Graph Data Mining and Learning: Modern applications, challenges, and paradigms

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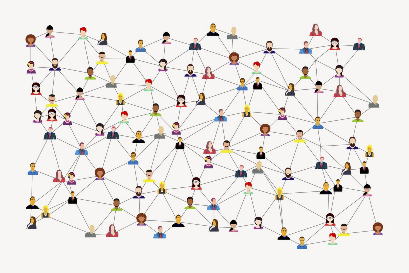
Post-doc
Nanyang Technological University, Singapore (2021-2024)
PhD
National University of Singapore (2020)

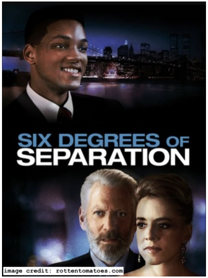
January 23, 2025

Outline

Slides

Graphs before..





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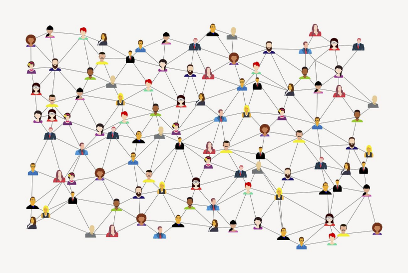
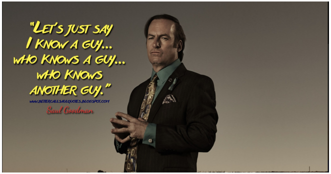
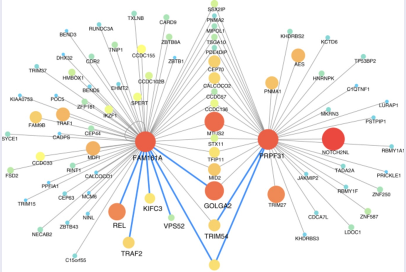




Graphs now..

Well, they are everywhere

Biology



Protein-protein interactions

Image credit: Kovács, István A., et al. "Network-based prediction of protein interactions." Nature comm., 2019

Graphs now..

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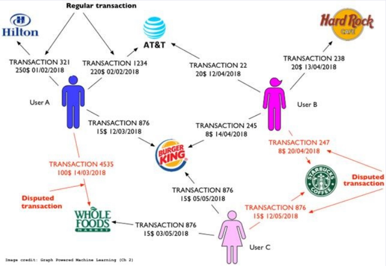
Finance



Financial transactions

Graphs now..

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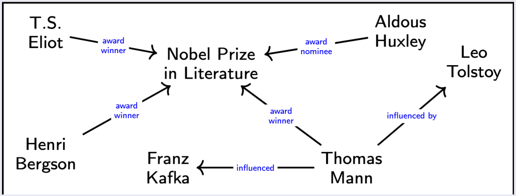
Human centered computing



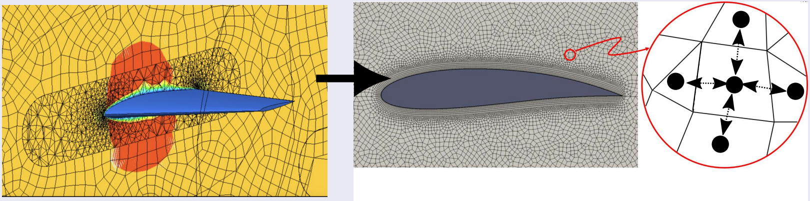
Knowledge graphs for explainable AI

Modern paradigm: Human-understandable explanation to black-box AI models. Why I was recommended *War and Piece*? Because I have read *The Magic Mountain* by Thomas Mann who was influenced by works of Tolstoy.

Graphs now..

Well, they are everywhere

Physics



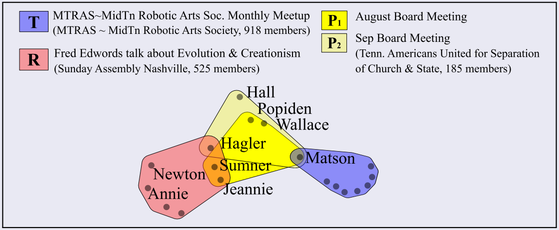
Fluid simulation at cross-section of an airplane wing (aka airfoil) and a close-up view

Modern paradigm: Modeling fluid flow as message passing on graphs.

Graphs now..

Well, they are everywhere

Public Health and Epidemiology

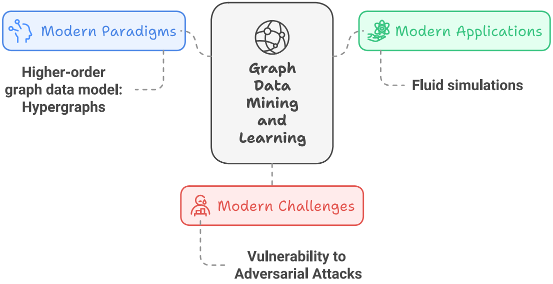


Social meet-ups (each meet-up event is a hyperedge)

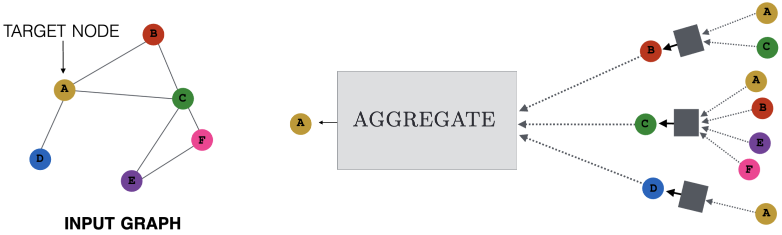
Modern paradigm: Modeling higher-order interactions as Hypergraphs.

My Research: Overview

How we can devise **efficient**, **scalable**, **robust**, **trustworthy**, and **impactful** solutions to problems in Graph data mining and learning?



My Research: Learning on Graph



Graph Neural Network

When GNNs are applied:

- Node classification (identifying fraudulant transactions)
- Link prediction (recommending movies, videos, posts, products)
- Graph classification (identifying toxic chemicals)

Basically, any learning task involving entities connected by relations.

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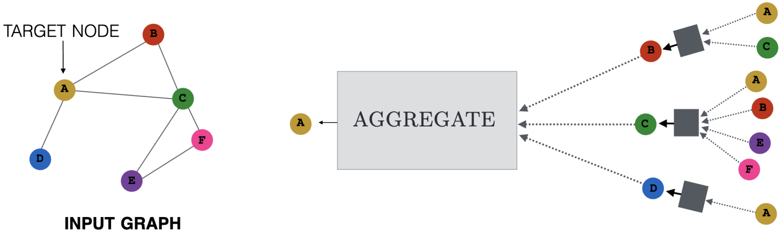

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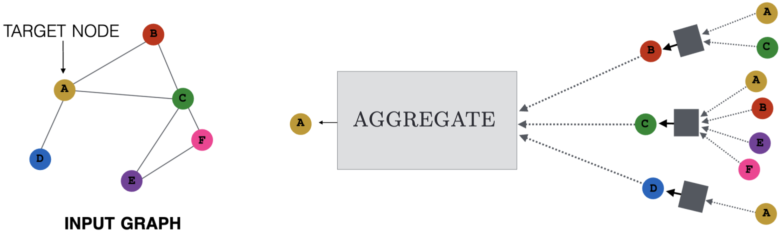

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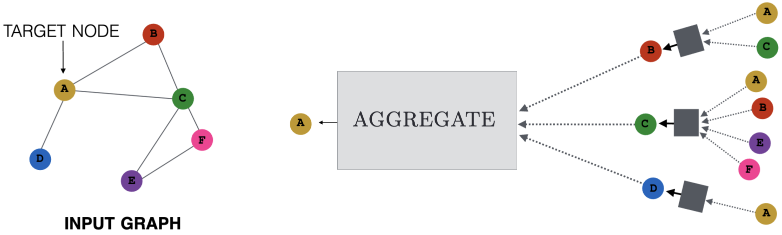

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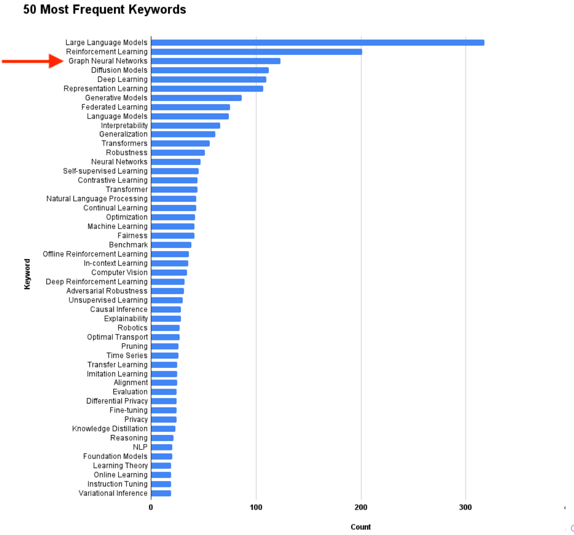
My Research: Why GNNs?

GNNs in Industry:

- Uber (food/restaurant recommendations)
- Alibaba (product recommendation)
- Snapchat (content recommendations)
- Pinterest (Pins recommendation)
- Google (Google Maps and Deepmind)
- Kumo.ai (fraud detection)
- Ant financial Services (fraud detection)
- Meta (preventing spread of misinformation, fake account detection)

GNNs in Academia: Top 50 keywords in submitted research papers at ICLR 2024.



Representative Works

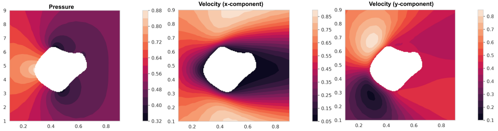
Fluid Simulation: a Modern Application of GNNs

Finite Volume Features, Global Geometry Representations, and Residual Training for Deep Learning-based CFD Simulation, ICML 2024 (spotlight)

Problem: Predict velocity, pressure at every point in the domain using AI.

Motivation:

- Numerical simulations of fluids are computationally expensive often requiring days.
- Recently, data-driven GNNs have been deployed as an efficient alternative. (e.g. MeshGraphNet from Deepmind)
- Can we improve the fidelity of data-driven GNNs?



Contributions

1. Geometric features to inform GNN nodes of long-range interactions.
2. Finite-volume features in the graph convolution layer.
3. *Super-resolution:* exploited residual training w/ low-res simulation data to ease the learning.

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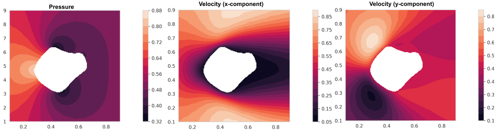

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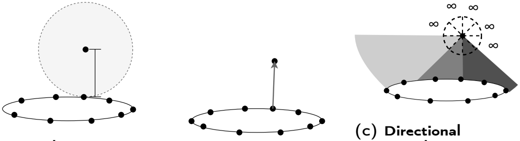

(a) **Signed Distance Function (SDF)** (b) **Shortest Vector (SV)** (c) **Directional Integrated Distance (DID)**

1. Existing geometric features (SDF) only indicate the presence of the closest boundary point. SV provides both distance and direction from the nearest boundary point. DID gives the average distance of all boundary points within a given angle range.
2. We showed that using cell characteristics, such as cell volume as node features, while face surface area, and face centroid as edge features improves the fidelity.
3. We improved the fidelity of MeshGraphNet by 41% (and others).
4. Patent at UK IP office.

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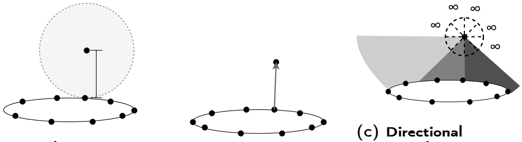

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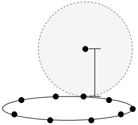

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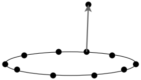

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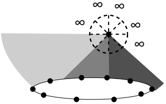

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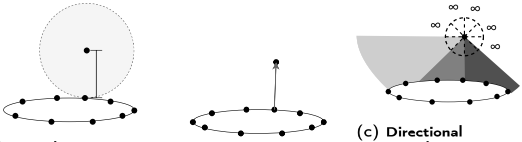

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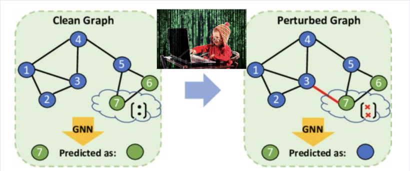
Adversarial attack: a Modern Challenge to GNNs

When Witnesses Defend: A Witness Graph Topological Layer for Adversarial Graph Learning. (AAAI'25)

Adversarial attack on Graph learning algorithms.

Attacker misleads a learning algorithm (e.g. GNN) into making incorrect predictions or classifications by deliberately perturbing a small number of edges (e.g. remove/add edges) or node features.



Adversarial perturbation (around target node 7) causes misclassification.

Contributions

1. We introduced a novel topological adversarial defense, namely, the *Witness Graph Topological Layer (WGTL)*.
2. WGTL integrates local and global higher-order graph characteristics and controls their potential defense role via a topological regularizer.

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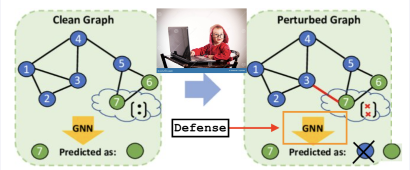

Design a defense algorithm that mitigates the effect of adversarial attack

Contributions

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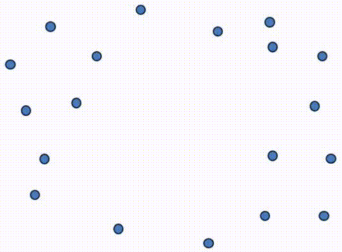
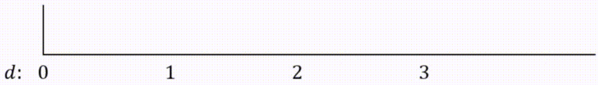
Topological Features

Example:



Record the barcode:



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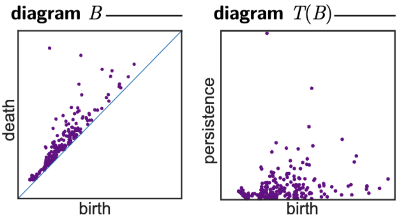
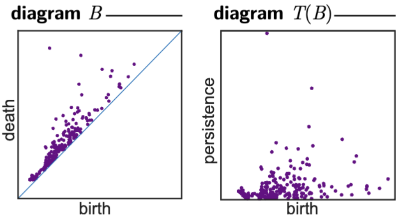


A persistence diagram is transformed using function $T : (x, y) \to (0, y - x)$.

Why Topological features?

Stability theorem: Small change in the data (graph) only result in small changes in the persistence diagram.

Topological Features



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Impact of this work

1. This is the first work that shows that topological features can make GNNs robust against adversarial perturbations.
2. Effective against several types of attacks, for instance,
   - Targetted poisoning attack (Graybox, modify the neighbors of a target node and their features)
   - Global poisoning attack (Graybox, instead of targetting specific neighborhood modify whichever edges minimizes the model accuracy)
   - Adaptive attacks (White-box, the model architecture, parameters and defense mechanisms are known to the attacker)
   - Node feature attack
3. WGTL improves existing defenses such as Pro-GNN, GNNGuard, and SimP-GCN respectively by 5%, 15%, and 5%.

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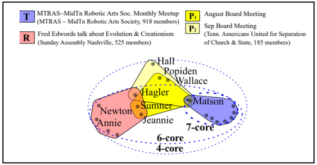
Hypergraphs: a modern paradigm in higher-order graph data mining

Neighborhood based hypergraph core decomposition (VLDB 2023).

Neighborhood-based core decomposition

Decomposition of a hypergraph into nested, maximal subhypergraphs/cores such that all nodes in the k-core have at least k neighbors in that subhypergraph.



The set of events $H = \{T, R, P_1, P_2\}$ **forms a hypergraph. 6-core =>** $\{T, R\}$, **7-core =>** $\{T\}$

Contributions

- We introduced this novel core decomposition.
- We proposed an efficient local algorithm that scales to million-node hypergraph.
- **Applications**:
  - **Densest subhypergraph extraction.** Our novel volume-densest subhypergraphs capture important meetup events.
  - **Diffusion intervention.** Our decomposition is more effective than other graph-based decompositions in intervening diffusion e.g. epidemic spread.

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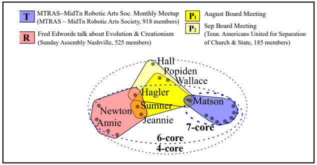

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Impact of this work

1. Fastest hypergraph core-decomposition algorithm to date: can decompose ArnetMiner hypergraph with 27M nodes and 17M hyperedges in-memory within 91 seconds.
2. Laid the foundation for more recent core decomposition methods such as (k,g)-core [CIKM'23], (k,t)-hypercore [ECML-PKDD'23], and Dual-Layer Hierarchy [CIKM'24].

Future Plans

(Brief) Future Plans

Problems I want to study and relevant impact areas:

1. Cyber-security/healthcare.
   - **Privacy-preserving graph neural networks** that are robust against adversaries.
     - ✓ These tools are vital for protecting sensitive public health data. Because adversaries can still exploit the graph structure to infer private (e.g. health) information, even when DP is applied.
   - Efficient **uncertainty estimation of GNNs.** We want increased trustworthiness of AI systems by providing transparency about model confidence. This is critical in sensitive applications such as medical diagnosis, autonomous systems, and cybersecurity. For instance,
     - ✓ In healthcare, uncertainty-aware GNNs can guide clinicians by highlighting areas where predictions are less certain, thereby supporting informed decision-making and mitigating risks.
     - ✓ In cybersecurity, uncertainty estimation can help prioritize high-risk alerts for further investigation.
2. Human-centered AI.
   - Can we develop benchmark datasets to assess the **deductive reasoning ability** of LLMs? new ICLR paper yesterday on LLM reasoning ability.
   - How to model rich datasets e.g. those arising from **multiple modalities and multiple sources** using a Knowledge Hypergraph? How to handle complex queries on such knowledge hypergraph?
3. Physical science.
   - **Explainability and reliability** of ML models in the **physics domain** e.g. fluid dynamics, additive manufacturing etc.

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    - **Explainability and reliability** of ML models in the **physics domain** e.g. fluid dynamics, additive manufacturing etc.

(Brief) Future Plans

Problems I want to study and relevant impact areas:

1. Cyber-security/healthcare.
   - **Privacy-preserving graph neural networks** that are robust against adversaries.
     - ✓ These tools are vital for protecting sensitive public health data. Because adversaries can still exploit the graph structure to infer private (e.g. health) information, even when DP is applied.
   - Efficient **uncertainty estimation of GNNs.** We want increased trustworthiness of AI systems by providing transparency about model confidence. This is critical in sensitive applications such as medical diagnosis, autonomous systems, and cybersecurity. For instance,
     - ✓ In healthcare, uncertainty-aware GNNs can guide clinicians by highlighting areas where predictions are less certain, thereby supporting informed decision-making and mitigating risks.
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Short term (years 1-2)

Funding Proposals

Year 1-2 (Foundations and Early Collaborations)

- Develop private+robust GNNs and series of collaborations with Virginia Tech, and GVSU colleagues. → NSF SatC 2.0, NSF CISE/CNS, NIST ITL MSE, NIH
- Develop and release benchmark dataset for assessing deductive reasoning in LLMs. → NSF HNDS, NSF CISE/IIS HCC
- Project AI4Engineering: Collaborative initative with GVSU engineering. (Planning and Funding phase) → DoE Office of Science

Mid term (years 3-4)

**Year 3-4
From Innovation
to Application)**

Funding
Proposals

- Extend the private+robust GNN solution to real-world, e.g., Fintech, IoT networks, personalized medicine and public health. → NSF SatC 2.0, NSF CISE/CNS, NIST ITL MSE, NIH
- Design a framework for efficient uncertainty estimation in GNNs. → NSF HNDS, NSF CISE/IIS HCC
- Develop Knowledge Hypergraph prototypes for multi-modal and multi-source data. Study and model complex queries. → DoE Office of Science
- Project AI4Engineering: Collaborative iniative with GVSU engineering. (publication phase)

Long term (year 5)

Funding Proposals

Year 5 (Expansion and Long-term impact)

- Implement Uncertainty Estimation methods in collaboration with cybersecurity industry partners.
- Secure a multi-institutional grant for Graph Learning for cyber-security and Uncertainty estimation in GNNs. Organize and host a workshop. → To be decided
- Deploy Knowledge Hypergraph models in interdisciplinary applications (e.g., healthcare).
- Project AI4Engineering: Collaborative initiative with GVSU engineering. (Extend the scope to other disciplines) → To be decided

Interdisciplinary Works and Collaborations

Interdisciplinary collaboration

- **Rolls-Royce plc.**, Dept. of Mechanical & Aerospace Engineering (NTU)
  - 1 Patent @UK IP office, 1 ICML paper.
  - Rolls-Royce has plans to internally adopt our solution.

Collaborations across the world

- *North-America*:
  - Virginia Tech (AAAI'25)
  - University of California Riverside (AAAI'25)
  - **Purdue University**
  - **Pacific Northwest National Lab (PNNL)**
- *Europe*:
  - Aalborg University, Denmark (ICLR'25)
  - Max Planck Institute, Germany (ICLR'25)
  - Inria @ Univ. of. Lile, **France**
  - University of Vienna, **Austria**
  - CENTAI, **Italy**
- *Asia*: NUS, NTU (**Singapore**), BUET (**Bangladesh**).

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- *Asia*: NUS, NTU (**Singapore**), BUET (**Bangladesh**).

Thank You
Q&A

Slides

Email: `naheed_anjum@u.nus.edu`

Supplementary Slides