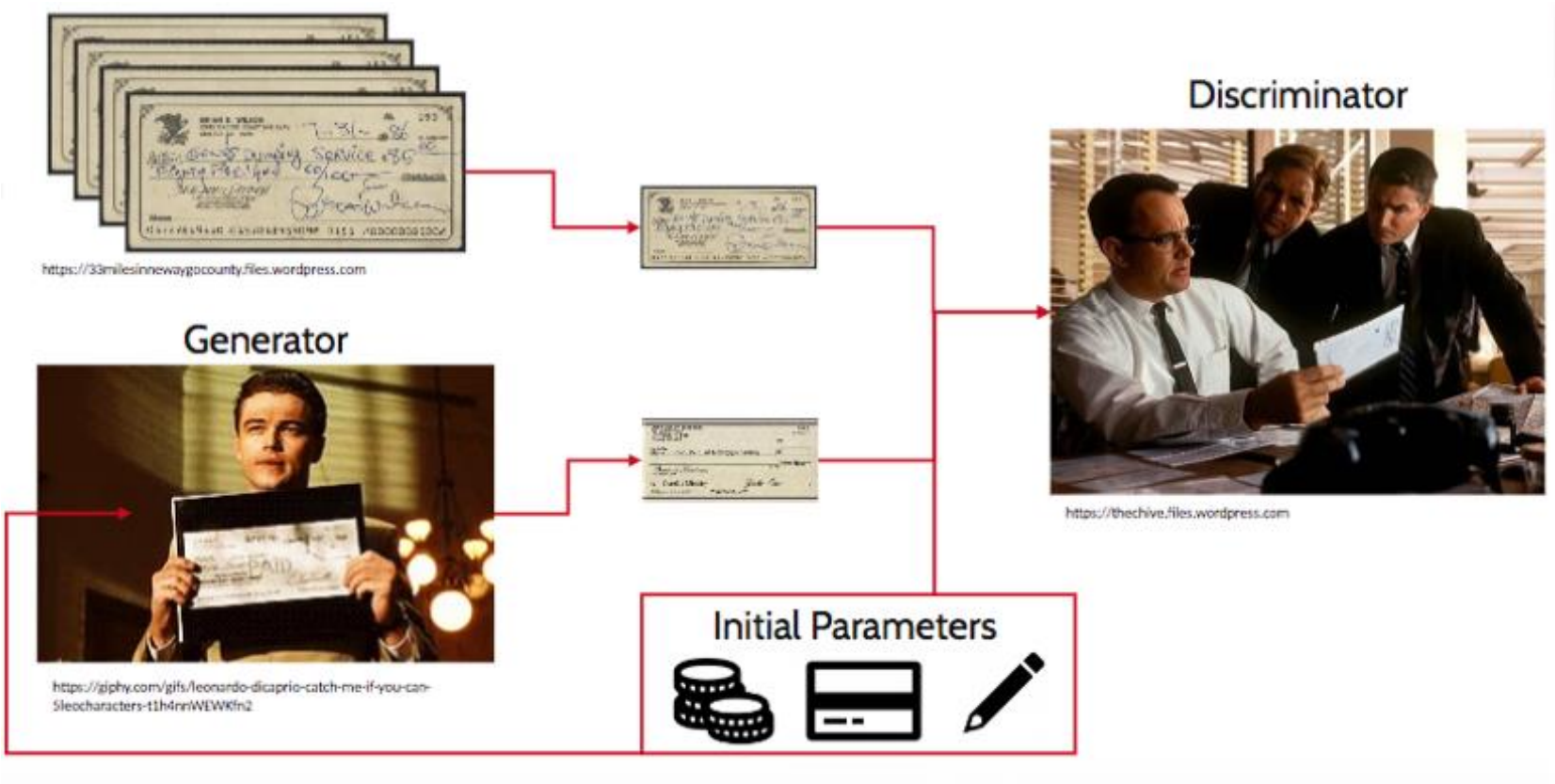
PH451, PH551

April 3, 2025

Generative Adversarial Networks



GAN

Generative Adversarial Networks

- Co-trained networks
  - first gradient **ascent** for **discriminator**
  - then gradient **descent** for **generator**
- **Game Theory:**
  - Nash Equilibrium, Minimax game
  - Watch out for “mode collapse”

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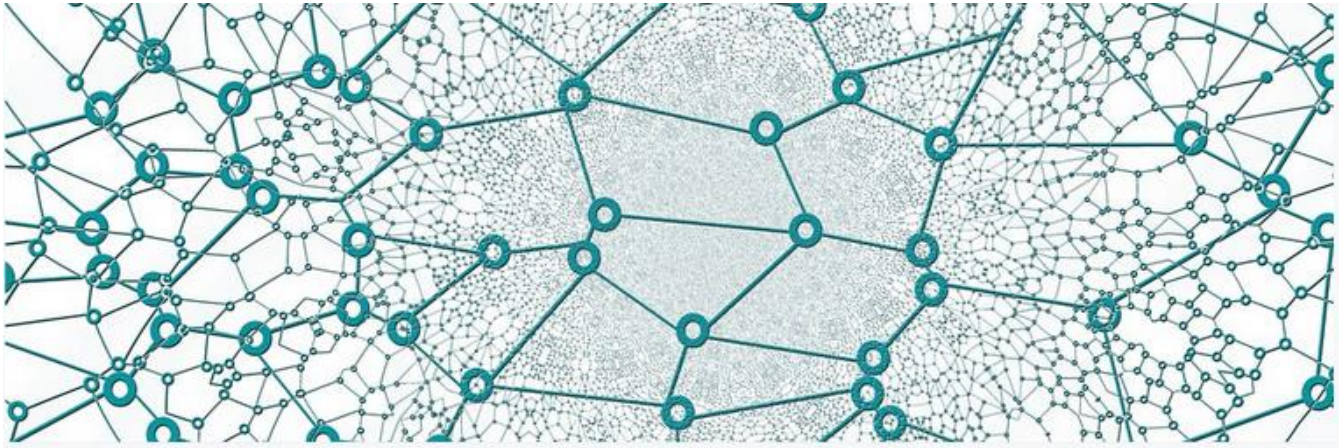
GAN

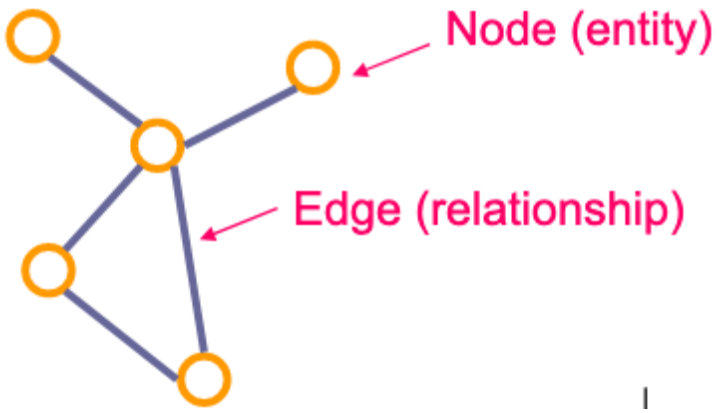
Graph Neural Networks



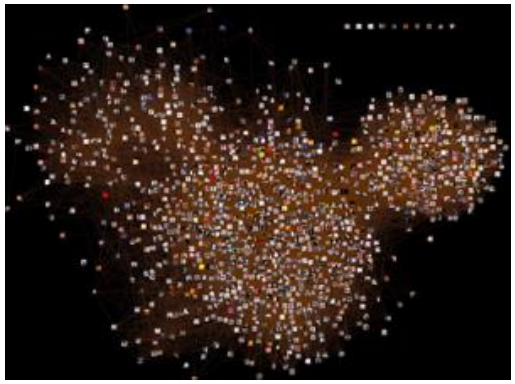
Graph Networks

Network definition:

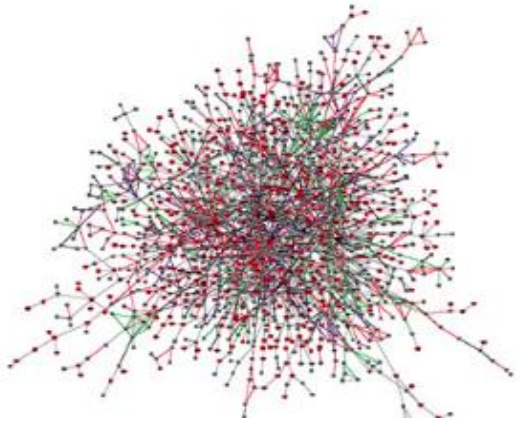
- collection of **entities (nodes)** joined by **relationships (edges)**
- Network = "**graph**"



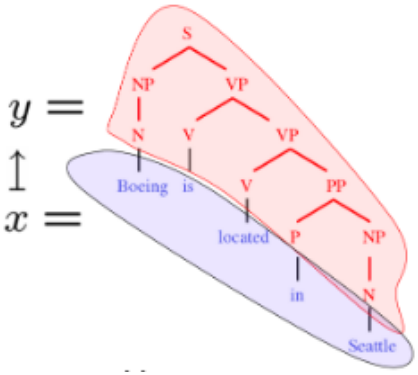
Examples



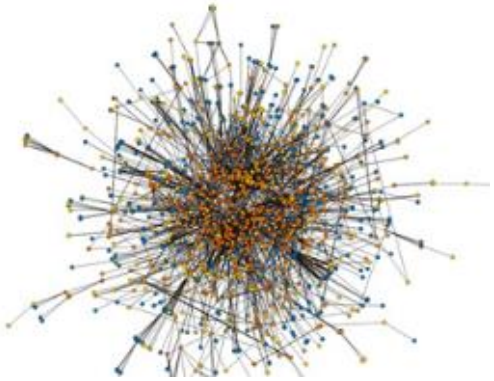
Social Network



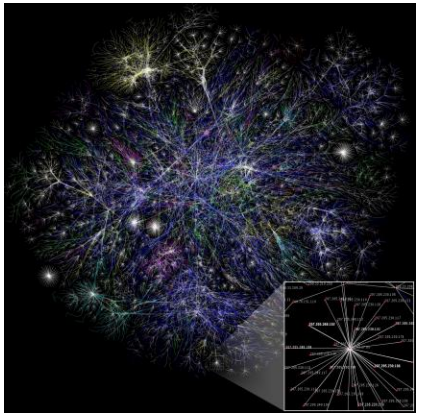
Protein-Protein Interactions



Natural Language Parsing



Genomic Associations

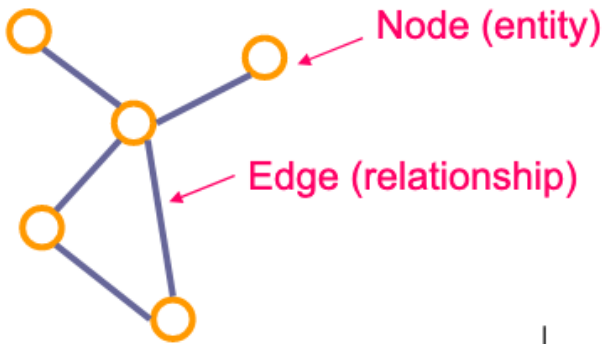


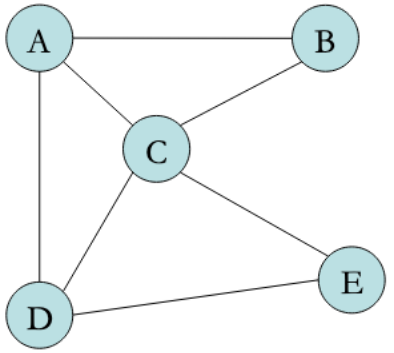
Internet Map

Graph Networks

How to build a simple graph

- Measure distance between **pairs**
- Connect each **entity** to its **k nearest neighbors**



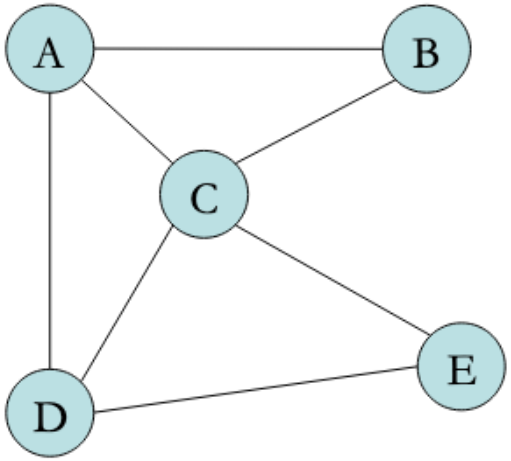


- Define: **Adjacency matrix**: A_{ij} weight of **edge** from i to j

Graph Networks

	1	1	1	
1		1		
1	1		1	1
1		1		1
		1	1	

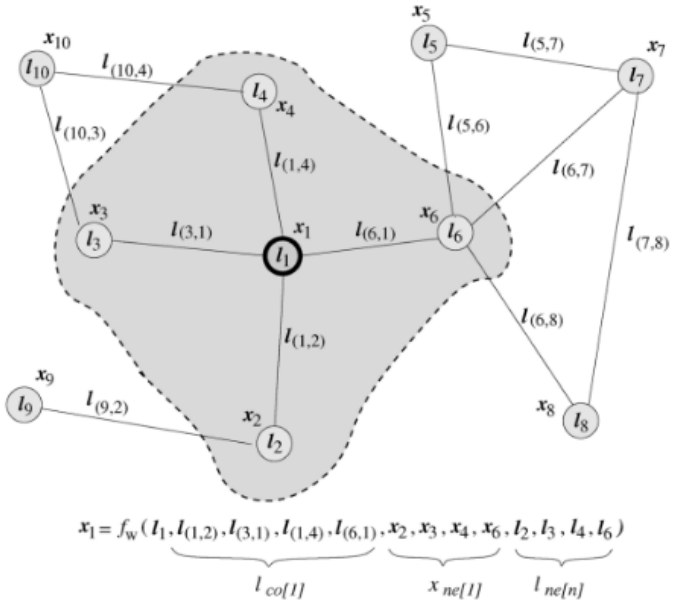
Adjacency matrix



Graph Neural Networks

Graph Neural Network:

- State of the **node** depends on its **neighbors**
- Any **neural network** can be expressed as a **graph**
- Powerful approach for when your data is not inherently **Euclidian**
- Optimize by **energy minimization**

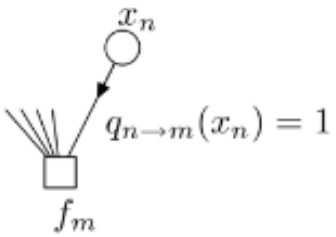


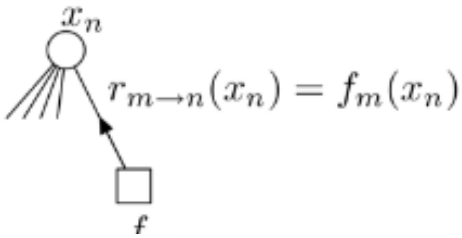
$$x_i = \sum_{j \in \mathcal{N}(i)} f(l_i, l_{i,j}, x_j, l_j)$$

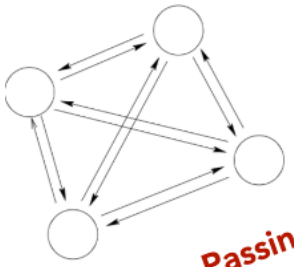
Message Passing

Message Passing Graph Neural Network:

- Message Passing
- Key idea: each **graph node** has a feature vector **hidden state**
  - Update the **hidden state** with **message from previous** hidden state (possibly also edges)



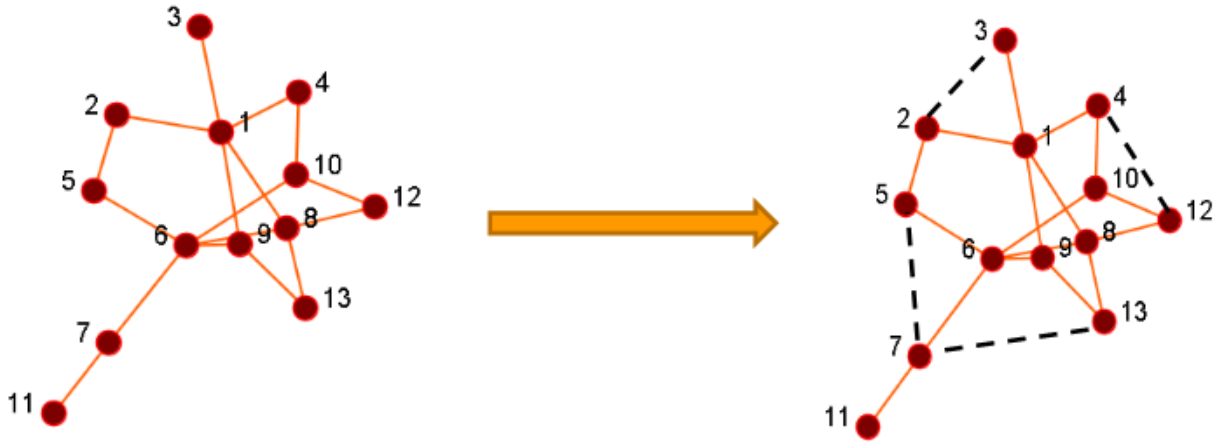




Graph Networks

Example: link prediction

- Which nodes are likely to get connected

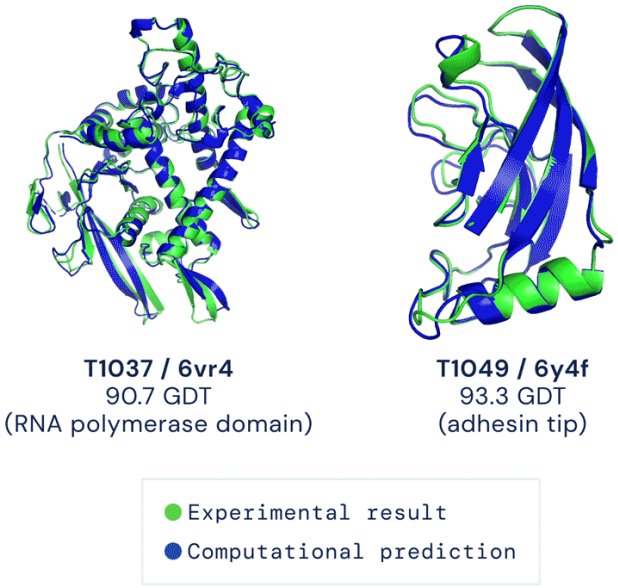


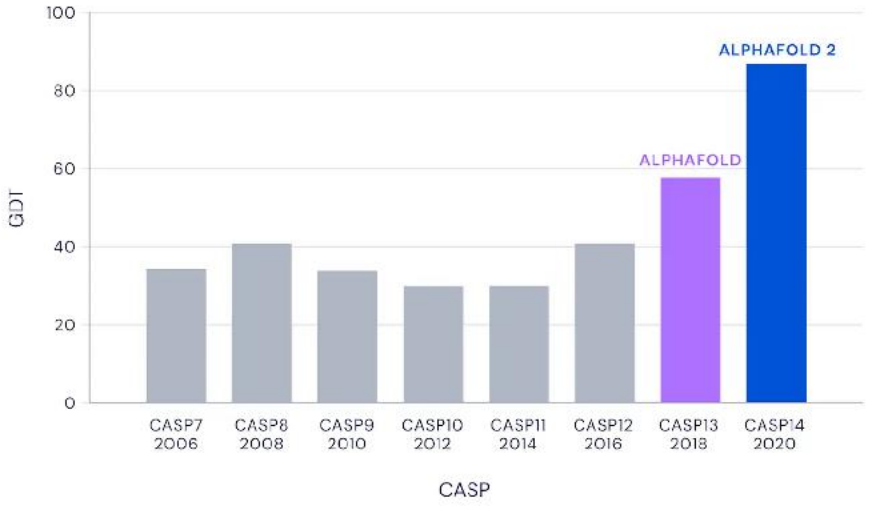
- i.e. Social network connection recommendations

Graph Networks

Example: protein folding

- Predicting which shapes proteins fold into





- Alphafold 2 (DeepMind 2020)