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Part I

Introduction and Fundamentals

Lecture 01

Importance of GNNs

- Explore the significance of graph neural networks (GNNs).
- Understand the role of graphs in various domains and their importance in data representation.
- Highlight the crucial aspect of graph learning.
- Spotlight the unique strengths of GNNs compared to other methods.

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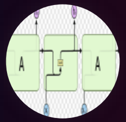
TRADITIONAL DL TOOLBOX
GRAPH-STRUCTURED DATA
GRAPH LEARNING
TYPES OF GL TASKS

Traditional Deep Neural Networks

- Traditional deep learning toolbox is designed for simple **sequences** or **grids**

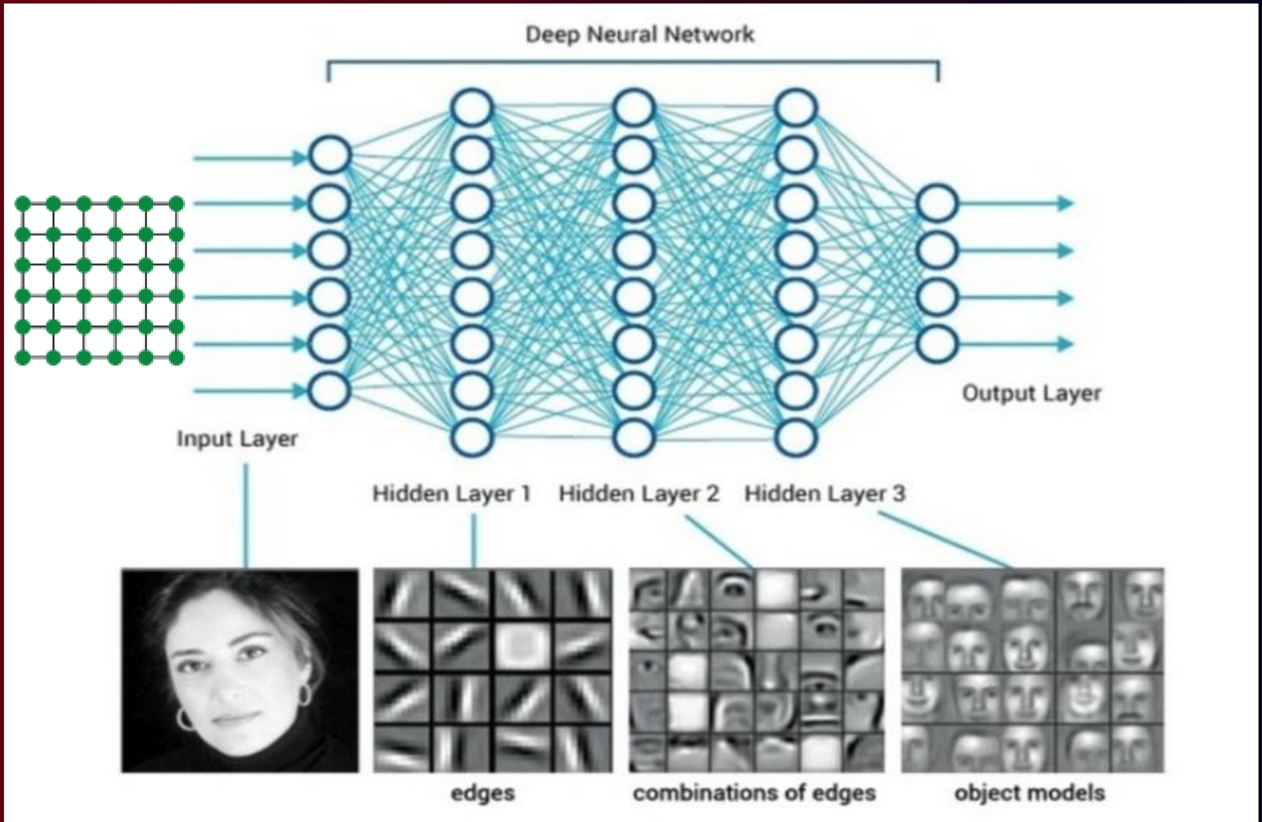
DNN

DNNs for fixed-size images/grids...



RNN

RNNs or word2vec for text/audio sequences...



Hold on! | But not everything can be represented as a **sequence** or a **grid**.

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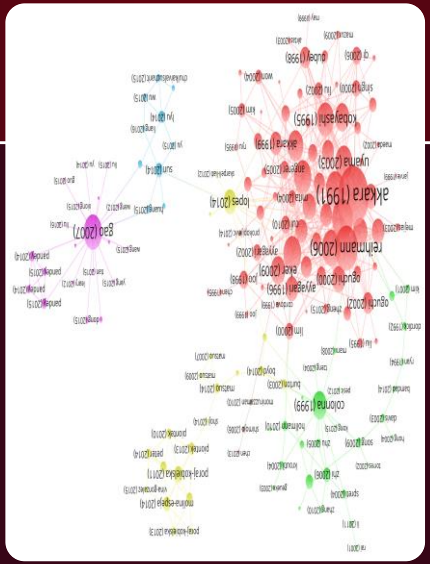
Many Types of Data are Graphs

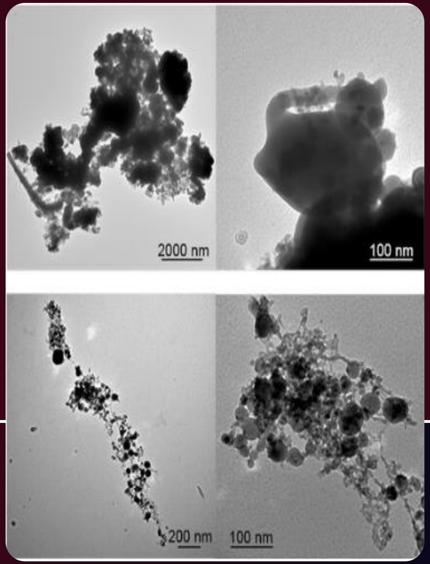
- ❑ A lot of real-world data does not "live" on grids or sequences.

Computer Networks



Citation Networks

Particle Networks



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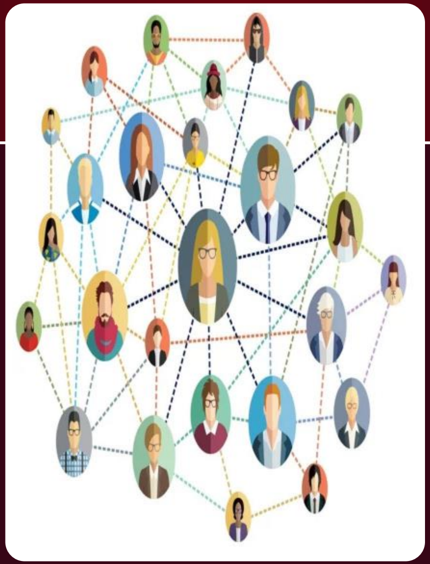
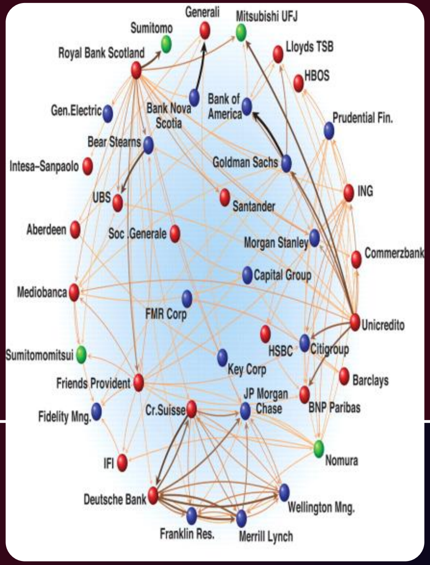
Underground Networks



Social Networks

Economic Networks



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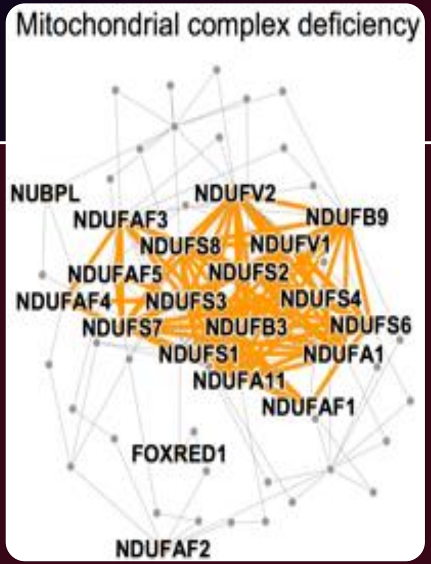
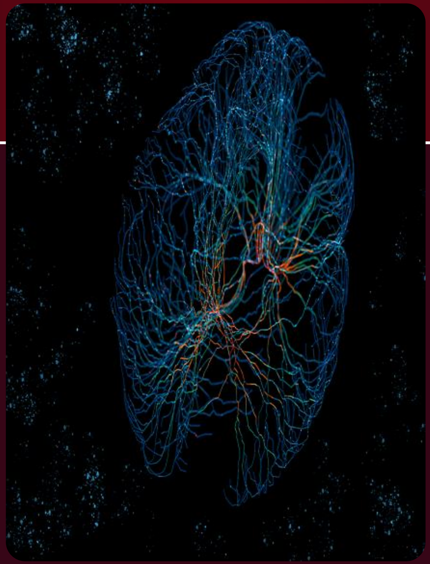
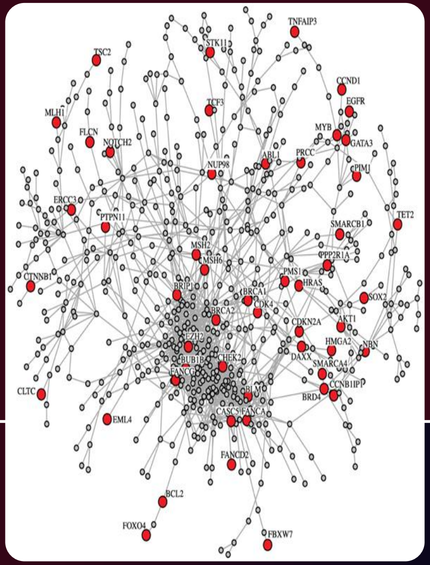


Disease Pathways



Networks of Neurons

Gene Regulatory Networks



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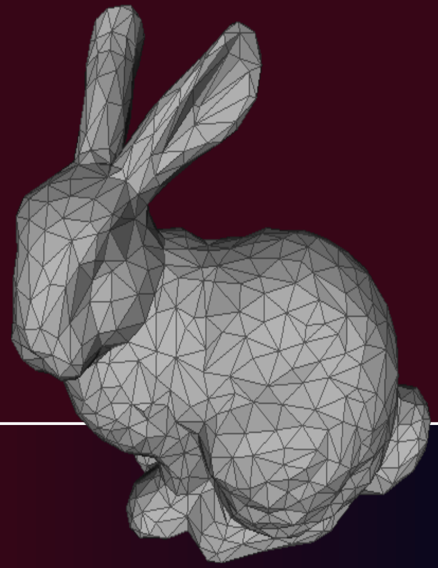
Many Types of Data are Graphs

- ❑ A lot of real-world data does not "live" on grids or sequences.

Internet

Molecules

3D Shapes



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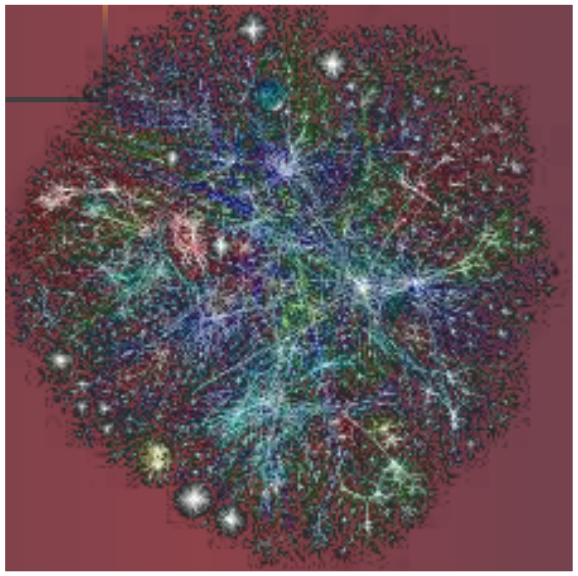
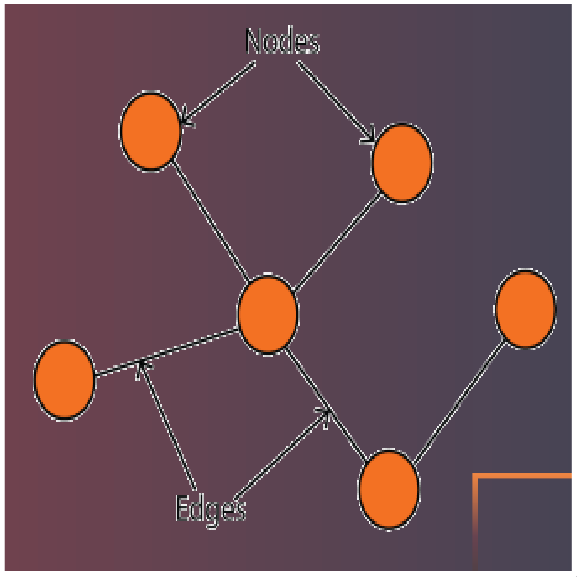
Importance of Graphs

- ❑ **Graphs** matter because they offer a versatile framework to understand complex systems and relationships.
- ❑ By representing entities and their interactions, **graphs** unlock insights in various domains of applications.



Graph Theory

- ❑ The mathematical study of graphs that emerges as a fundamental tool for understanding complex systems and its relationships.



What are Graphs?

- ❑ **Graphs** → a general language for describing and analyzing entities with relations/interactions,
- ❑ A **graph** visually captures nodes and edges, offering a framework to decipher patterns and structures.

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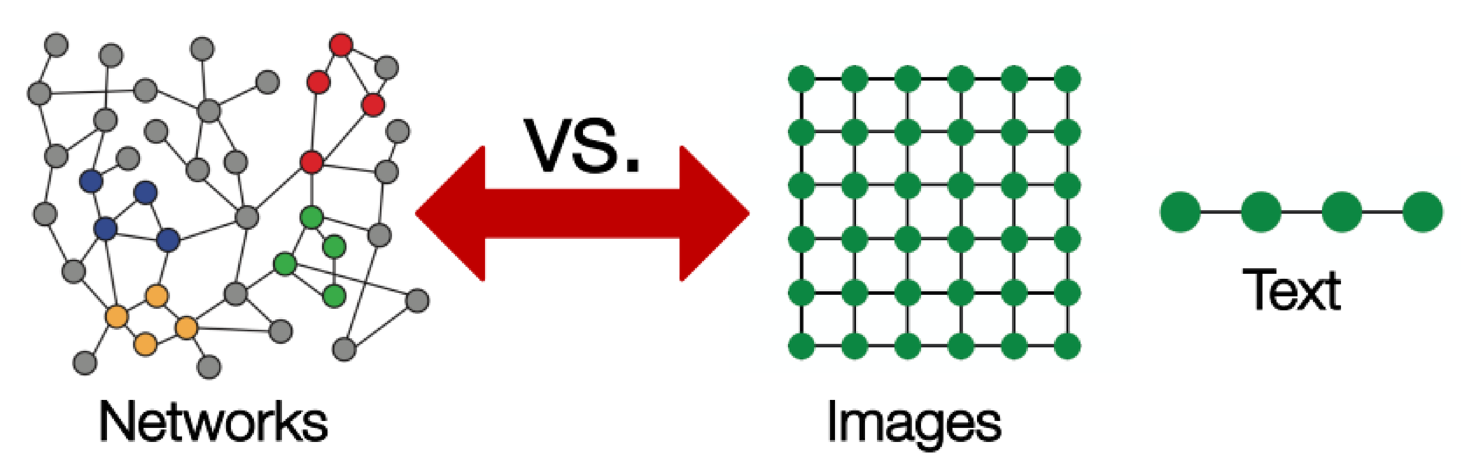
Graph Complexity?

- ❑ Arbitrary size and complex topological structure.
- ❑ No fixed node ordering or reference point.
- ❑ Often dynamic and have multimodal features.



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Why Graph Learning?

Main Concerns of Classical DL:

- Standard **CNN** and **RNN** architectures don't work on this **graph-structured data.**

Graph Learning:

- New frontiers beyond **classic neural networks** that learn on **grids** and **sequences**.
- **Graph Neural Networks (GNNs)** are the new frontier of deep learning.

Main Challenges:

- How do we take advantage of **graph-relational structure** of such complex systems for better prediction?
- How can we develop neural networks that are much more broadly applicable for **graph-structured data**?

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Hot Subfield of DL

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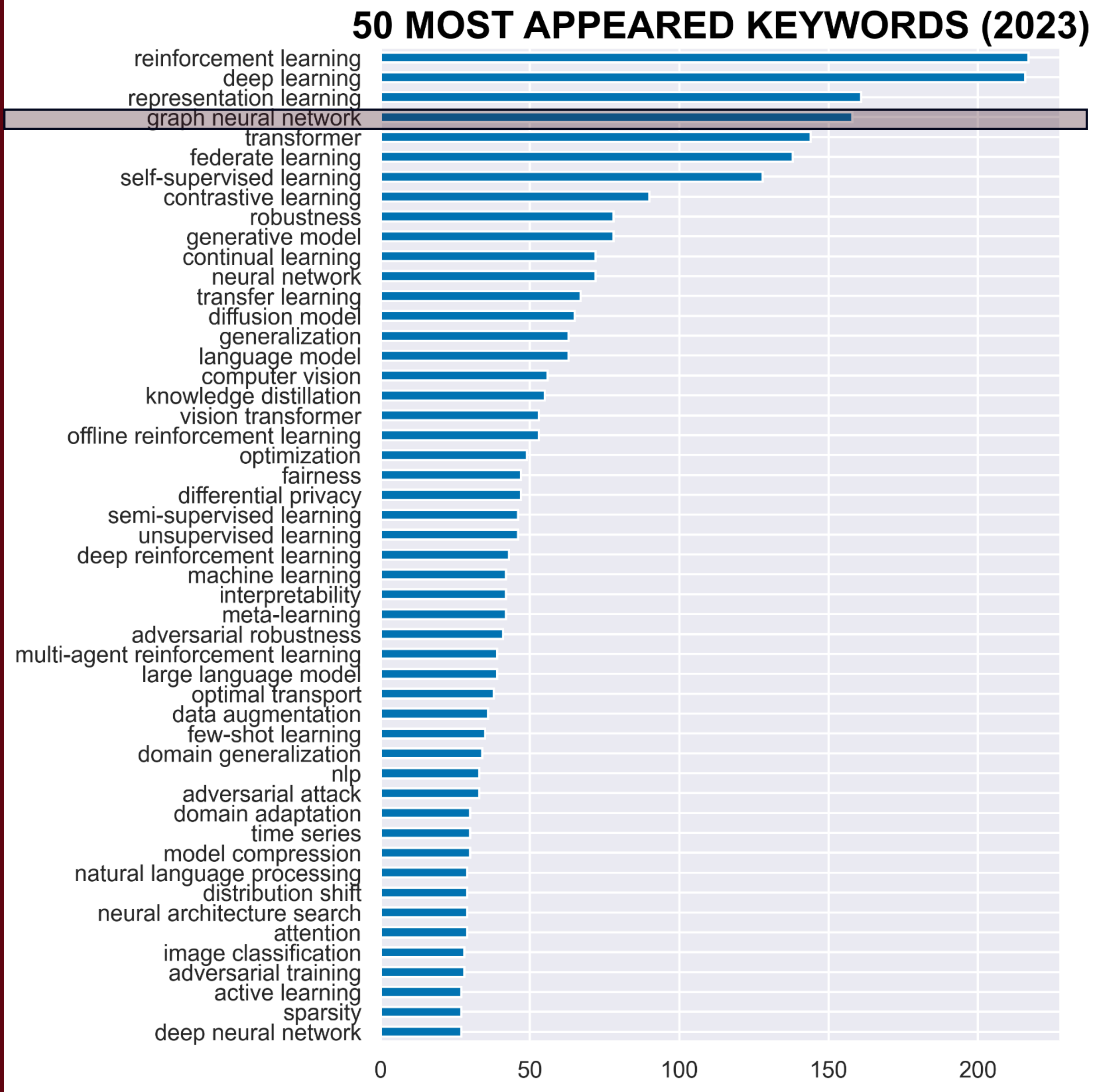
Staff Research Scientist @GoogleDeepMind | Affiliated Lecturer @Cambridge_Uni | Associate @clarehall_cam | GDL Scholar @ELLISforEurope. Algorithms. 🇷🇸 🇲🇪 🇧🇦

Petar Veličković
@PetarV_93

ICLR 2023 stats are in:
GNNs still the top studied model! 🔥 🕸️ 🌐 🧪 🧑‍🔬



- **Resource:** https://github.com/EdisonLeeeee/ICLR2023-OpenReviewData. (International Conference on Learning Representations 2023)

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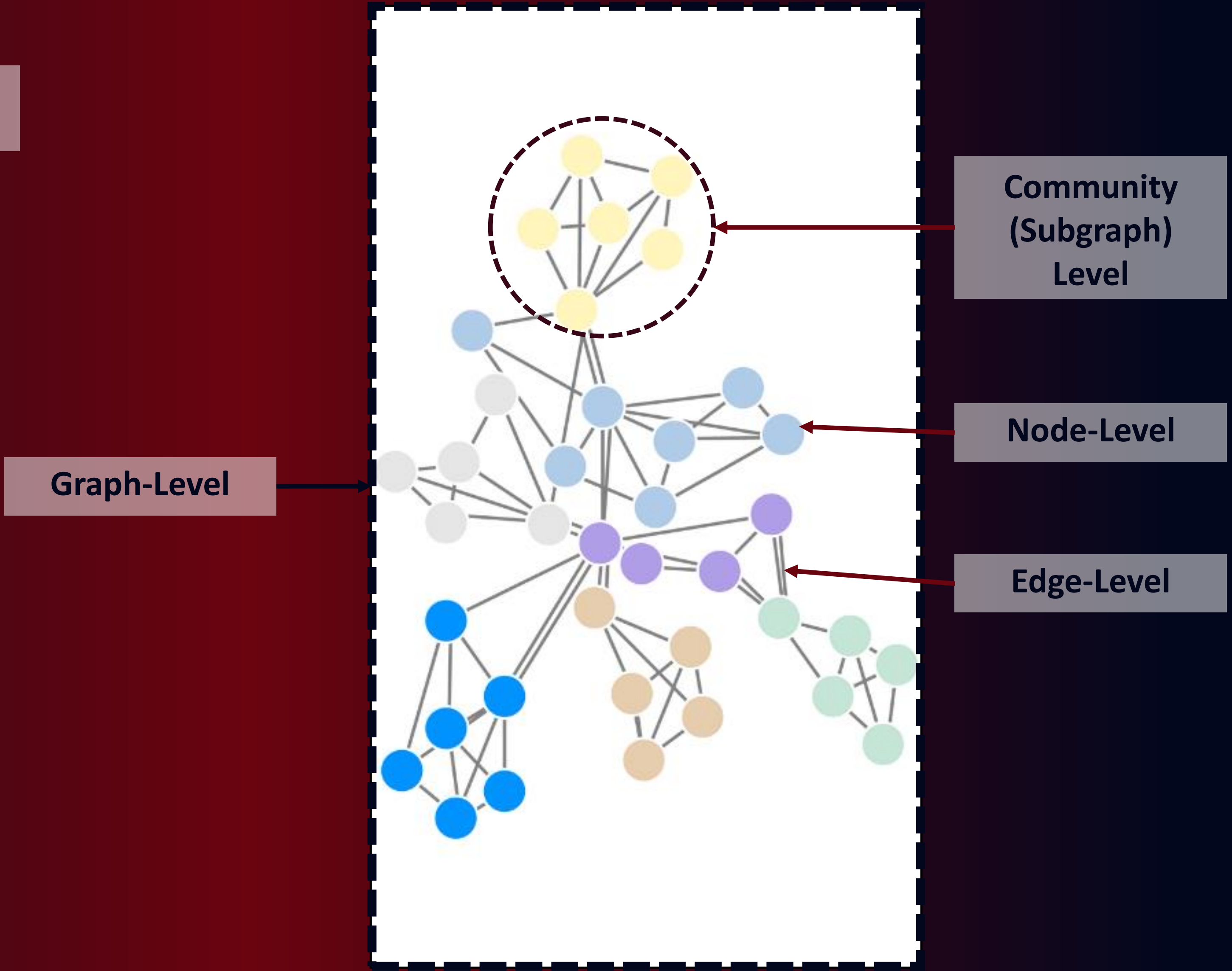
What is Graph Learning?

- **Graph Learning** ➔ the application of machine learning and Deep Learning techniques to **graph data**.
- **The study area** ➔ encompasses **different types of tasks** aimed at understanding and manipulating **graph-structured data**.



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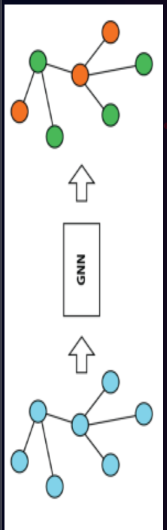
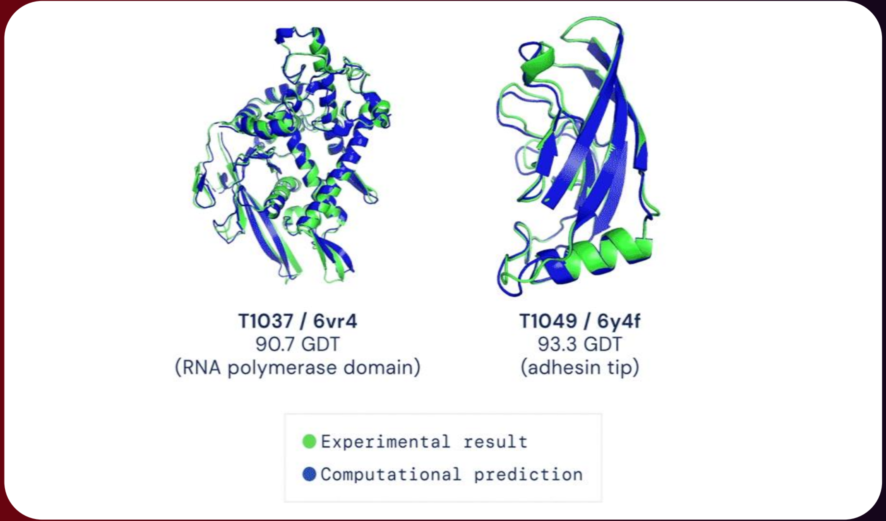


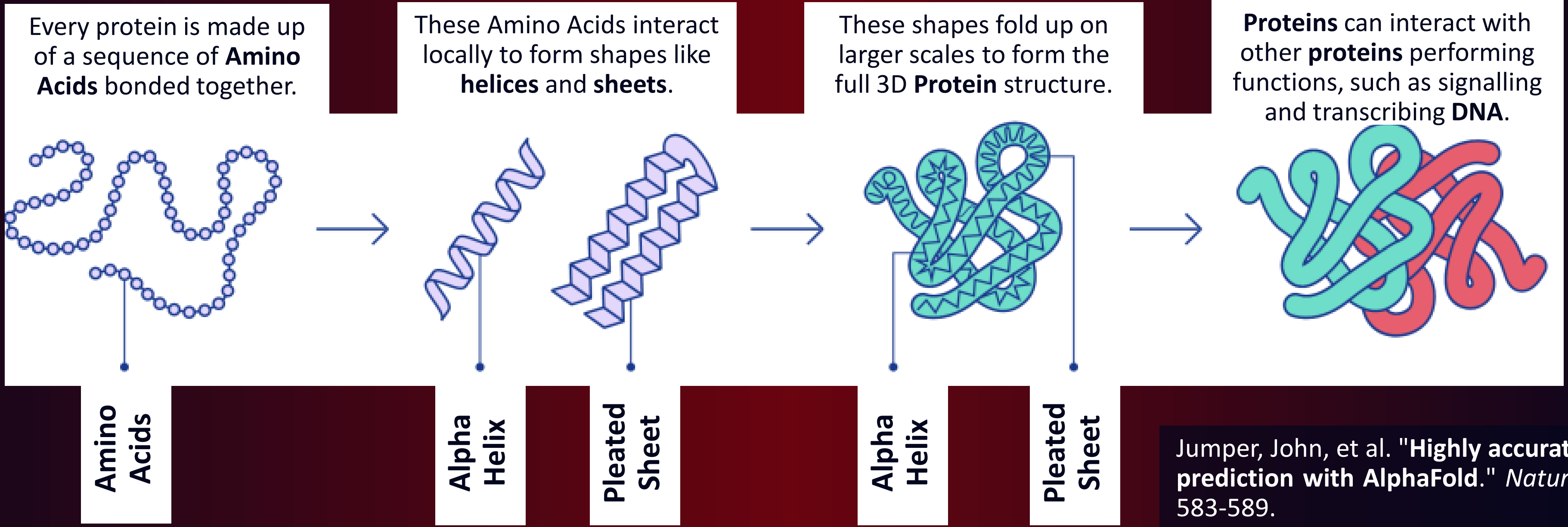
Node-Level Tasks

Key Idea
- ❑ Nodes → Amino acids in a protein sequence
- ❑ Edges → Proximity between amino acids

- ❑ **Node Classification:** Predicting the category (class) of a **node** in a graph.
- ❑ **Example: AlphFold** Google Project from DeepMind - Solving Protein Folding.
  - **AlphaFold** → State-of-the-art GNN-based DL model for predicting the 3D structure of proteins from their amino acid sequence.
  - Has significant implications for fields such as Drug Discovery, Protein Engineering, and Synthetic Biology.



Computationally **predict a protein's 3D structure** based solely on its **amino acid sequence**



Jumper, John, et al. "**Highly accurate protein structure prediction with AlphaFold.**" *Nature* 596.7873 (2021): 583-589.

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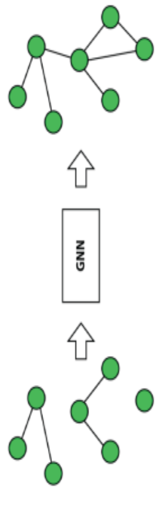
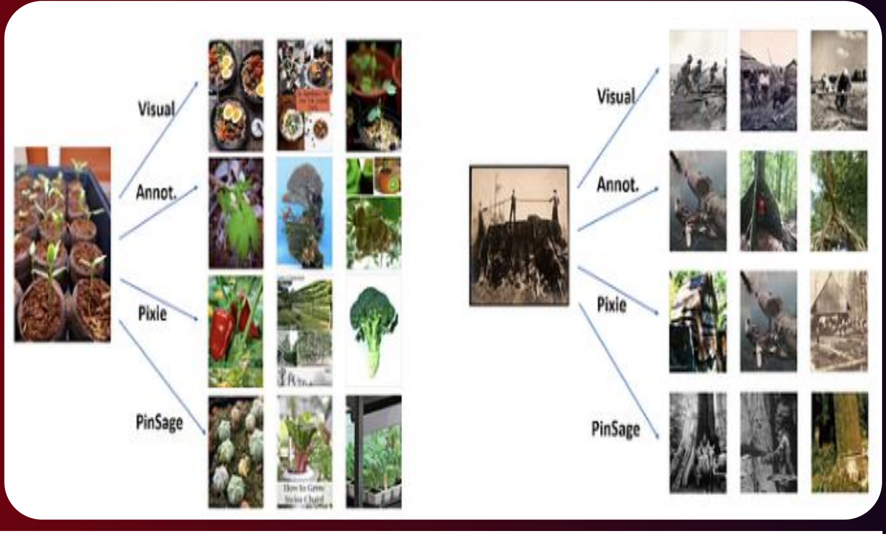


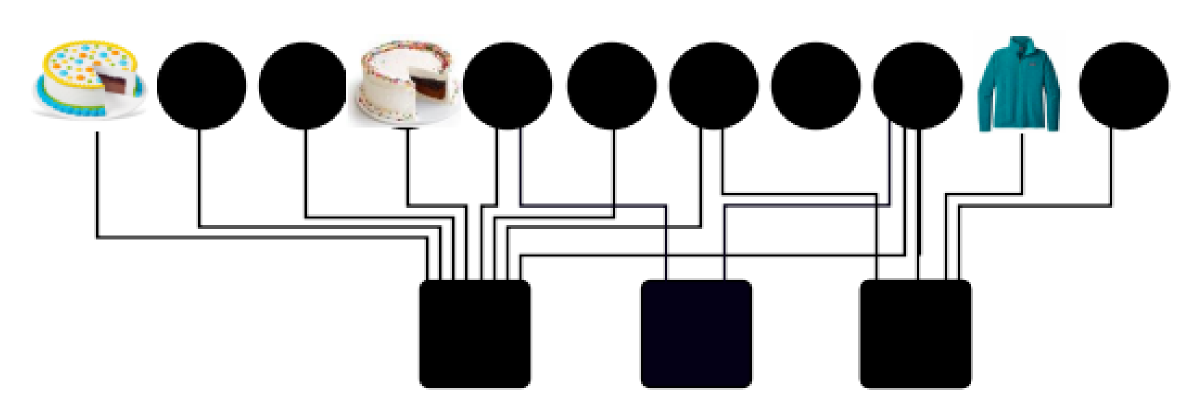
Edge-Level Tasks

Key Idea
- Nodes ➔ User Query pin image
- Edges ➔ User-Item Interactions

- **Link Prediction:** Predicting missing **links** between pairs of nodes in a graph.
- **Example: PinSage - Graph Based Recommender from Pinterest Lab** (**3** billion **nodes** and **18** billion **edges**)
  - **PinSage** ➔ A GNN-based rec-system for providing personalized recommendations to Pinterest users.
  - It models the user-item interaction graph which allows to recommend related pins to users.



Computationally **Predict whether two nodes in a graph are related.**



A **user** can click on a **product** or an **Ad**, he can follow a **board**. A **pin** can belong to a **board**, a **user** can enter a **search-query** and then click on a **pin**.

Learn node embeddings to predict whether two nodes in a graph are related.

Ying, Rex, et al. "**Graph convolutional neural networks for web-scale recommender systems.**" Proceedings of the 24th ACM SIGKDD international conference on knowledge discovery & data mining. 2018.

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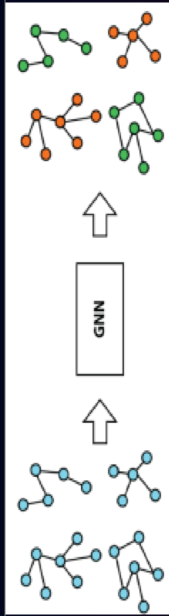
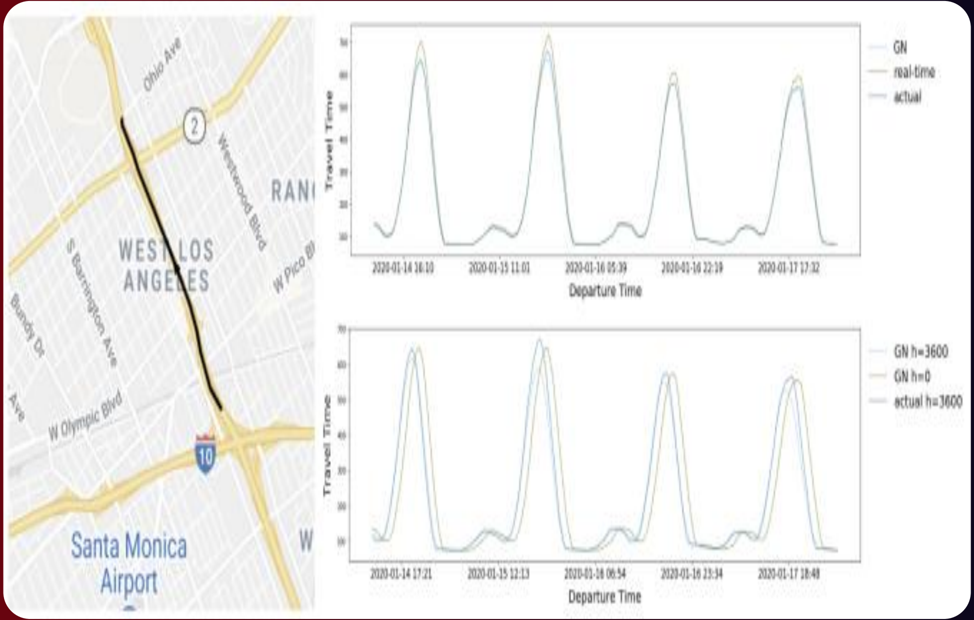


SubGraph-Level Tasks

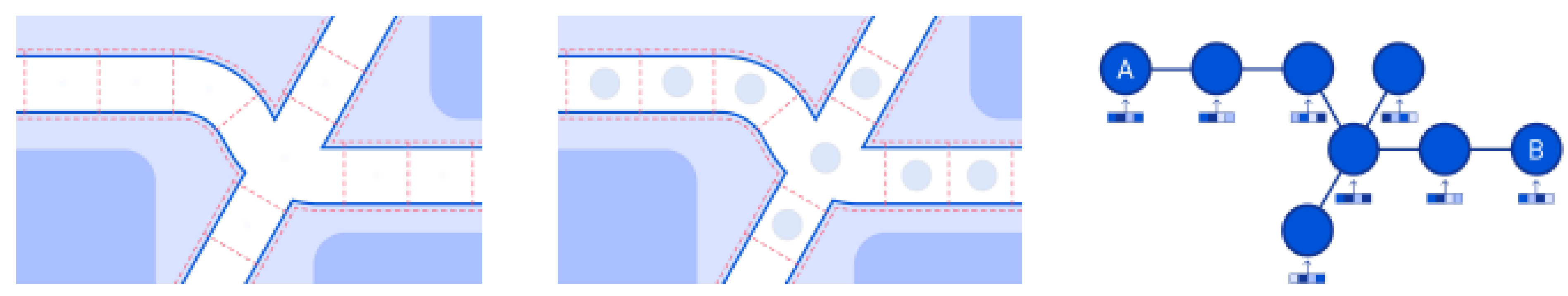
- ❑ **Graph Classification:** Categorizing different graphs into predefined categories.
- ❑ **Example: Estimated Time of Arrival (ETA) Prediction in Google Maps – A DeepMind Traffic Prediction Google Project.**
  - **ETA Prediction** ➔ A cutting-edge GNN technology that enables more accurate location estimates.
  - It analyses graph structure of road networks to capture complex relationships between locations and improve the accuracy of eta predictions. (has numerous applications, including route optimization, traffic prediction, …)

Key Idea

- ❑ Nodes ➔ Road segments
- ❑ Edges ➔ Connectivity between road segments



Computationally Predicting Time of Arrival with Graph Neural Networks



An example **road network** with shared traffic volume, which is partitioned into **segments of interest** (**left**). Each **segment** is treated as a **node** (**middle**), with adjacent **segments** connected by **edges**, thus forming a **supersegment** (**right**).

Derrow-Pinion, Austin, et al. "**ETA prediction with graph neural networks in google maps.**" Proceedings of the 30th ACM International Conference on Information & Knowledge Management. 2021.

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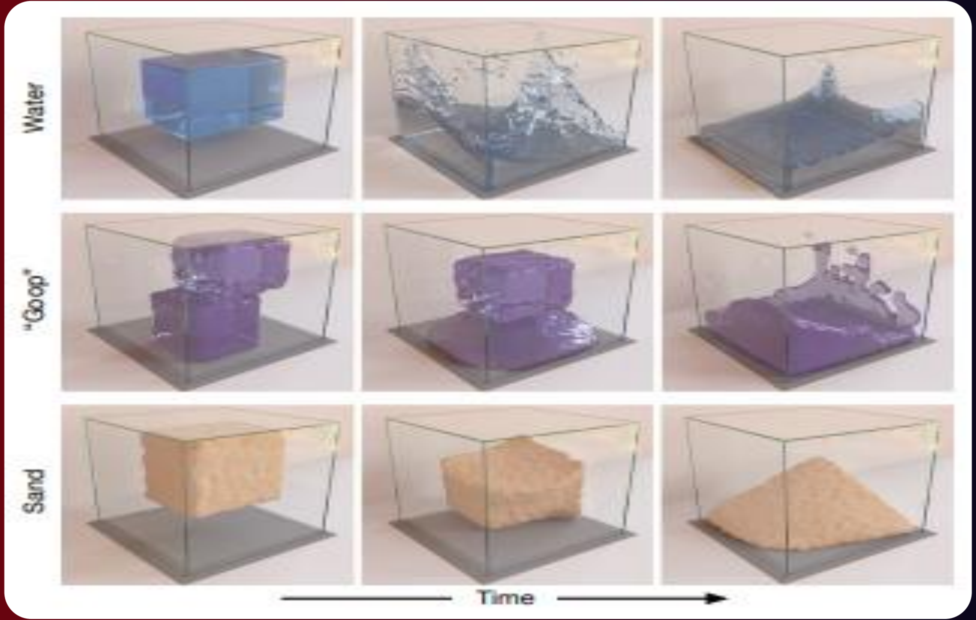
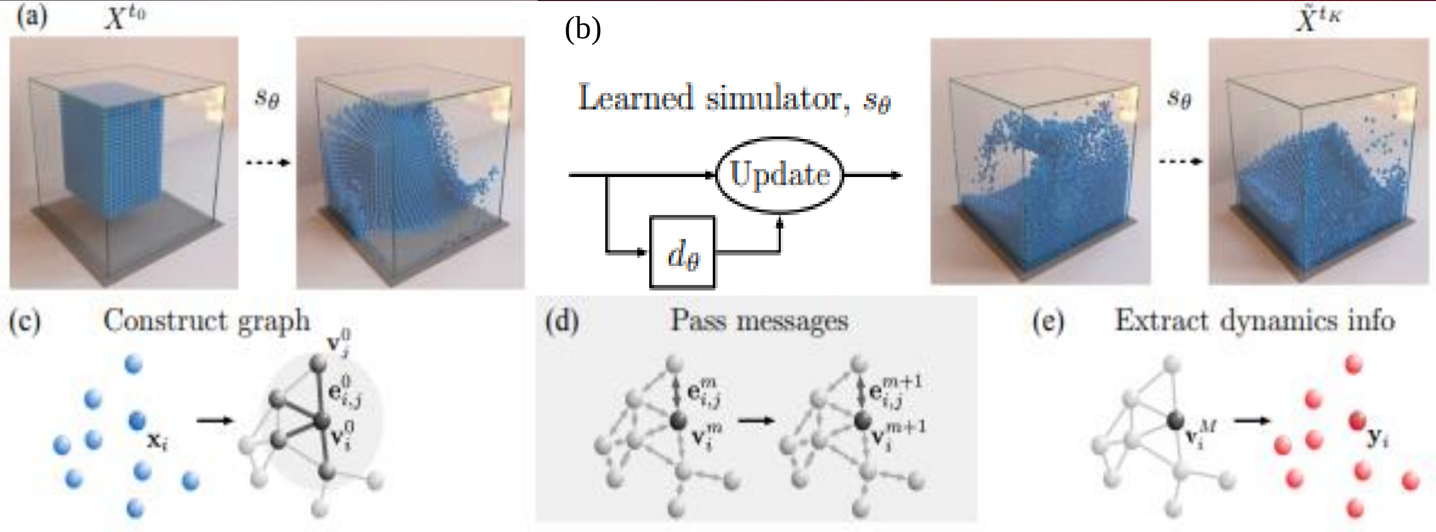
Graph-Level Tasks

- **Graph Generation:** Generating new graphs based on a set of desired properties.
- **Example: Physics Simulation as a Graph – A Stanford University Project.**
  - **Graph Bases Physical Simulation→** A cutting-edge GNN technology that enables learning to Simulate Complex Physics with Graph Networks.
  - It generates a totally new graph by updating an existed one that captures the complex relationships between physical particles systems and their interactions.

Key Idea
- Nodes → Particles
- Edges → Interaction between particles



Computationally **Predict how a graph will evolve over time.**



(a) Predicts future states represented as particles using its learned dynamics model, d_θ, and a fixed update procedure **(b)**. **(c)** Constructing graph, G_0 , from the input state, X. **(d)** Performing M rounds of learned message-passing over the graphs, G_0, . . . , G_M. **(e)** Extracting dynamics information, Y , from the final graph, G_M.

Sanchez-Gonzalez, Alvaro, et al. "**Learning to simulate complex physics with graph networks.**" International conference on machine learning. PMLR, 2020.

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THANK YOU