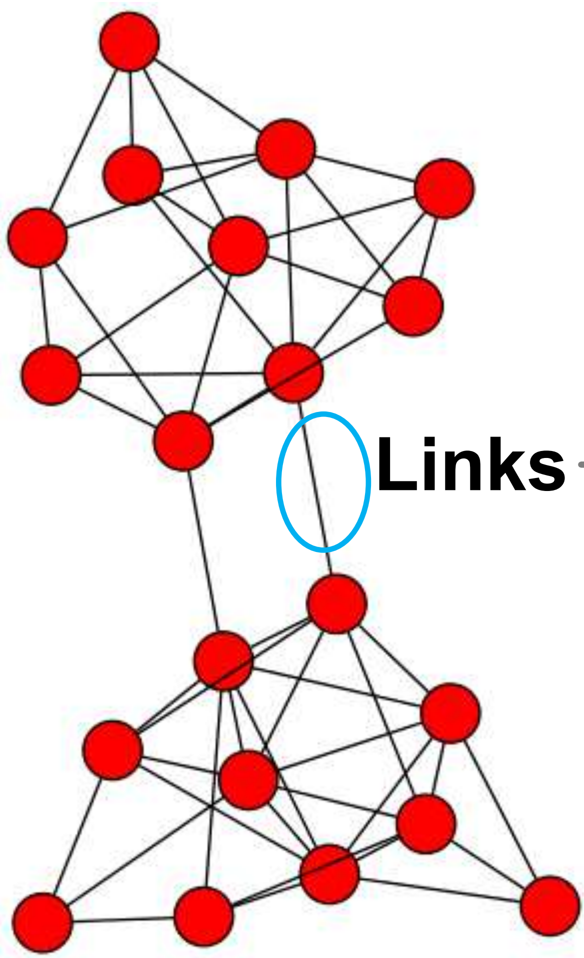


Physical Simulation

Graph is a common and general tool for modeling relational data!

Graph Machine Learning is Challenging

G = (V, E)



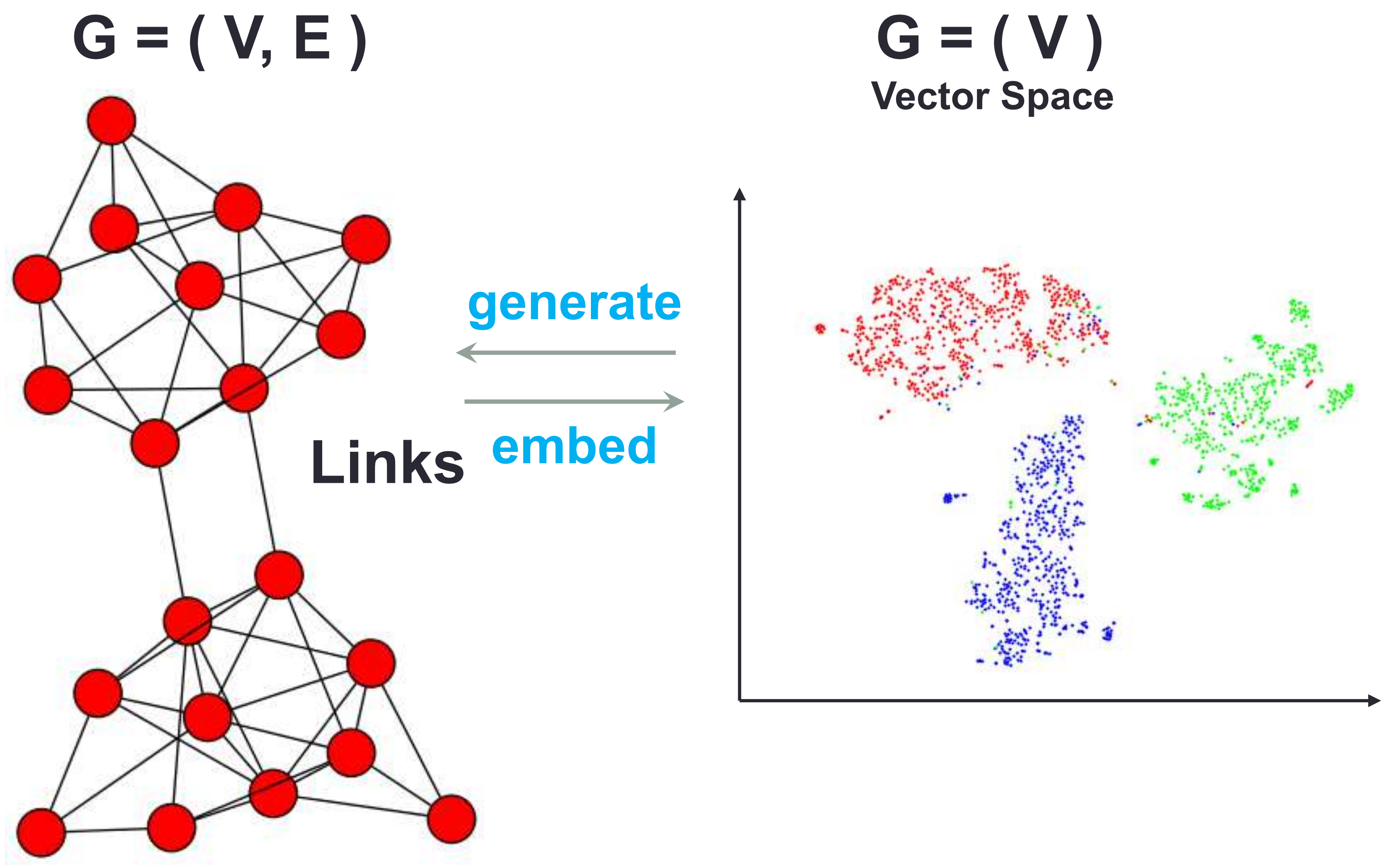
- Iterative & Combinatorial
- Coupling
- Dependency among nodes

Complexity

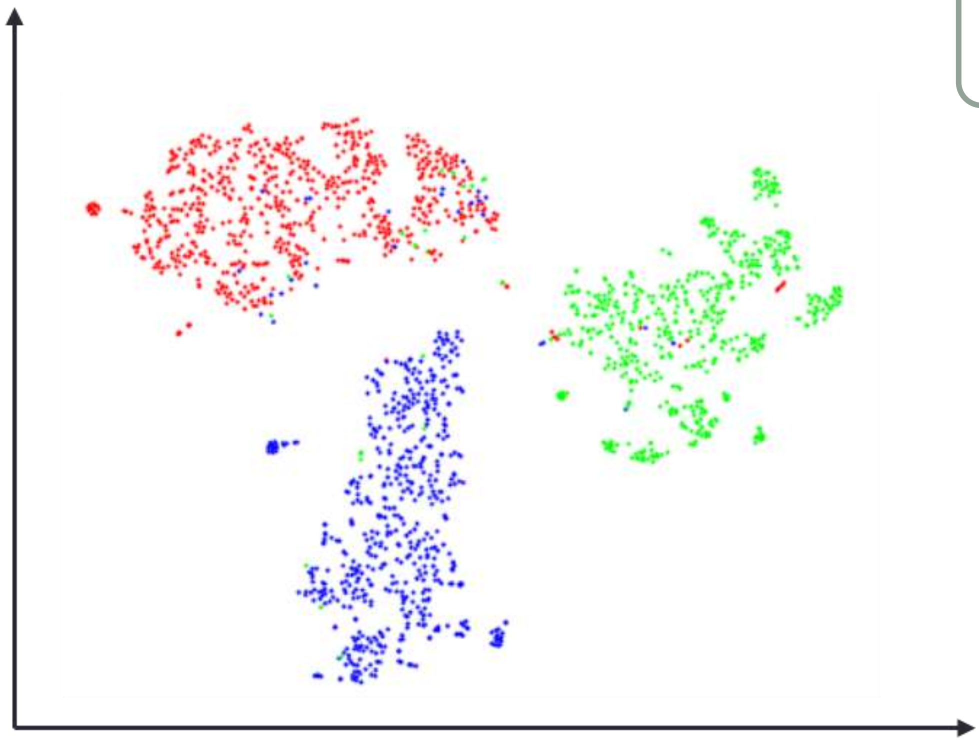
Parallelizability

Applicability of ML methods

Graph Representation Learning (GRL)



The ultimate goal of Graph Representation Learning



Descriptive and Predictive

- Node classification
- Link prediction
- Graph Classification
- Node importance
- Community detection
- Network distance
- Network evolution
- …

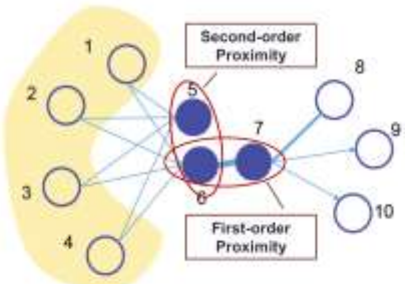
in the *Vector Space*

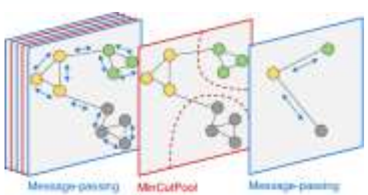
Requirement of Graph Representation Learning

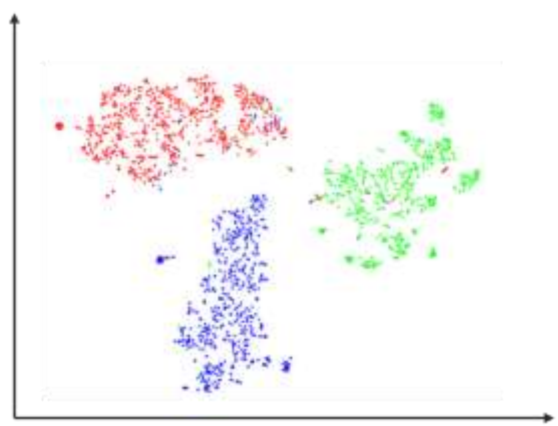
Goal: Support various graph analytical tasks

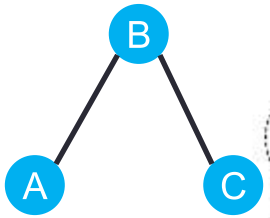
Reflect graph structure

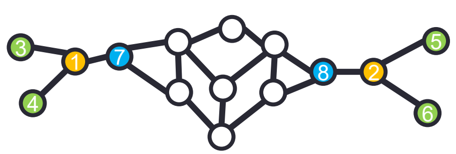
Maintain graph Properties





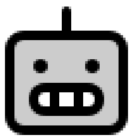






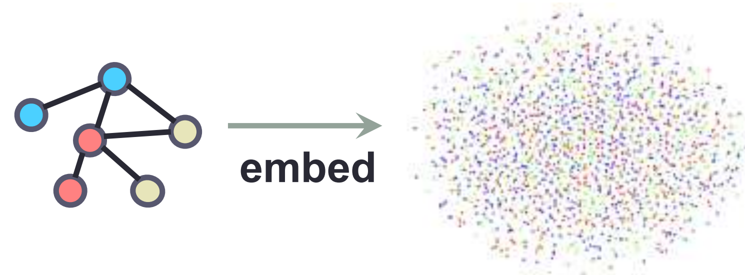
GRL should preserve essential characteristics of graphs

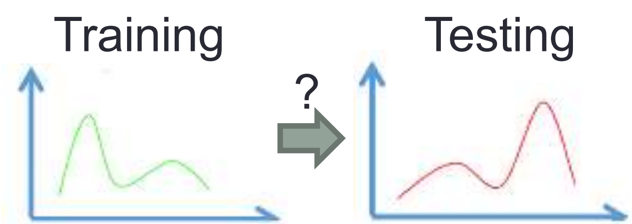
However, GRL is usually imperfect …



GRL Model1

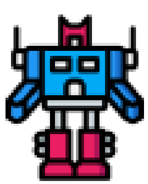
I cannot learn sufficiently meaningful representation





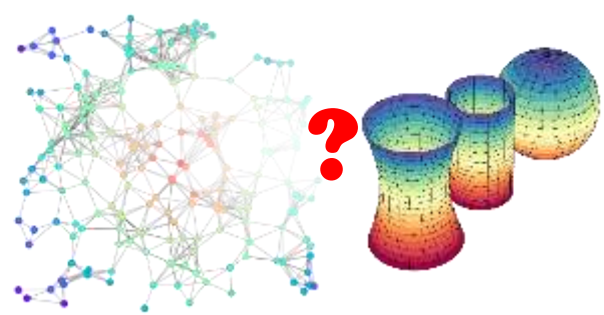
I have learned well on the training data, but even a slight perturbation in the data makes me fail

GRL Model2



GRL Model3

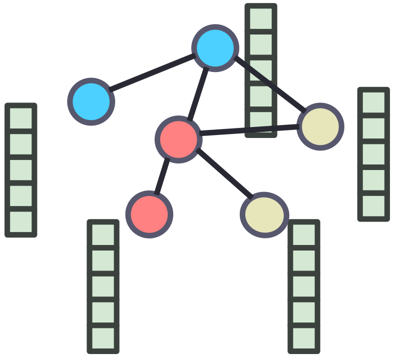
I have trouble maintaining the inherent graph characteristics



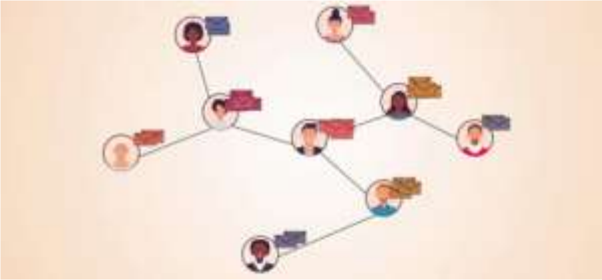
We generally refer to these phenomenon as "distortion"

What Causes Distortion in Graph Representation?

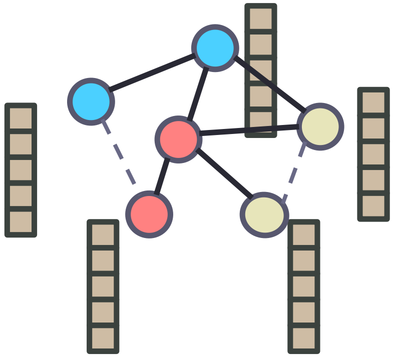
Graph Data



GRL Models



Representation



Spurious relationship
Imbalance (label, topology)
Noise (label, structure)
…

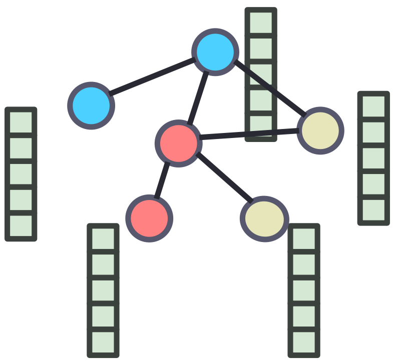
Over-smoothing
Over-squashing
Structural simplification
…

Limited dimensionality
Representation bias
Low discriminability
…

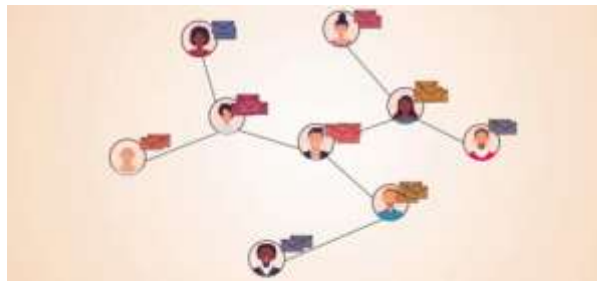
!! Distortion !!

Understanding and Addressing Distortion

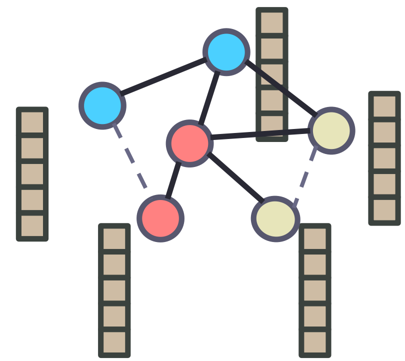
Graph Data



GRL Models



Representation



Low-Distortion Graph Representation Learning

Invariance-guided Graph Representation Learning

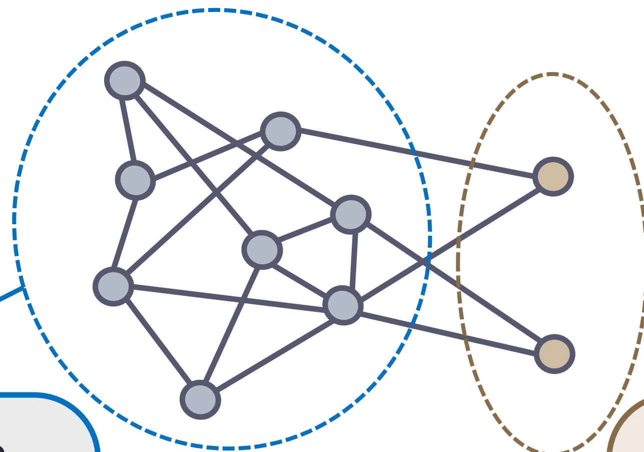
Information-theoretic Graph Representation Learning

Geometry-guided Graph Representation Learning

Understanding and Addressing Distortion

① Invariance-guided | ② Information-theoretic | ③ Geometry-guided

Distinguish the **invariant/variant structures/features** in the graph data



Invariant Parts

- Stability/Causal
- Generalization
- Core information

Variant Parts

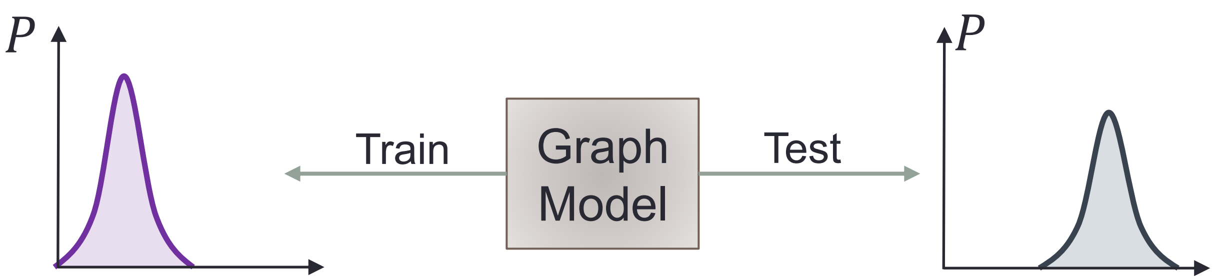
- Environments
- Short-cuts or noises
- Auxiliary information

Understanding and Addressing Distortion

① **Invariance-guided** | ② Information-theoretic | ③ Geometry-guided

Distortion: Learned representations **fail** to fully capture **invariant features**, which makes them struggle with **distribution shift** problem.

- E.g., train on small graphs, test on large graphs.
- Mislead by spurious correlations.



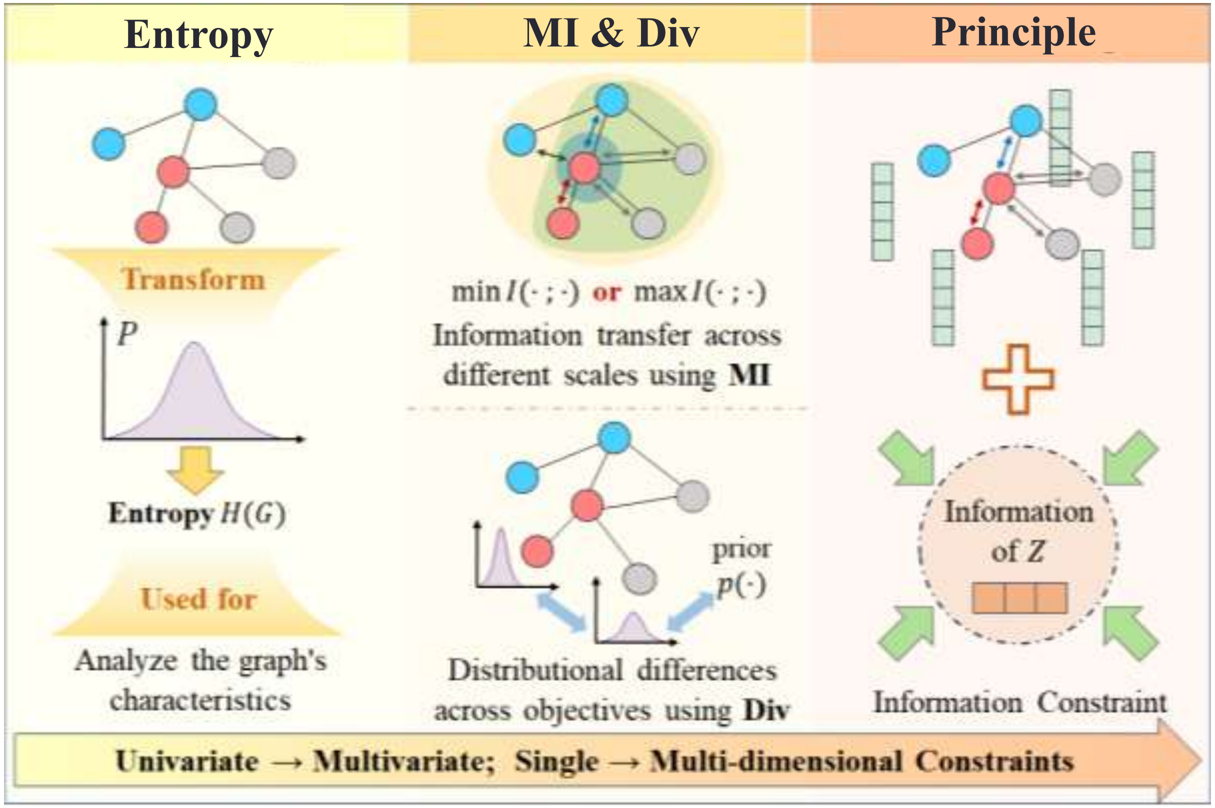
Distinguish invariant and variant structures/features under distribution shift

Reduce distortion and improve generalization

Understanding and Addressing Distortion

① Invariance-guided | ② Information-theoretic | ③ Geometry-guided

Analyze and **extract information** from complex node features and irregular structure



Understanding and Addressing Distortion

① Invariance-guided | **② Information-theoretic** | ③ Geometry-guided

Distortion: The model **loses information** during encoding, message passing, or decoding

- ☐ Message passing causes feature information loss
- ☐ Structure simplification causes structural information loss

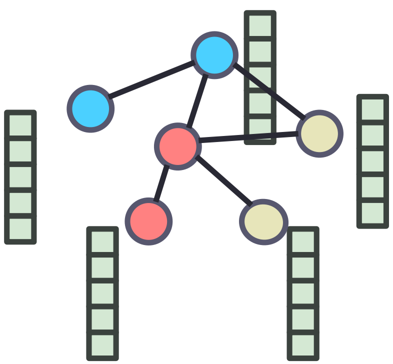
Formulate the trade-off between information acquisition and compression in graph learning

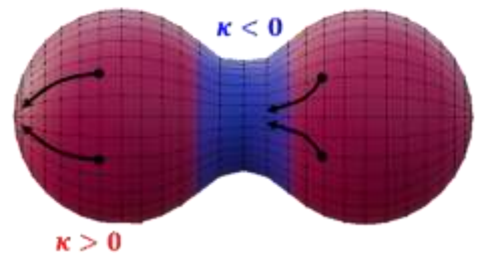
Reduce distortion and improve interpretability

Understanding and Addressing Distortion

① Invariance-guided | ② Information-theoretic | ③ **Geometry-guided**

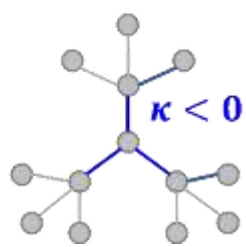
Extend graph learning to the **continuous** Riemannian /**discrete** curvature space



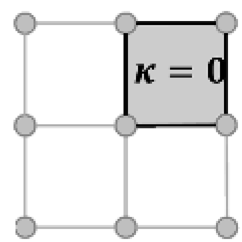


Ricci Flow

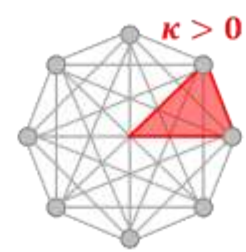
Continuous Riemannian space



Tree



Grid



Clique

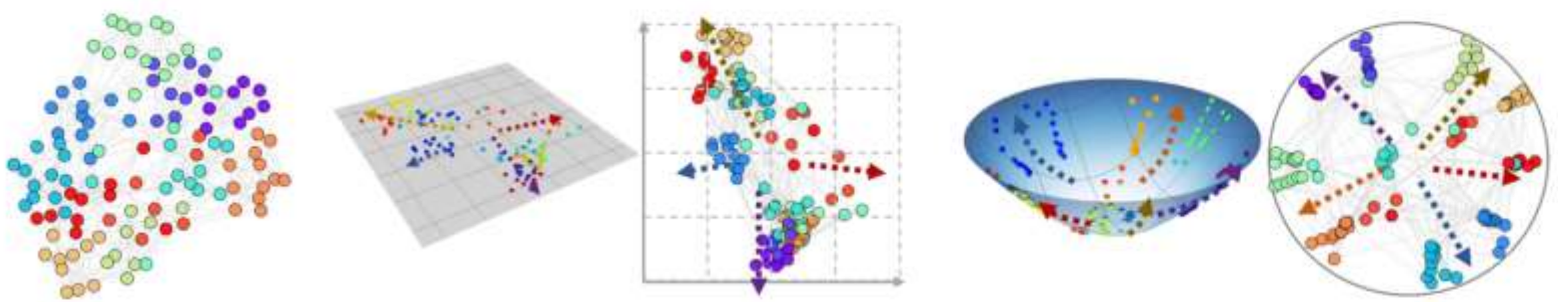
Discrete curvature-based space

Understanding and Addressing Distortion

① Invariance-guided | ② Information-theoretic | ③ Geometry-guided

Distortion: The embedding space **mismatches** the geometric relations

- Mapping to Euclidean space without considering graph characteristics
- Insufficient information storage capacity in low-dimensional space



(a) Original structure. (b) Euclidean latent space. (c) Hyperbolic latent space.

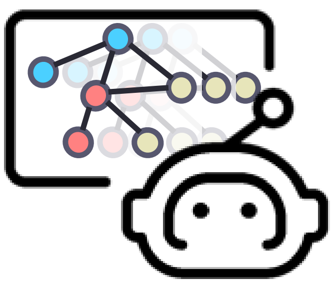
Learn representations in non-Euclidean spaces (Riemannian space & curvature-based space)

Reduce distortion and improve expressiveness

Advanced Directions

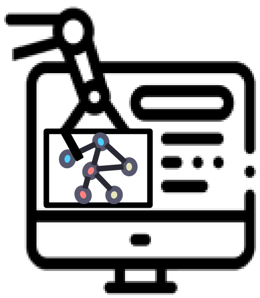
Graph Foundation Model

- Inspired by LLMs, GNNs with cross-task zero-shot generalization
- One pre-train, use everywhere
- Scaling Law



Graph RAG

- Construct knowledge graphs
- Capture complex relations across documents and across facts
- Enhance multi-hop reasoning



Graph World Model

Now, let’s move towards

low-distortion graph representation!