Stanford CS224W: Fast Neural Subgraph Matching and Counting

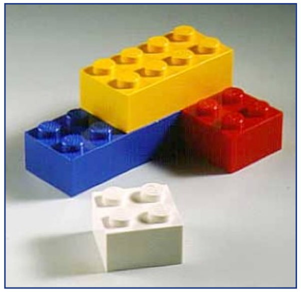
CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

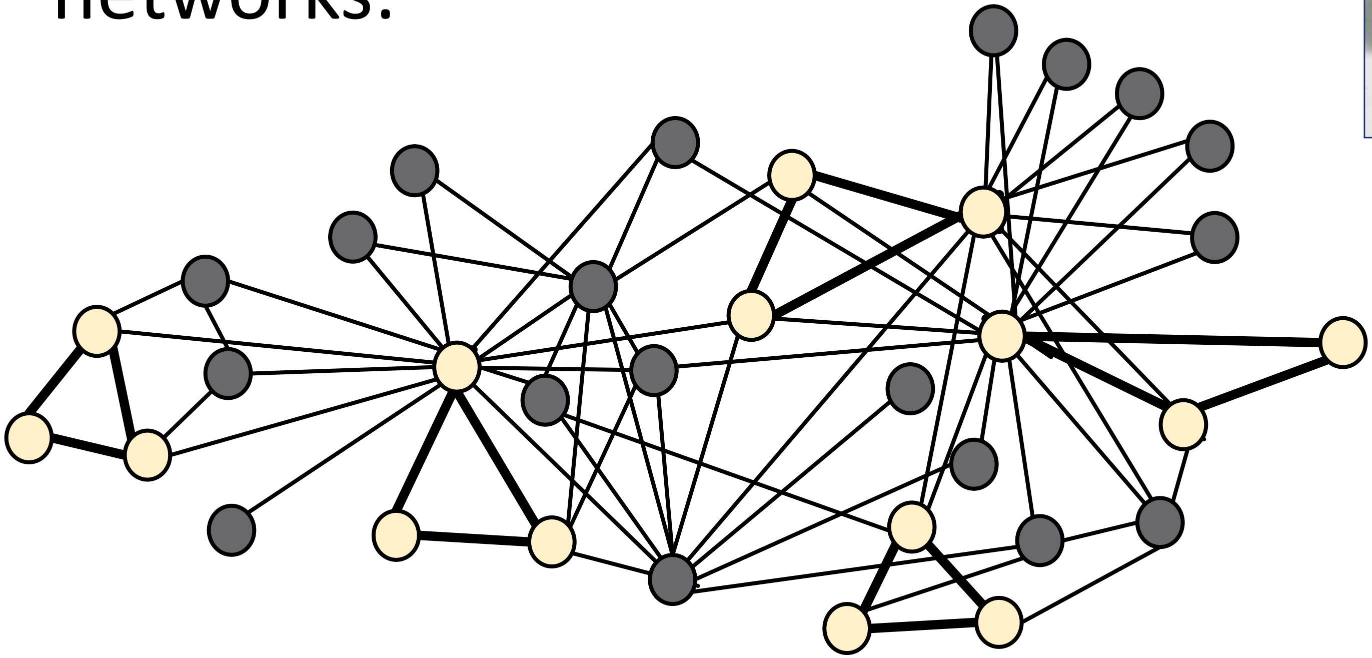
ANNOUNCEMENTS

- **No class next Tuesday! (11/02 - Democracy Day)**
- **Homework 2 due today**
  - Thanks for attending group OH! We will hold another one for Homework 3
  - Recordings are available on Canvas
- **Later today:**
  - Homework 3 out (due in two weeks on 11/11)
  - Colab 2 & Project Proposal grades released

Subgraphs

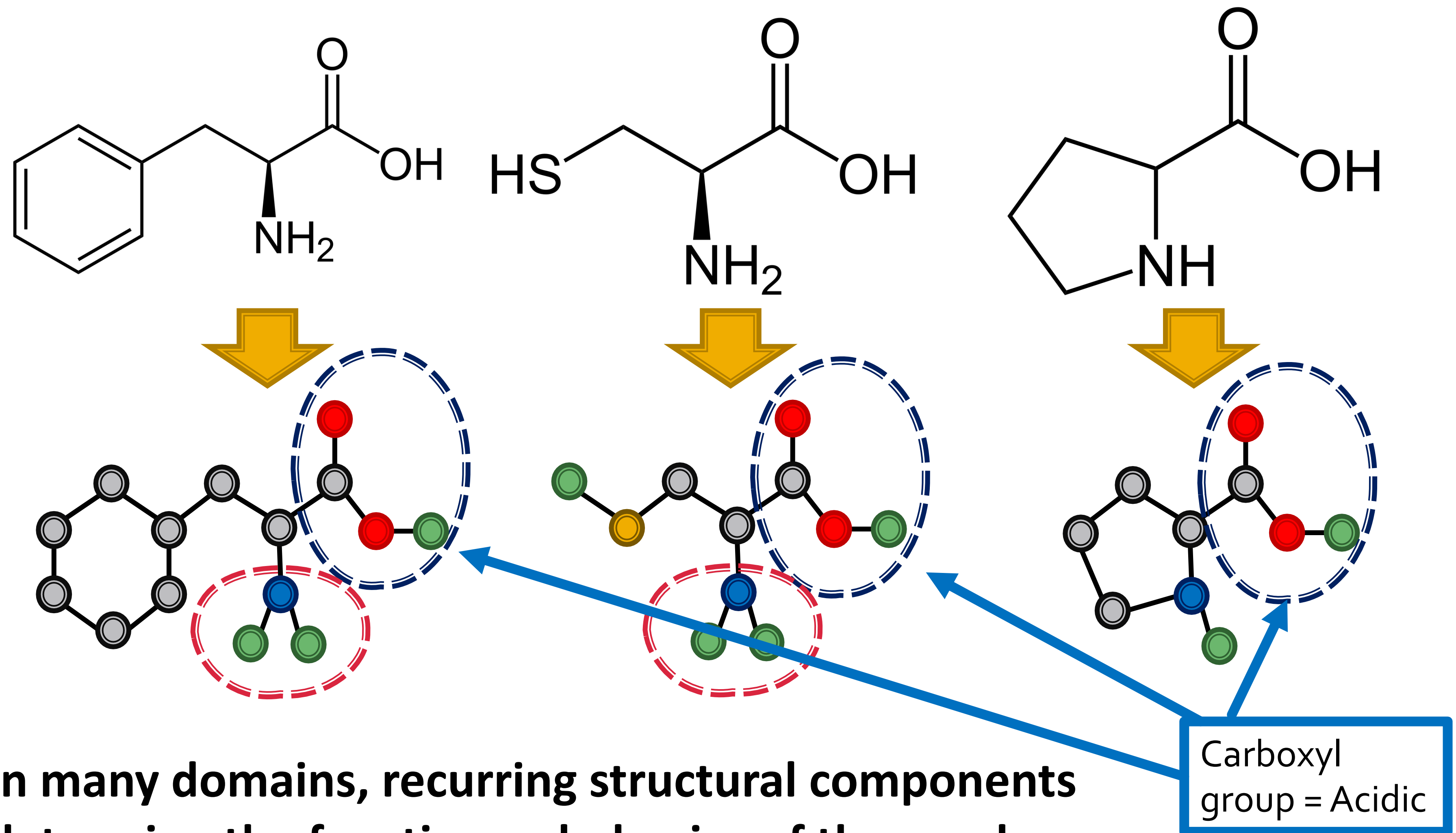
- **Subgraphs** are the building blocks of networks:





- They have the power to **characterize** and **discriminate** networks

Building Blocks of Networks



In many domains, recurring structural components determine the function or behavior of the graph

Plan for Today

1) Subgraphs and motifs

- Defining Subgraphs and Motifs
- Determining Motif Significance

2) Neural Subgraph Representations

3) Mining Frequent Motifs

Stanford CS224W: Subgraphs and Motifs

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Definition: Subgraph (1)

Two ways to formalize "network building blocks"

- Given graph $\boldsymbol{G} = (\boldsymbol{V}, \boldsymbol{E})$:

Def 1. Node-induced subgraph: Take subset of the **nodes** and all edges induced by the nodes:

- $G' = (V', E')$ is a node induced subgraph iff
  - $V' \subseteq V$
  - $E' = \{(u, v) \in E \mid u, v \in V'\}$
  - G' is the subgraph of G **induced** by V'

- **Alternate terminology:** "induced subgraph"

Definition: Subgraph (2)

Two ways to formalize "network building blocks"

- Given graph $\boldsymbol{G = (V, E)}$:

Def 2. Edge-induced subgraph: Take subset of the edges and all corresponding nodes

- $G' = (V', E')$ is an edge induced subgraph iff
  - $E' \subseteq E$
  - $V' = \{v \in V \mid (v, u) \in E'$ for some $u\}$

- **Alternate terminology:** "non-induced subgraph" or just "subgraph"

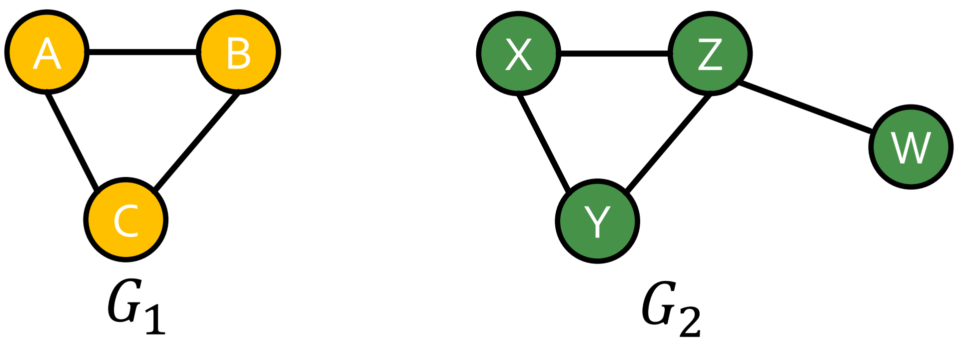
Definition: Subgraph (3)

Two ways to formalize "network building blocks"

- The best definition depends on the domain! **Examples:**
  - **Chemistry**: Node-induced (functional groups)
  - **Knowledge graphs**: Often edge-induced (focus is on edges representing logical relations)

Definition: Subgraph (4)

- The preceding definitions define subgraphs when $V' \subseteq V$ and $E' \subseteq E$, i.e. nodes and edges are taken from the original graph G.
- **What if V' and E' come from a totally different graph?** Example:



- **We would like to say that G_1 is "contained in" G_2**

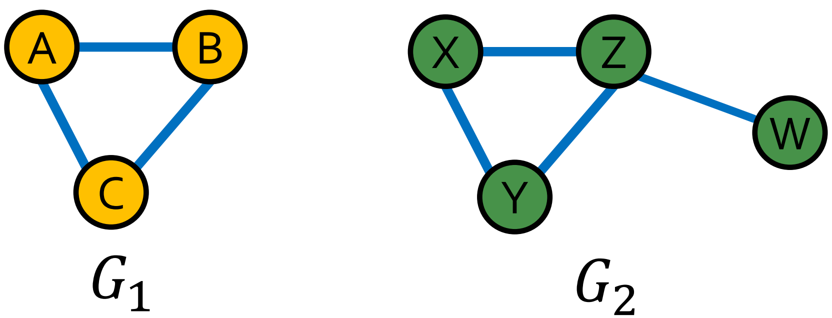
Graph Isomorphism

- **Graph isomorphism problem:** Check whether two graphs are identical:
  - $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are **isomorphic** if there exists a bijection $f: V_1 \to V_2$ such that $(u, v) \in E_1$ iff $\left(f(u), f(v)\right) \in E_2$
    - f is called the **isomorphism:**

- We do not know if graph isomorphism is NP-hard, nor is any polynomial algorithm found for solving graph isomorphism.

Subgraph Isomorphism

- G_2 is **subgraph-isomorphic** to G_1 if some subgraph of G_2 is isomorphic to G_1
  - We also commonly say G_1 is a subgraph of G_2
  - We can use either the node-induced or edge-induced definition of subgraph
  - **This problem is NP-hard**



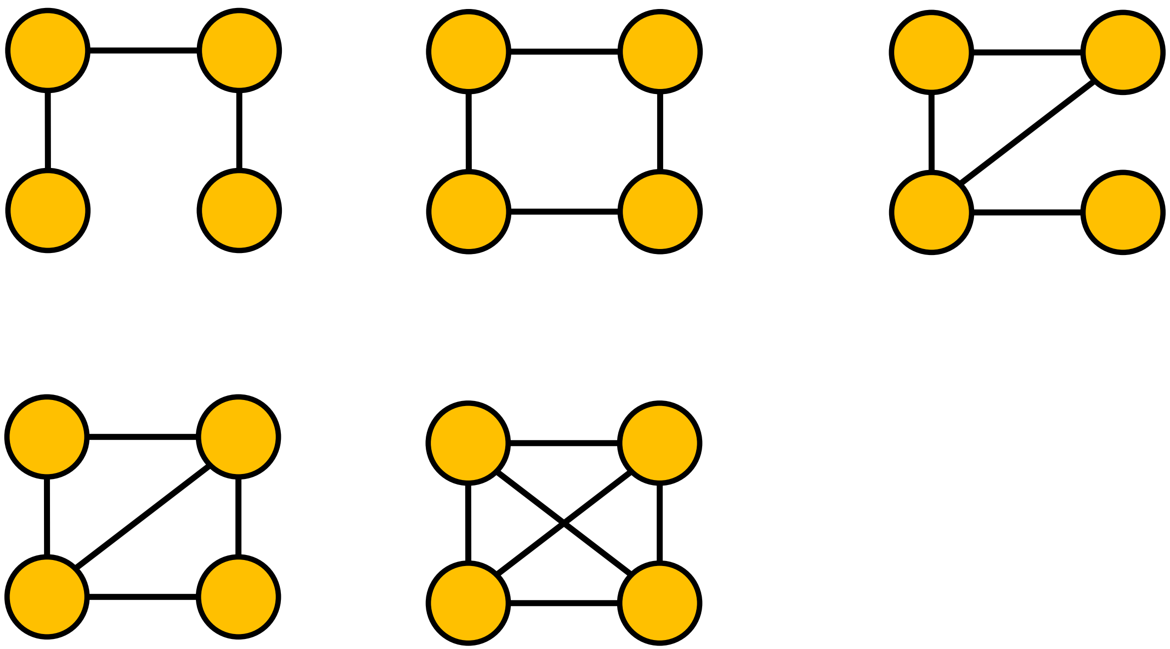
f:

V_1	V_2
A	X
B	Y
C	Z

A-B-C matches with X-Y-Z: There is a subgraph isomorphism between G1 and G2.

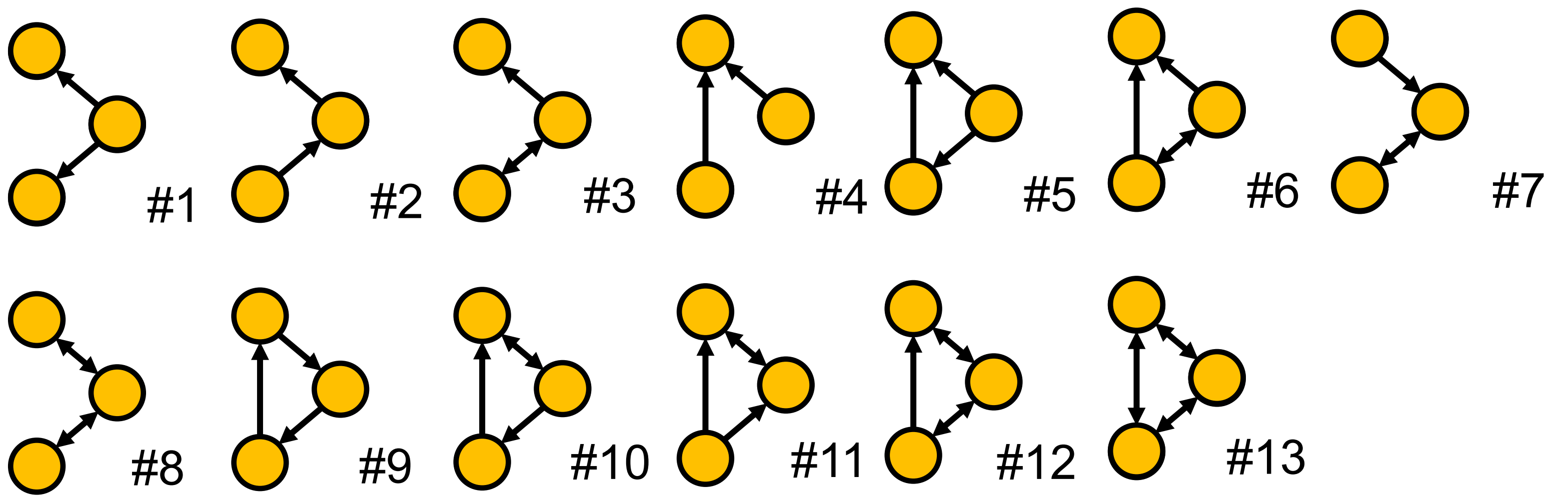
Case Example of Subgraphs (1)

All non-isomorphic, connected, undirected graphs of size 4



Case Example of Subgraphs (2)

All non-isomorphic, connected, directed graphs of size 3



Network Motifs

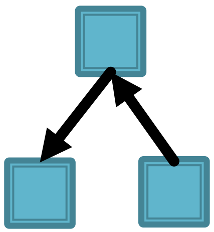
- **Network motifs:** "recurring, significant patterns of interconnections"

- **How to define a network motif:**
  - **Pattern:** Small (node-induced) subgraph
  - **Recurring:** Found many times, i.e., with high frequency **How to define frequency?**
  - **Significant:** More frequent than expected, i.e., in randomly generated graphs?

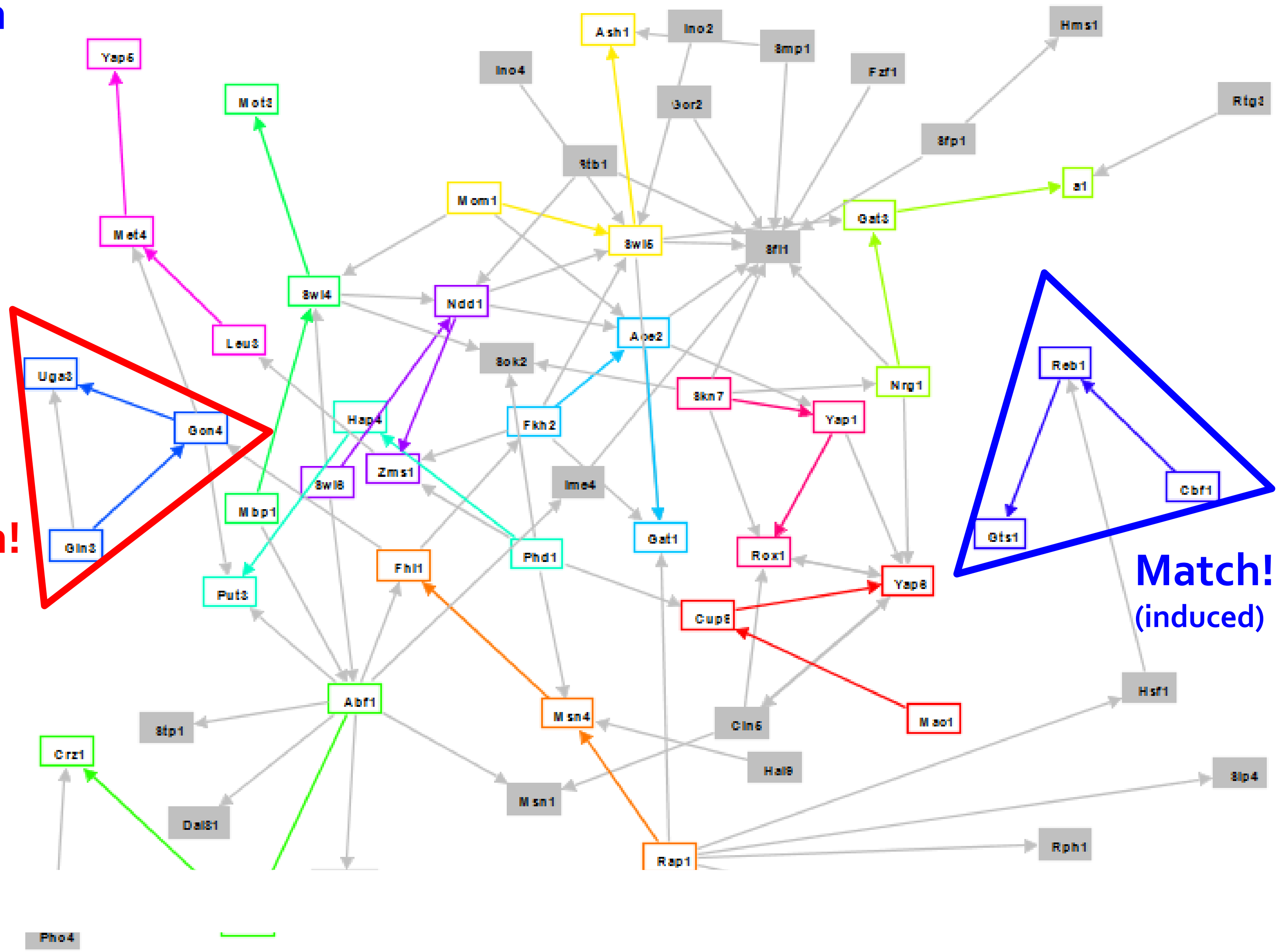
How to define random graphs?

Motifs: Induced Subgraphs

Induced subgraph
of interest
(aka Motif):

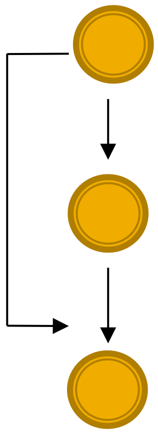


No match!
(not induced)



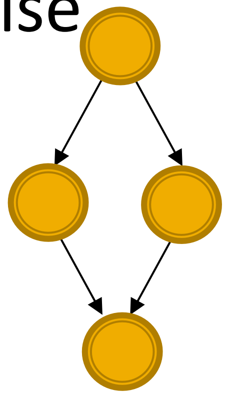
Why Do We Need Motifs?

- **Motifs:**
  - Help us understand how graphs work
  - Help us make predictions based on presence or lack of presence in a graph dataset

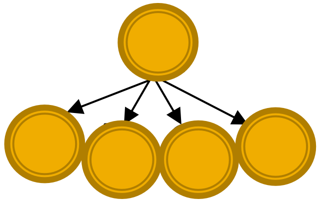


Feed-forward loop

- **Examples:**
  - **Feed-forward loops:** Found in networks of neurons, where they neutralize “biological noise”
  - **Parallel loops:** Found in food webs
  - **Single-input modules:** Found in gene control networks



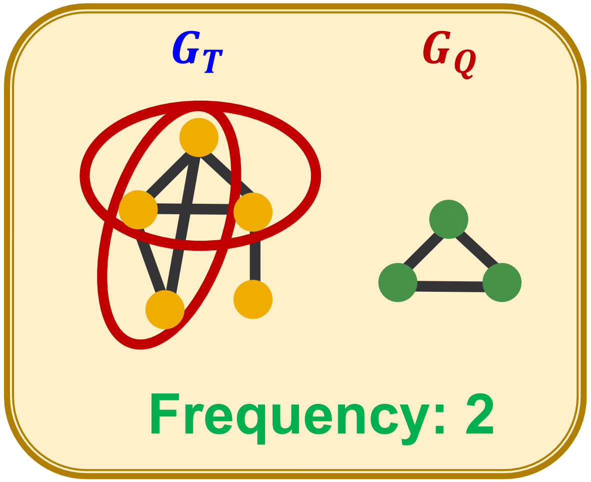
Parallel loop

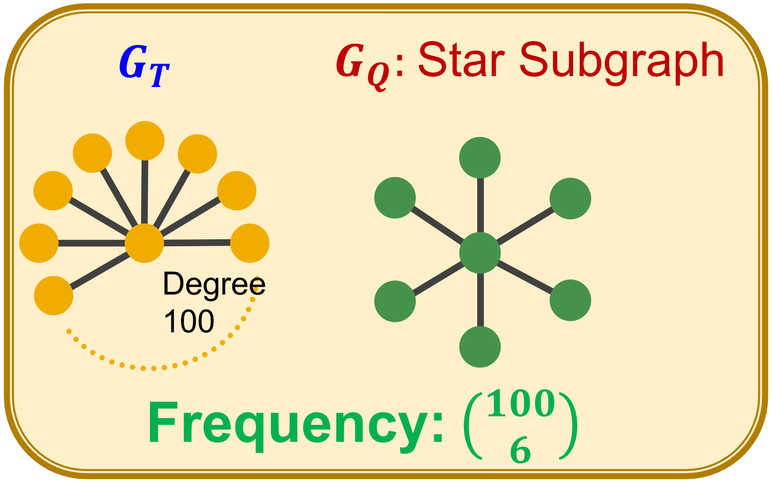


Single-input module

Subgraph Frequency (1)

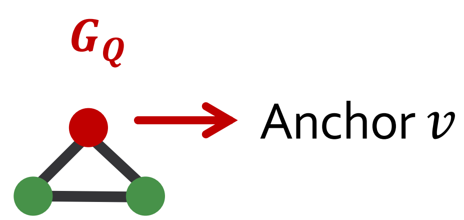
- Let G_Q be a small graph and G_T be a target graph dataset.
- **Graph-level Subgraph Frequency Definition**
  Frequency of G_Q in G_T: number of unique subsets of nodes V_T of G_T for which the subgraph of G_T induced by the nodes V_T is isomorphic to G_Q

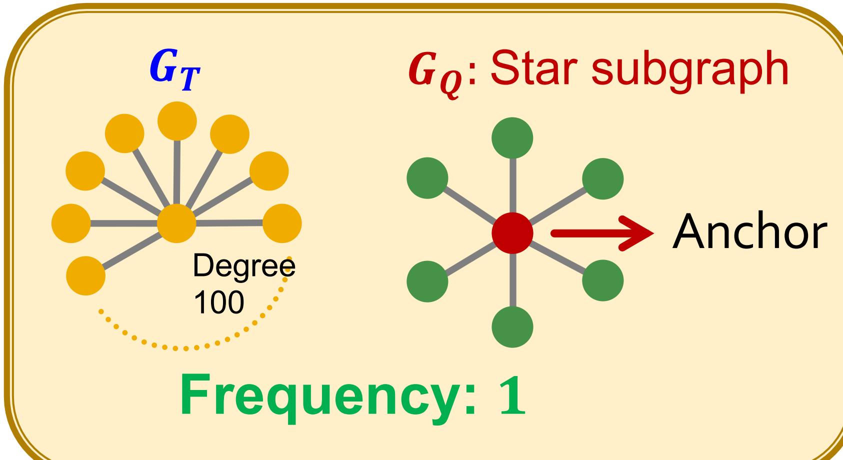




Subgraph Frequency (2)

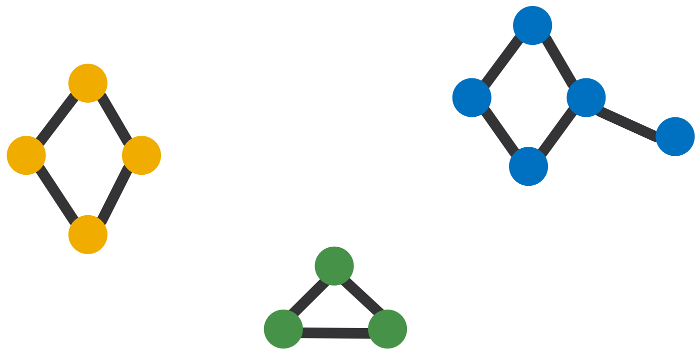
- Let G_Q be a small graph, v be a node in G_Q (the "anchor") and G_T be a target graph dataset.
- **Node-level Subgraph Frequency Definition:** The number of nodes u in G_T for which some subgraph of G_T is isomorphic to G_Q and the isomorphism maps node u to v
- Let (G_Q, v) be called a **node-anchored** subgraph
- Robust to outliers





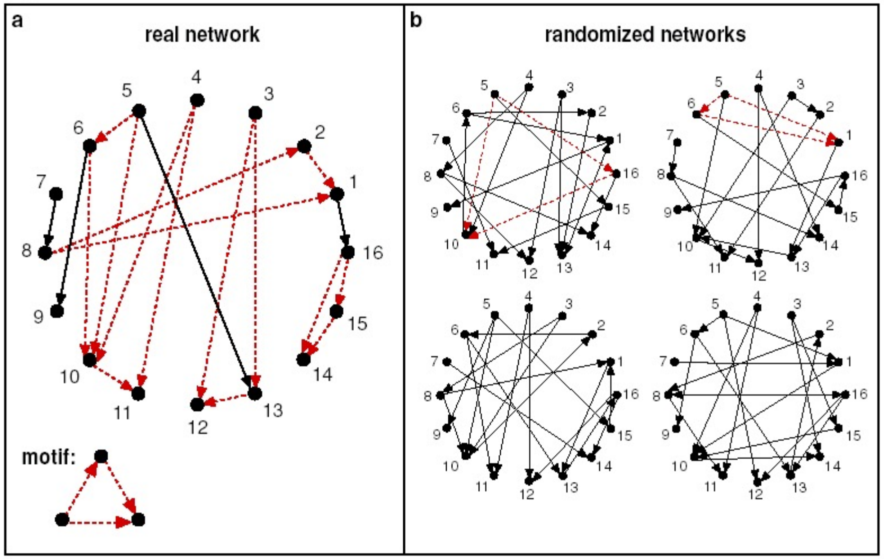
Subgraph Frequency (3)

- **What if the dataset contains multiple graphs, and we want to compute frequency of subgraphs in the dataset?**
- **Solution:** Treat the dataset as a giant graph G_T with disconnected components corresponding to individual graphs.



Defining Motif Significance

- To define significance, we need to have a null-model (i.e., point of comparison).
- **Key idea:** Subgraphs that occur in a real network much more often than in a random network have functional significance.

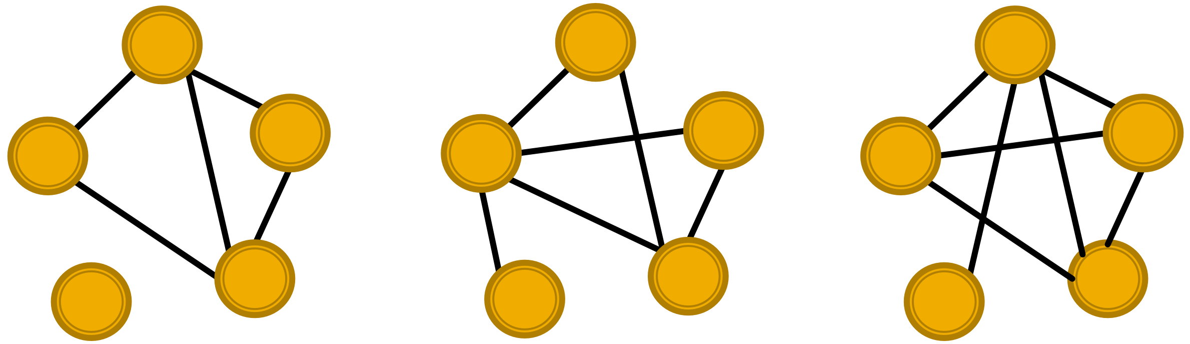


Milo *et. al.*, Science 2002

Defining Random Graphs

Erdős–Rényi (ER) random graphs:

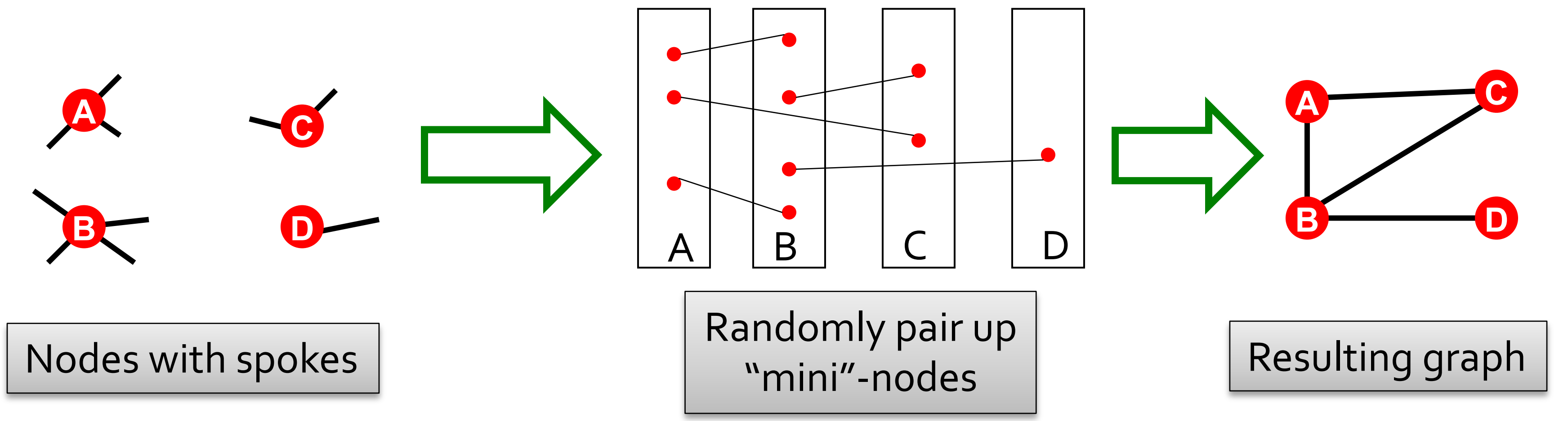
- $\boldsymbol{G_{n,p}}$: undirected graph on n nodes where each edge (u, v) appears i.i.d. with probability p
  - **How to generate the graph:** Create n nodes, for each pair of nodes (u, v) flip a biased coin with bias p
- Generated graph is a result of a random process:



Three random graphs drawn from $\boldsymbol{G_{5,0.6}}$

New Model: Configuration Model

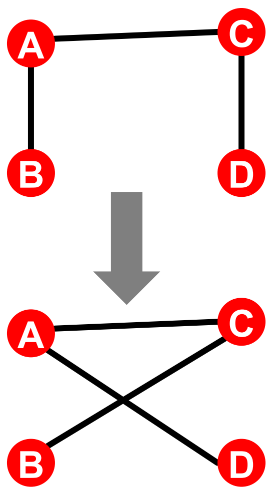
- **Goal:** Generate a random graph with a given **degree sequence** $k_1, k_2, \ldots k_N$
- **Useful as a "null" model of networks:**
  - We can compare the real network G^{real} and a "random" G^{rand} which has the same degree sequence as G^{real}
- **Configuration model:**



We ignore double edges and self-loops when creating the final graph

Alternative for Spokes: Switching

- Start from a **given graph G** Q is a constant parameter
- Repeat **the switching step** $Q \cdot |E|$ times:
  - Select a pair of edges A→B, C→D at random
  - **Exchange** the endpoints to give A→D, C→B
    - Exchange edges only if no multiple edges or self-edges are generated



- **Result:** A randomly rewired graph:
  - Same node degrees, randomly rewired edges
- Q is chosen large enough *(e.g., $Q = 100$)* for the process to converge

Motif Significance Overview

- **Intuition:** Motifs are **overrepresented** in a network when compared to **random graphs:**
- **Step 1: Count motifs** in the given graph (G^{real})
- **Step 2: Generate random graphs** with similar statistics (e.g. number of nodes, edges, degree sequence), and count motifs in the random graphs
- **Step 3: Use statistical measures** to evaluate how significant is each motif
  - Use **Z-score**

Z-score for Statistical Significance

- Z_i captures **statistical significance of motif i:**

$$Z_i = (N_i^{\mathrm{real}} - \bar{N}_i^{\mathrm{rand}}) / \mathrm{std}(N_i^{\mathrm{rand}})$$

  - N_i^{real} is #(motif i) in graph G^{real}
  - $\bar{N}_i^{\mathrm{rand}}$ is average #(motifs i) in random graph instances
- **Network significance profile (SP):**

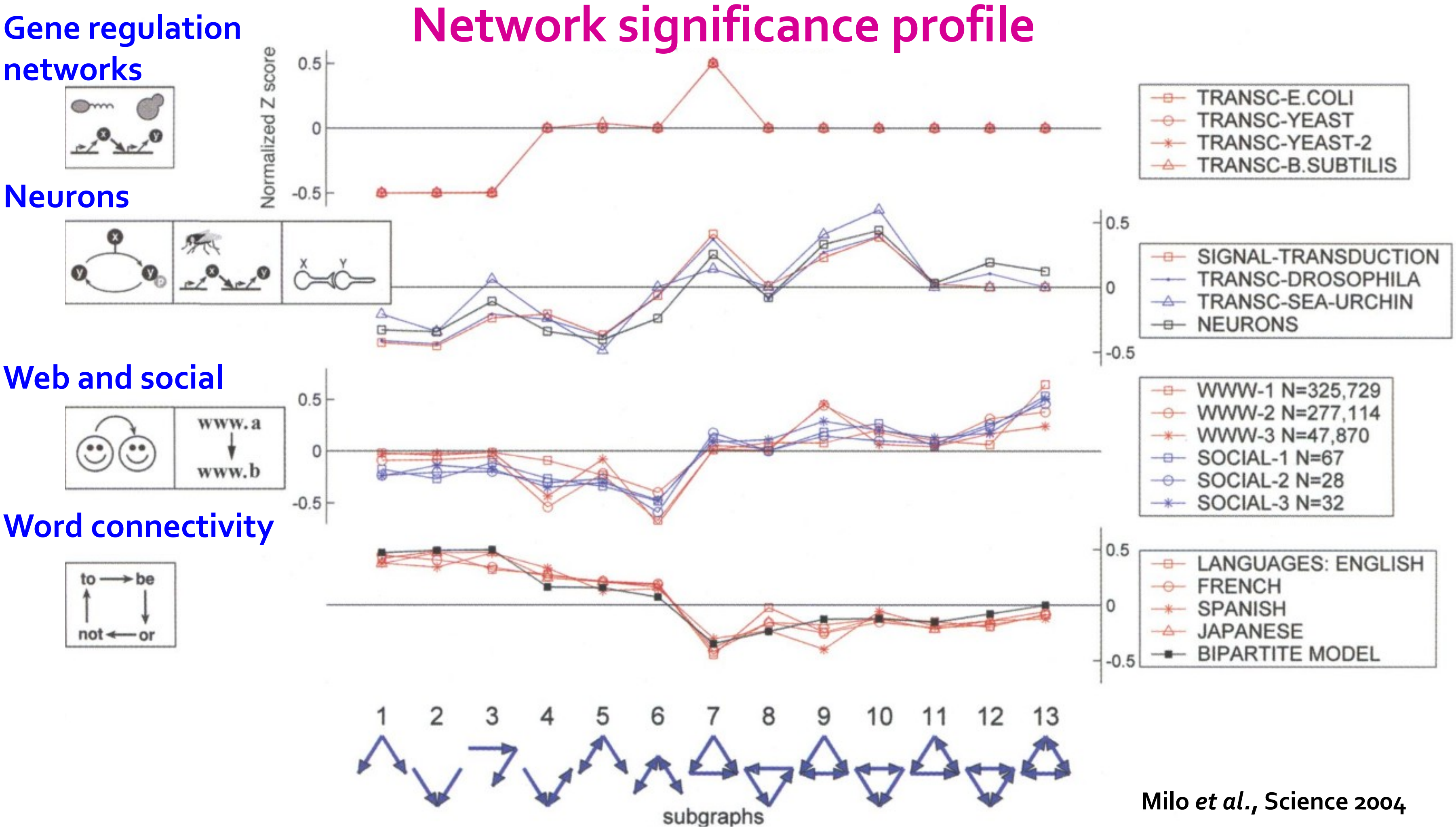
$$SP_i = Z_i / \sqrt{\sum_j Z_j^2}$$

  - SP is a vector of **normalized Z-scores**
  - The dimension depends on number of motifs considered
  - SP emphasizes relative significance of subgraphs:
    - Important for comparison of networks of different sizes
    - Generally, larger graphs display higher Z-scores

Significance Profile

- **For each subgraph:**
  - z-score metric is capable of classifying the subgraph "significance":
    - Negative values indicate **under-representation**
    - Positive values indicate **over-representation**
- We create a **network significance profile:**
  - A feature vector with values for all subgraph types
- **Next:** Compare profiles of different graphs with **random graphs**:
    - Regulatory network (gene regulation)
    - Neuronal network (synaptic connections)
    - World Wide Web (hyperlinks between pages)
    - Social network (friendships)
    - Language networks (word adjacency)

Example Significance Profile



Milo *et al.*, Science 2004

Networks from the same domain have similar significance profiles

Summary: Detecting Motifs

- Count subgraphs i in G^{real}
- Count subgraphs i in random graphs G^{rand}:
  - **Null model:** Each G^{rand} has the same #(nodes), #(edges) and degree distribution as G^{real}

- Assign **Z-score** to motif i:
  - $Z_i = (N_i^{\text{real}} - \bar{N}_i^{\text{rand}})/\text{std}(N_i^{\text{rand}})$
  - **High Z-score:** Subgraph i is a **network motif of G**

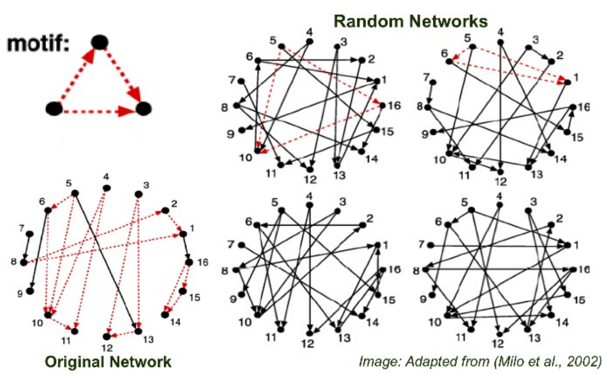
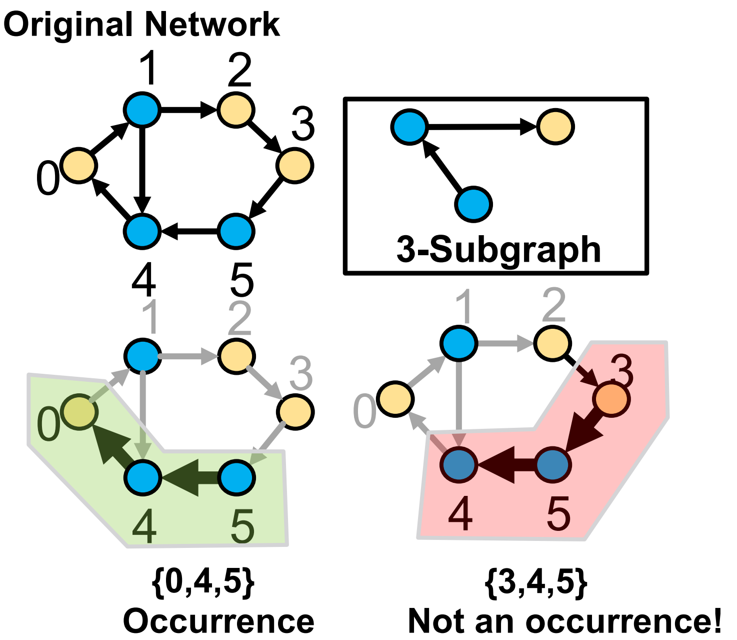
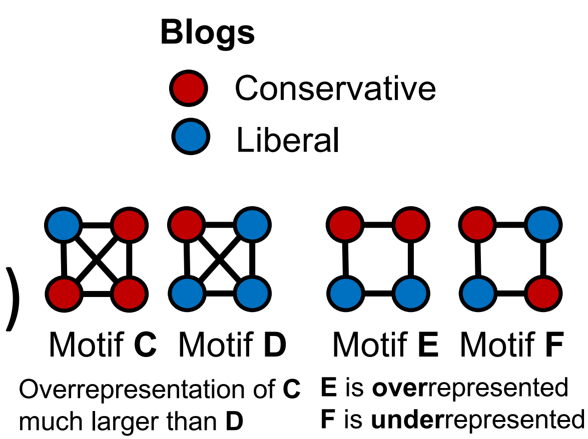


Image: Adapted from (Milo et al., 2002)

Variations on the Motif Concept

- **Extensions:**
  - Directed and undirected
  - Colored and uncolored
  - Temporal and static motifs
- **Variations on the concept:**
  - Different frequency concepts
  - Different significance metrics
  - Under-Representation (**anti-motifs**)
  - Different null models





Summary: Motifs

- Subgraphs and motifs are the **building blocks** of graphs
  - Subgraph isomorphism and counting are NP-hard
- Understanding which motifs are frequent or significant in a dataset gives insight into the unique characteristics of that domain
- Use **random graphs** as null model to evaluate the significance of motif via **Z-score**

Stanford CS224W: Neural Subgraph Matching

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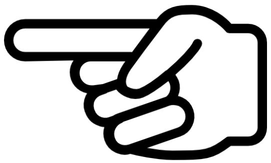
Plan for Today

1) Subgraphs and Motifs

- Defining Subgraphs and Motifs
- Determining Motif Significance

2) Neural Subgraph Representations

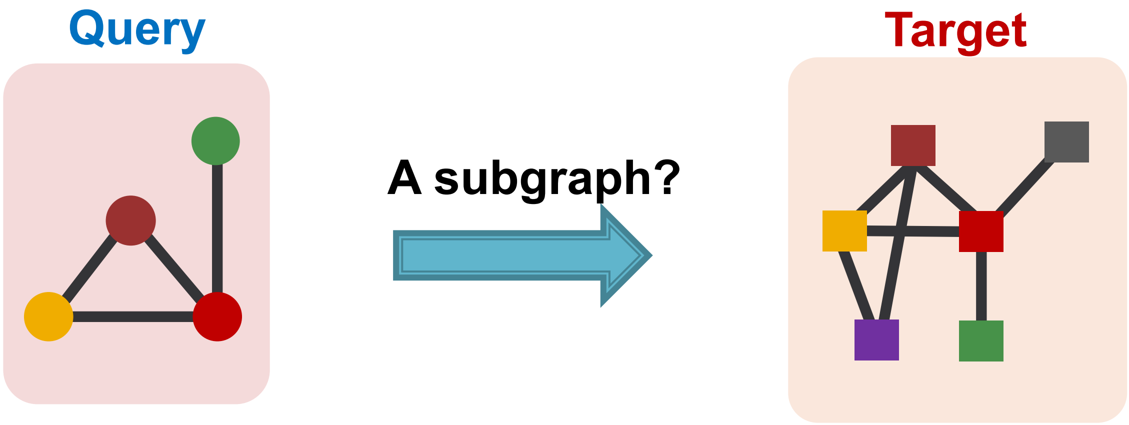


3) Mining Frequent Motifs

Subgraph Matching

Given:
- Large target graph (can be disconnected)
- Query graph (connected)

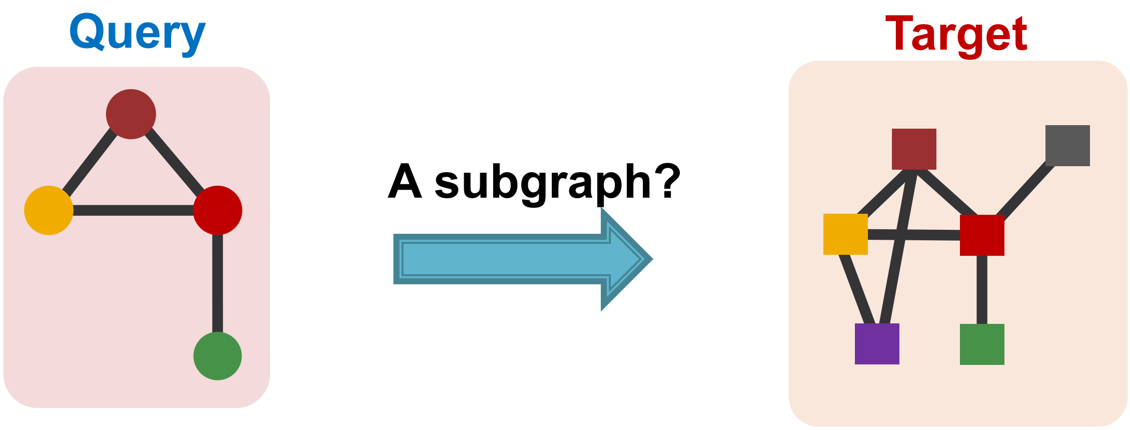
Decide:
- Is a query graph a subgraph in the target graph?



- Node colors indicate the correct mapping of the nodes

Isomorphism as an ML Task

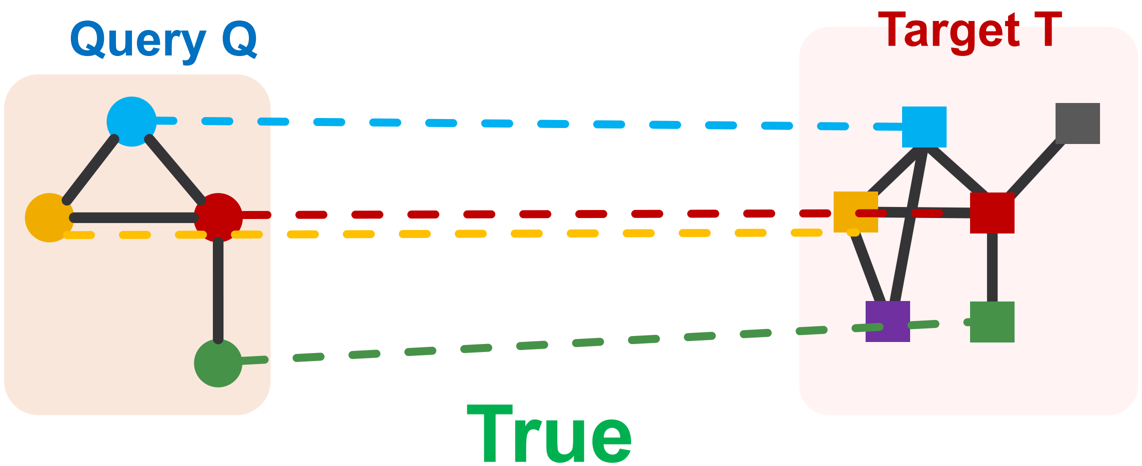
- Large target graph (can be disconnected)
- Query graph (has to be connected)
- **Use GNN to predict subgraph isomorphism:**



- **Intuition:** Exploit the **geometric shape** of **embedding space** to capture the properties of subgraph isomorphism

Task Setup

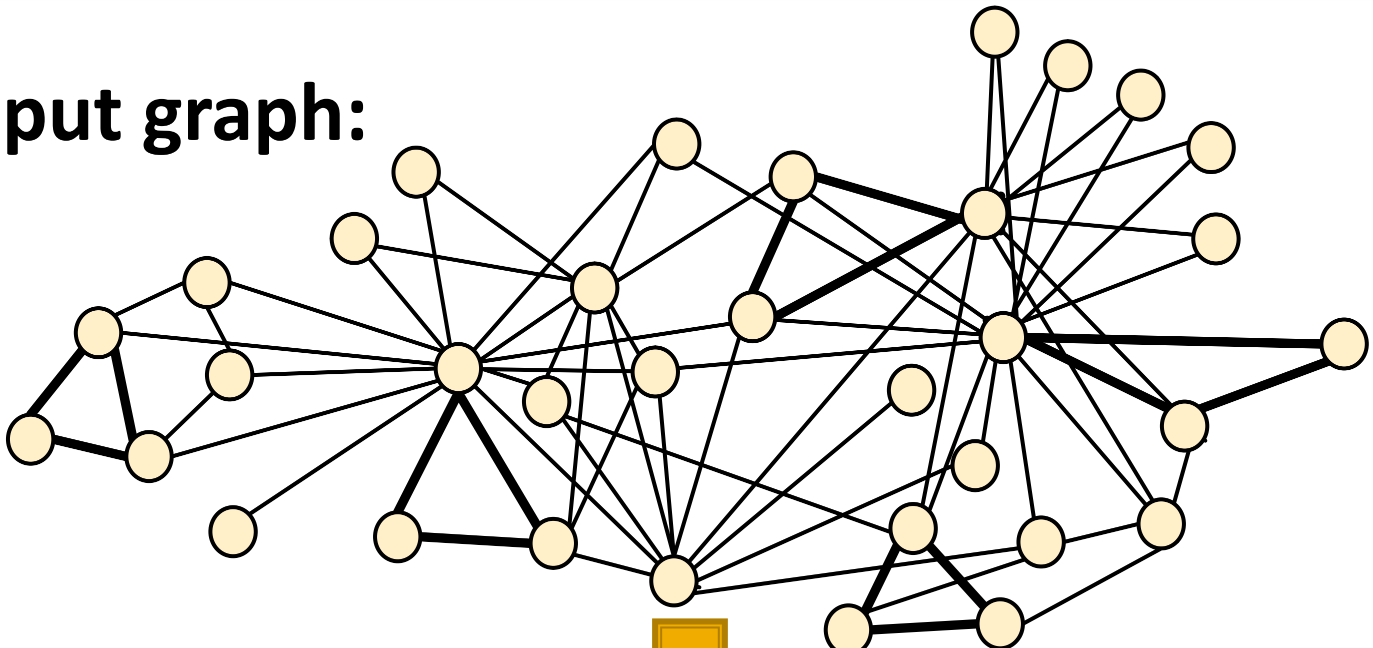
- **Consider a binary prediction:** Return **True** if query is isomorphic to a subgraph of the target graph, else return False

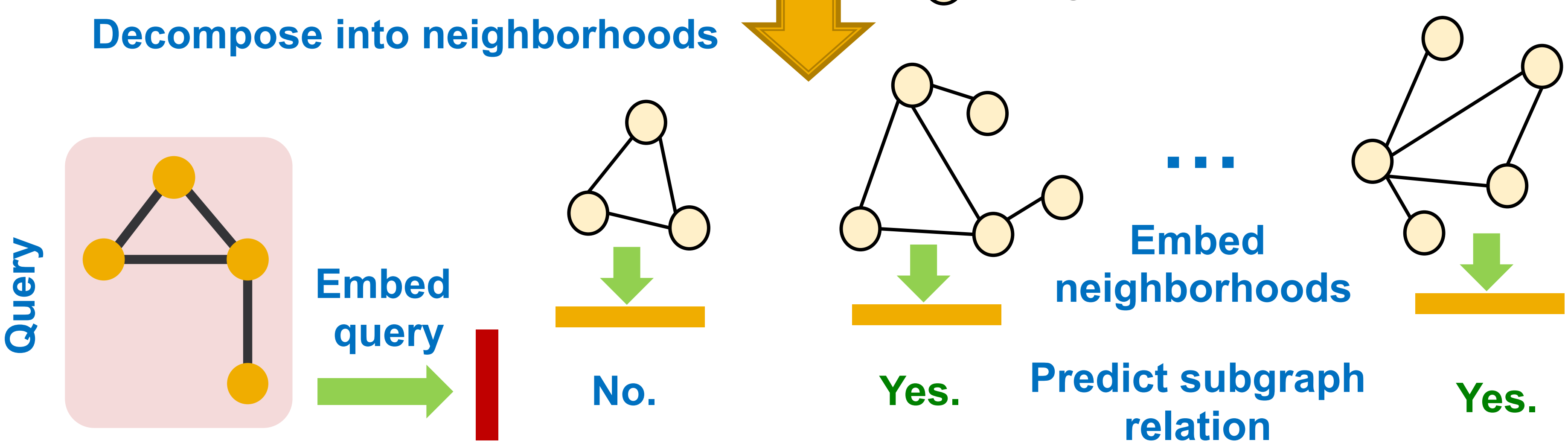


Finding node correspondences between Q and T is another challenging problem, which will not be covered in this lecture.

Overview of the Approach

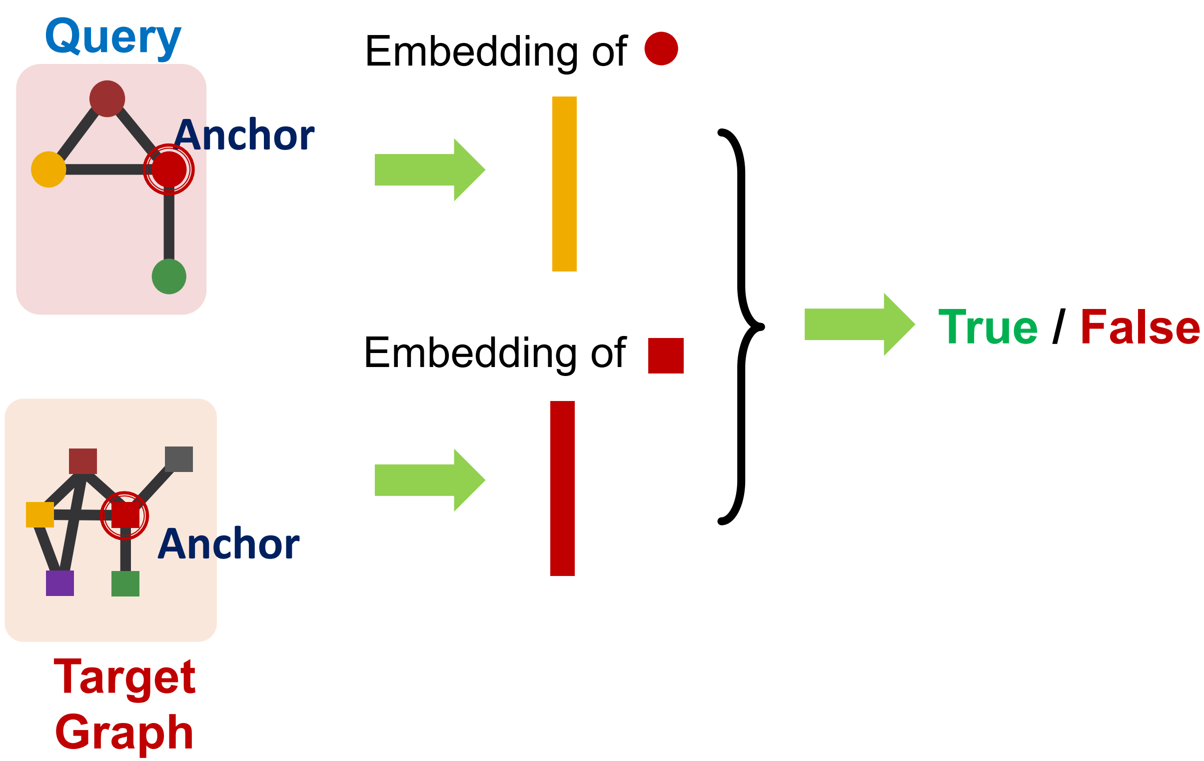
- **Input graph:**





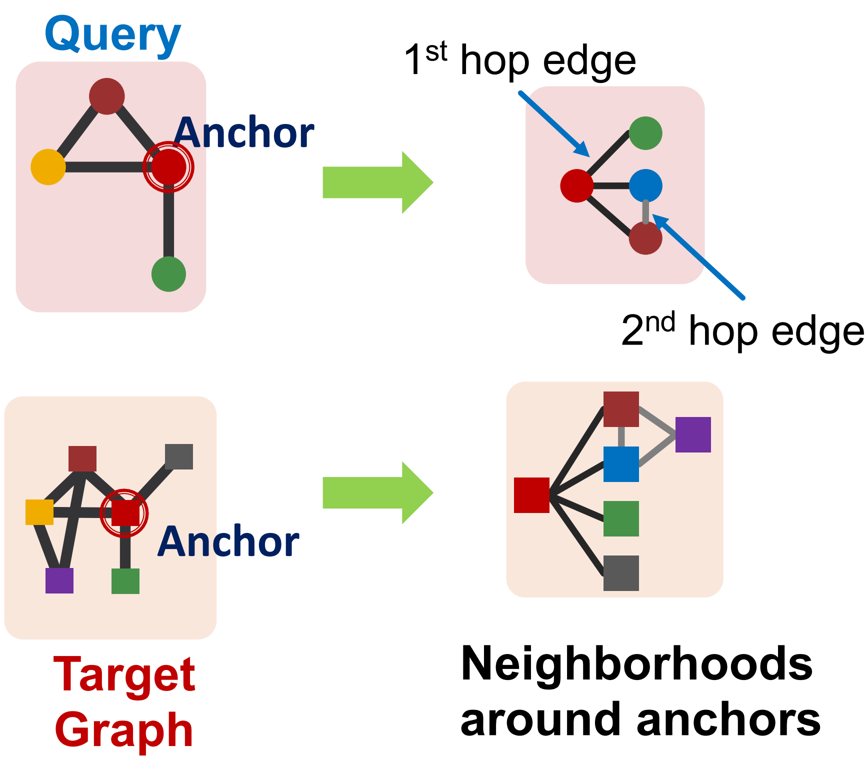
Neural Architecture for Subgraphs (1)

- **(1)** We are going to work with **node-anchored definitions**:



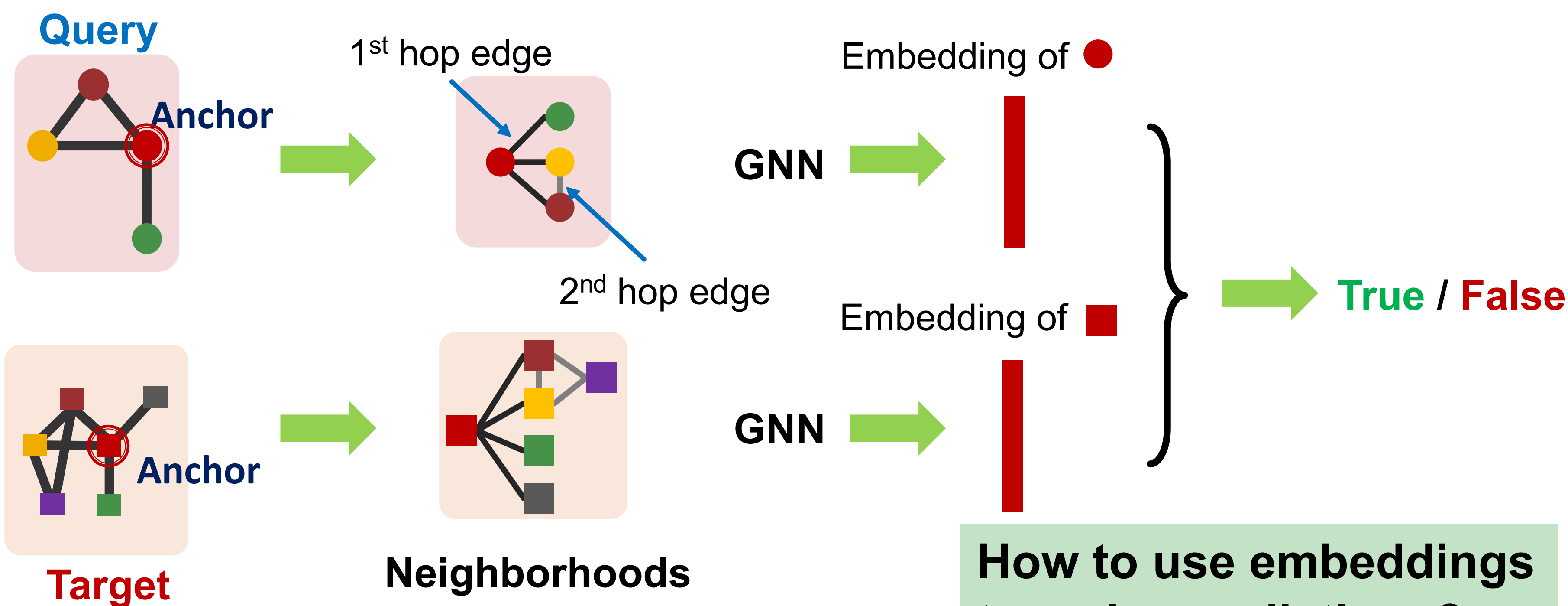
Neural Architecture for Subgraphs (2)

- **(2)** We are going to work with **node-anchored neighborhoods**:



Neural Architecture for Subgraphs (3)

- Use GNN to obtain representations of u and v
- **Predict if node u's neighborhood is isomorphic to node v's neighborhood:**



How to use embeddings to make predictions?

Why Anchor?

- **Recall node-level frequency definition:**
  The number of nodes u in G_T for which some subgraph of G_T is isomorphic to G_Q and the isomorphism maps u to v
- We can compute **embeddings** for u and v using GNN
- Use embeddings to decide if neighborhood of u is isomorphic to subgraph of neighborhood of v
- We not only predict if there exists a mapping, but also **a identify corresponding nodes** (u and v)!

Decomposing G_T into Neighborhoods

- **For each node in G_T:**
  - Obtain a **k-hop neighborhood** around the anchor
  - Can be performed using **breadth-first search** (BFS)
  - The depth k is a hyper-parameter (*e.g.* 3)
    - Larger depth results in more expensive model
- Same procedure applies to G_Q to obtain the neighborhoods
- We embed the neighborhoods using a GNN
  - By computing the **embeddings for the anchor** nodes in their respective neighborhoods

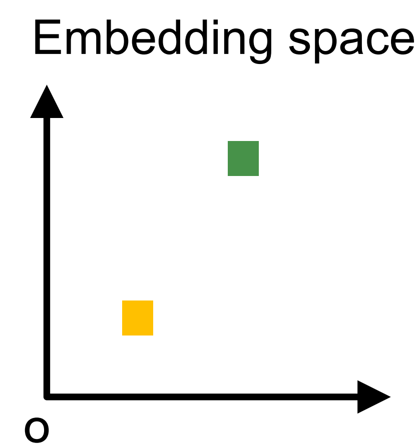
Order Embedding Space

Map graph A to a point z_A into a high-dimensional (e.g. 64-dim) embedding space, such that z_A is **non-negative in all dimensions**

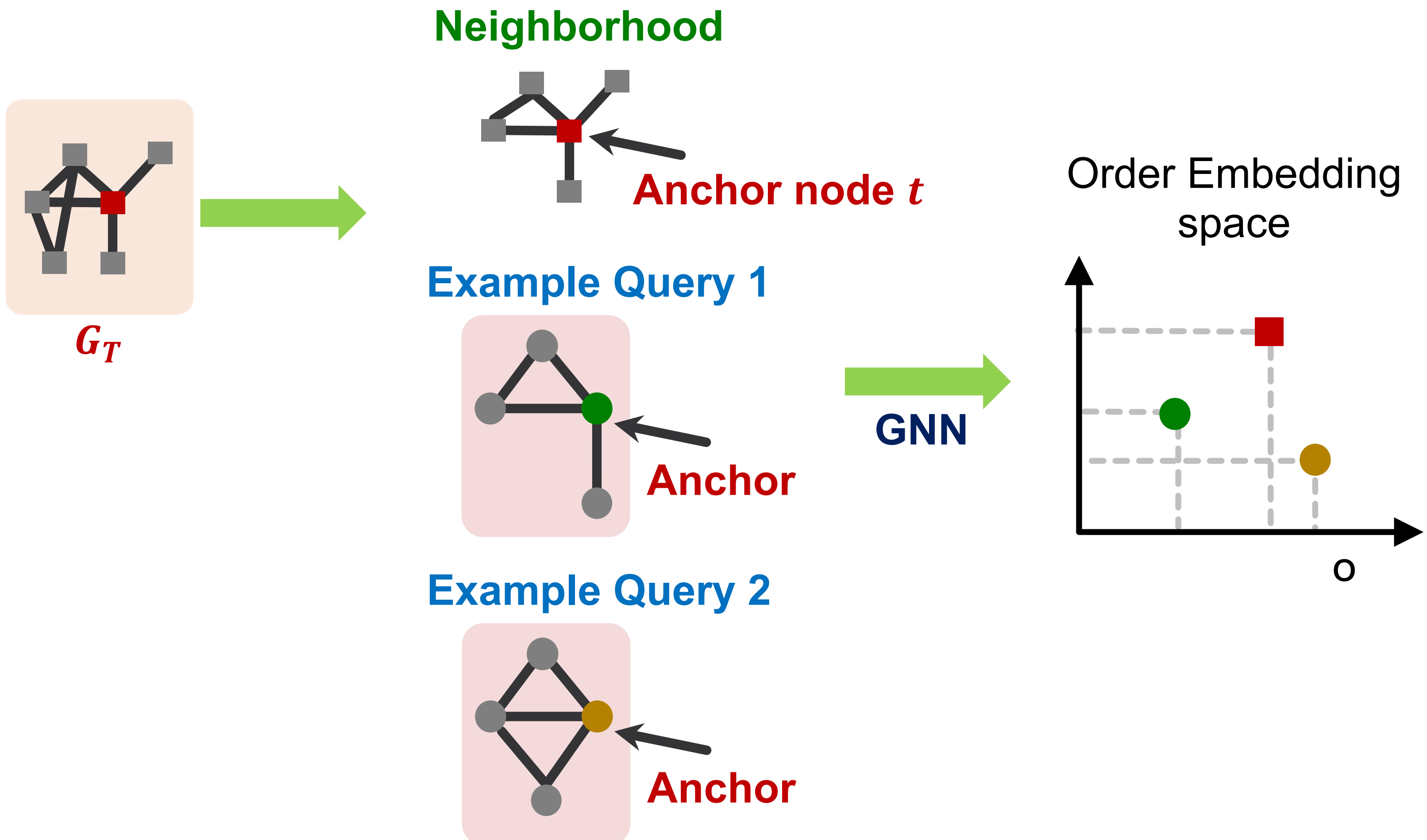
Capture partial ordering (transitivity):

- We use ■ $\preccurlyeq$ ■ to denote that the embedding of ■ is less than or equal to ■ in **all of its coordinates**
- If ■ $\preccurlyeq$ ■, ■ $\preccurlyeq$ ■ then ■ $\preccurlyeq$ ■

Intuition: subgraph is to the lower-left of its supergraph (in 2D)



Subgraph Order Embedding Space



By comparing the embedding, we find that ● $\preccurlyeq$ ■ but ● $\not\preccurlyeq$ ■ ,
Indicating that only query 1 is a subgraph of the neighborhood of t

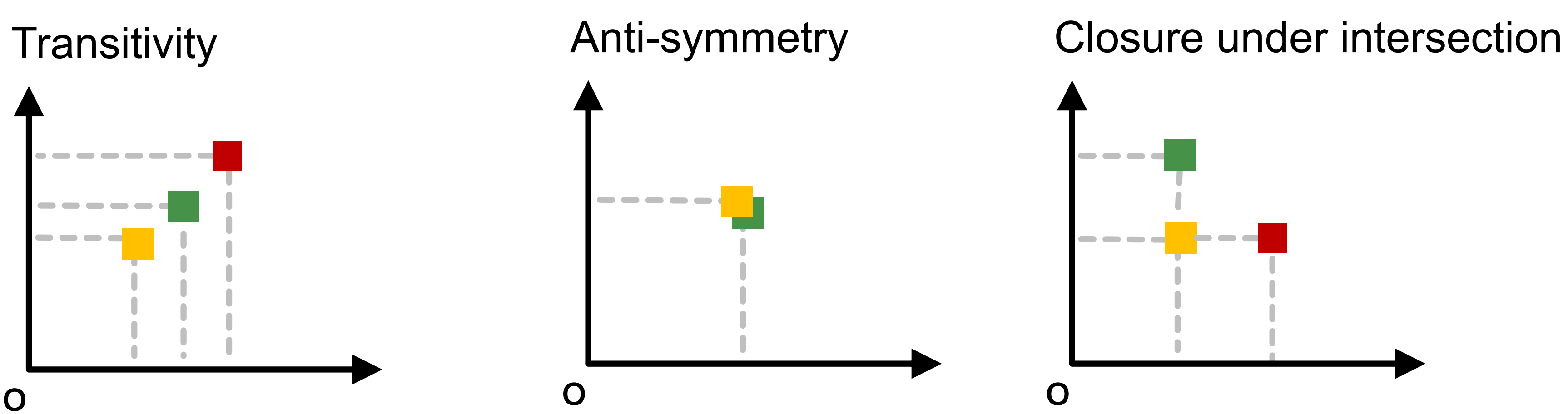
Why Order Embedding Space?

- **Subgraph isomorphism relationship** can be nicely encoded in **order embedding space**
  - **Transitivity**: If G_1 is a subgraph of G_2, G_2 is a subgraph of G_3, then G_1 is a subgraph of G_3
  - **Anti-symmetry**: If G_1 is a subgraph of G_2, and G_2 is a subgraph of G_1, then G_1 is isomorphic to G_2
  - **Closure under intersection**: The trivial graph of 1 node is a subgraph of any graph
  - **All properties have their counter-parts in the order embedding space**

Why Order Embedding Space?

- **Subgraph isomorphism relationship** can be nicely encoded in order embedding space
  - **Transitivity**: If 🟨 ≼🟩, 🟩≼🟥 then 🟨≼🟥
  - **Anti-symmetry**: If 🟨 ≼ 🟩 and 🟩 ≼ 🟨 , then 🟨 = 🟩
  - **Closure under intersection**: The 0 embedding satisfies 0 ≼🟨 for any order embedding 🟨 since all dimensions of order embedding are non-negative
    - Corollary: If 🟨≼🟩 and 🟨≼🟥 then 🟨 has a valid embedding

0 embedding: Trivial graph with one node



Order Constraint (1)

- We use a GNN to learn to embed neighborhoods and preserve the **order embedding** structure
- **What loss function should we use, so that the learned order embedding reflects the subgraph relationship?**
- We design loss functions based on the **order constraint:**
  - Order constraint specifies the ideal order embedding property that reflects subgraph relationships

Order Constraint (2)

We specify the order constraint to ensure that the subgraph properties are preserved in the order embedding space

Embedding dimension

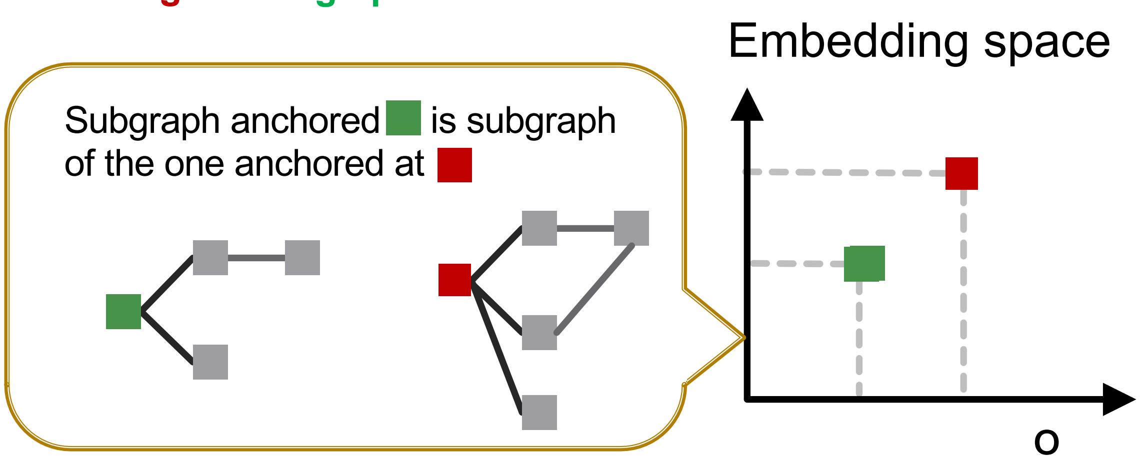
$$\forall_{i=1}^{D} z_q[i] \leq z_t[i] \ \text{ iff } \ G_Q \subseteq G_T$$

trained with max-margin loss

Query embedding

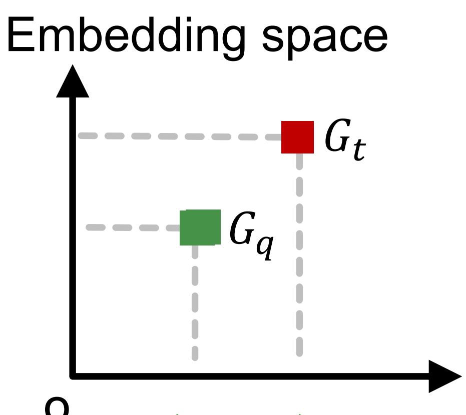
Target embedding

Subgraph Relation



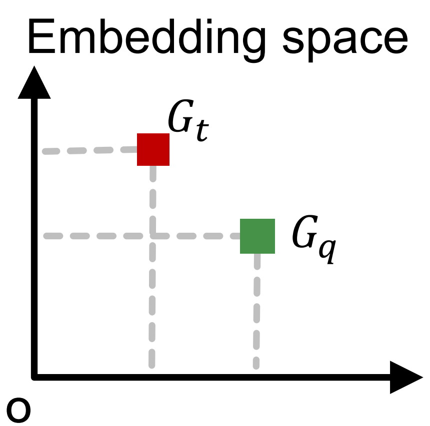
Loss Function: Order Constraint

- GNN Embeddings are learned by minimizing a **max-margin** loss
- Define $E(G_q, G_t) = \sum_{i=1}^{D}(\max(0, z_q[i] - z_t[i]))^2$ as the "margin" between graphs G_q and G_t



$E(G_q, G_t) = 0$

According to the order embedding, G_q is a subgraph of G_t!



$E(G_q, G_t) > 0$

According to the order embedding, G_q is **not** a subgraph of G_t!

Loss Function

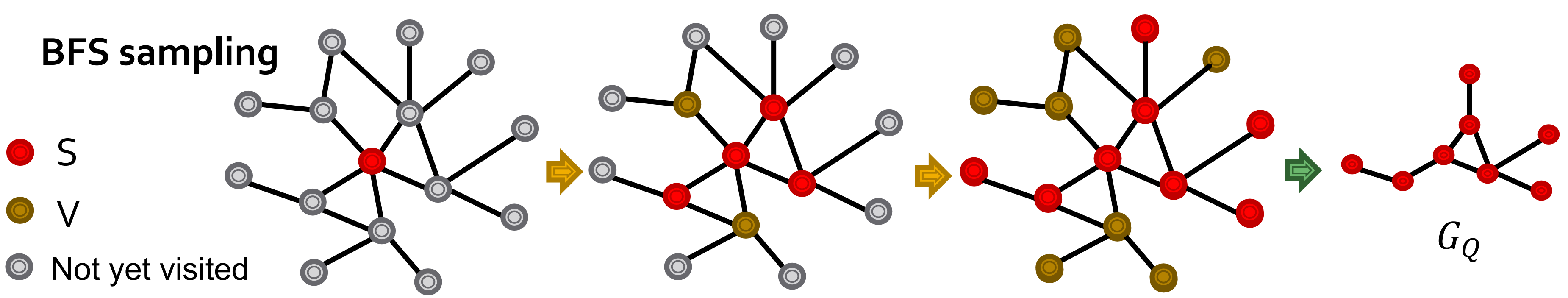
- Embeddings are learned by minimizing a **max-margin** loss
- Let $E(G_q, G_t) = \sum_{i=1}^{D} (\max(0, z_q[i] - z_t[i]))^2$ be the "margin" between graphs G_q and G_t
- **To learn the correct order embeddings, we want to learn $\boldsymbol{z_q, z_t}$ such that**
  - $E(G_q, G_t) = 0$ when G_q **is** a subgraph of G_t
  - $E(G_q, G_t) > 0$ when G_q **is not** a subgraph of G_t

Training Neural Subgraph Matching

- To learn such embeddings, **construct training examples** (G_q, G_t) where half the time, G_q is a subgraph of G_t, and the other half, it is not
- Train on these examples by minimizing the following **max-margin loss**:
  - **For positive examples:** Minimize $E(G_q, G_t)$ when G_q is a subgraph of G_t
  - **For negative examples:** Minimize $\max(0, \alpha - E(G_q, G_t))$
    - Max-margin loss prevents the model from learning the degenerate strategy of moving embeddings further and further apart forever

Training Example Construction

- Need to generate training queries G_Q and targets G_T from the dataset G
- Get G_T by choosing a random anchor v and taking all nodes in G within distance K from v to be in G_T
- **Positive examples:** Sample induced subgraph G_Q of G_T. Use **BFS sampling:**
  - Initialize $S = \{v\}, V = \emptyset$
  - Let $N(S)$ be all neighbors of nodes in S. At every step, sample 10% of the nodes in $N(S) \setminus V$, put them in S. Put the remaining nodes of $N(S)$ in V.
  - After K steps, take the subgraph of G induced by S anchored at q
- **Negative examples** (G_Q not subgraph of G_T): "corrupt" G_Q by adding/removing nodes/edges so it's no longer a subgraph.



Training Details

- **How many training examples to sample?**
  - At every iteration, we sample new training pairs
  - **Benefit**: Every iteration, the model sees different subgraph examples
  - Improves performance and avoids **overfitting** – since there are exponential number of possible subgraphs to sample from
- **How deep is the BFS sampling?**
  - A hyper-parameter that trades off **runtime and performance**
  - Usually use 3-5, depending on size of the dataset

Subgraph Predictions on New Graphs

- **Given**: query graph G_q anchored at node q, target graph G_t anchored at node t
- **Goal**: output whether the query is a node-anchored subgraph of the target
- **Procedure**:
  - If $E(G_q, G_t) < \epsilon$, predict "True"; else "False"
  - ϵ is a hyper-parameter
- To check if G_Q is isomorphic to a subgraph of G_T , repeat this procedure for all $q \in G_Q$, $t \in G_T$. Here G_q is the neighborhood around node $q \in G_Q$.

Summary: Neural Subgraph Matching

- Neural subgraph matching uses a **machine learning-based approach** to learn the NP-hard problem of subgraph isomorphism
  - Given query and target graph, it embeds both graphs into an order embedding space
  - Using these embeddings, it then computes $E(G_q, G_t)$ to determine whether query is a subgraph of the target
- Embedding graphs within an **order embedding space** allows subgraph isomorphism to be efficiently represented and tested by the relative positions of graph embeddings

Stanford CS224W: Finding Frequent Subgraphs

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

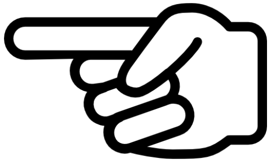
Plan for Today

1) Subgraphs and Motifs

- Defining Subgraphs and Motifs
- Determining Motif Significance

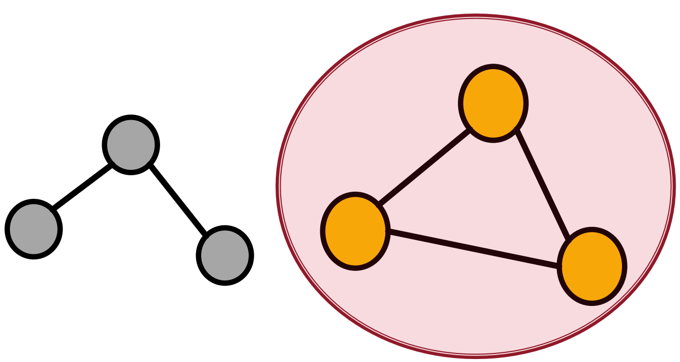
2) Neural Subgraph Representations

3) Mining Frequent Subgraphs

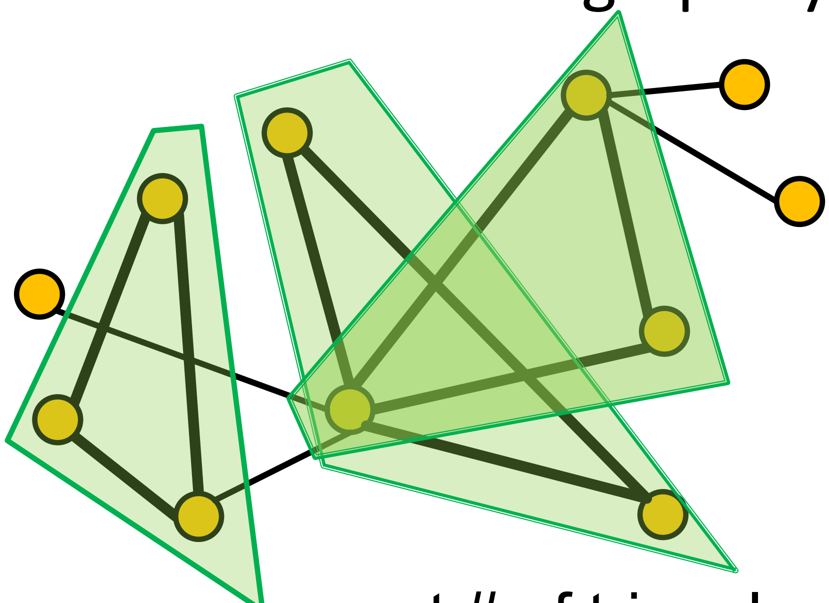


Intro: Finding Frequent Subgraphs

- Generally, finding the most frequent size-k motifs requires solving two challenges:
  - **1) Enumerating** all size-k connected subgraphs
  - **2) Counting** #(occurrences of each subgraph type)



Possible size-3 motifs



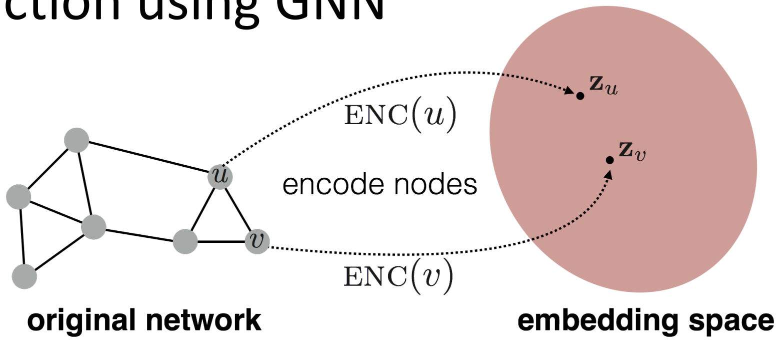
count # of triangle motifs

Why is it Hard?

- **Just knowing if a certain subgraph exists in a graph, is a hard computational problem!**
  - Subgraph isomorphism is NP-complete
- **Computation time grows exponentially as the size of the subgraphs increases**
  - Feasible motif size for traditional methods is relatively small (3 to 7)

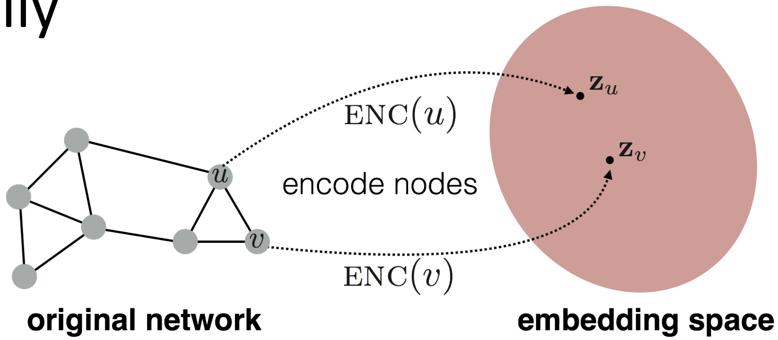
Solution with Representation Learning

- Finding frequent subgraph patterns is **computationally hard**
  - **Combinatorial explosion** of number of possible patterns
  - Counting **subgraph frequency** is NP-hard
- **Representation learning** can tackle these challenges:
  - **Combinatorial explosion** → organize the search space
  - **Subgraph isomorphism** → prediction using GNN



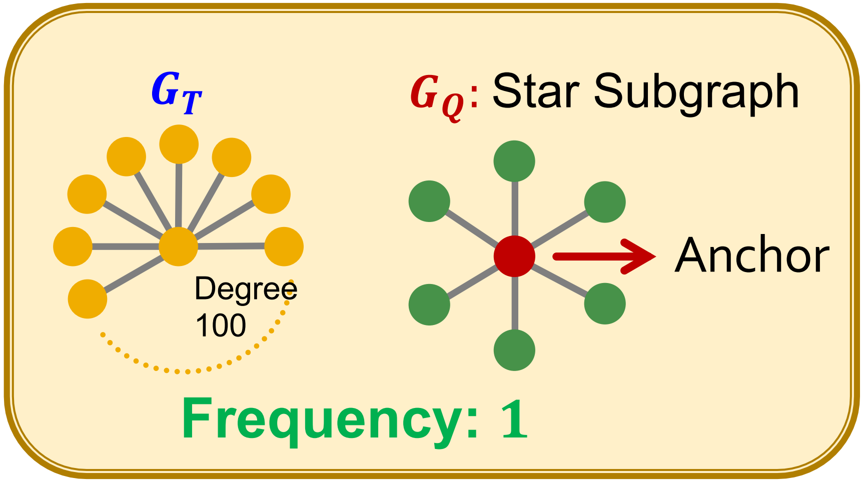
Solution with Representation Learning

- **Representation learning** can tackle these challenges:
  - **1) Counting** #(occurrences of each subgraph type)
    - **Solution:** Use GNN to "predict" the frequency of the subgraph.
  - **2) Enumerating** all size-k connected subgraphs
    - **Solution:** Don't enumerate subgraphs but construct a size-k subgraph incrementally
      - Note: We are only interested in high frequency subgraphs



Problem Setup: Frequent Motif Mining

- Target graph (dataset) G_T, size parameter k
- Desired number of results r
- **Goal**: Identify, among *all* possible graphs of k nodes, the r graphs with the highest frequency in G_T.
- **We use the node-level definition:** The number of nodes u in G_T for which some subgraph of G_T is isomorphic to G_Q and the isomorphism maps u to v.



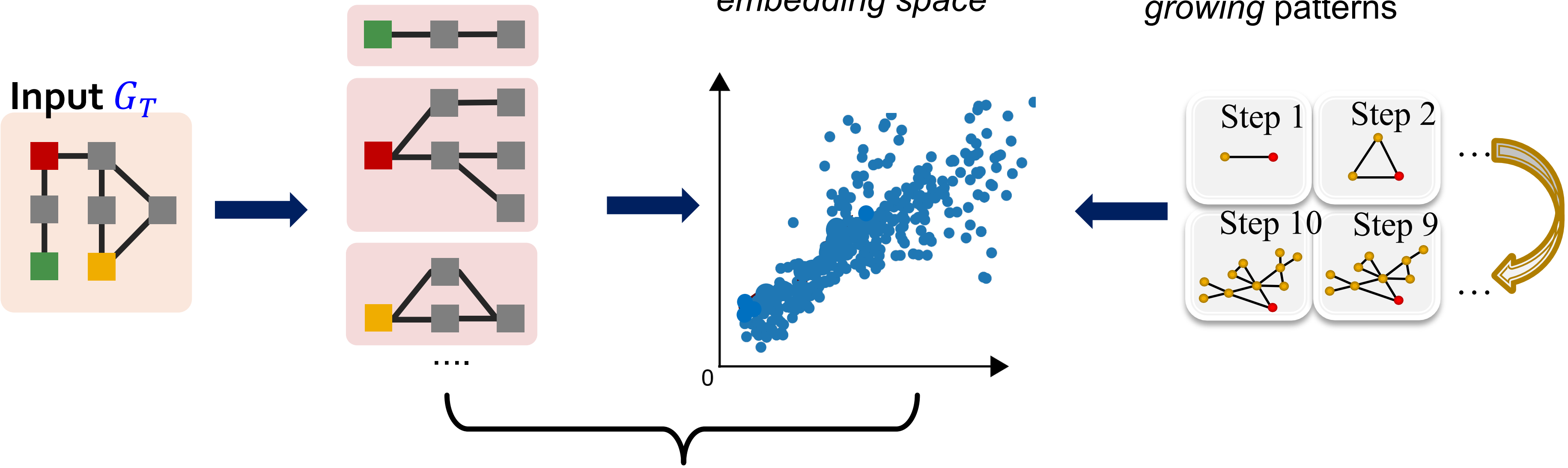
SPMiner: Overview

SPMiner: A neural model to identify frequent motifs

Decompose: Overlapping *node-anchored* neighborhoods

Encoder: Embed subgraphs into *order embedding space*

Search Procedure: Find frequent subgraphs by *growing* patterns



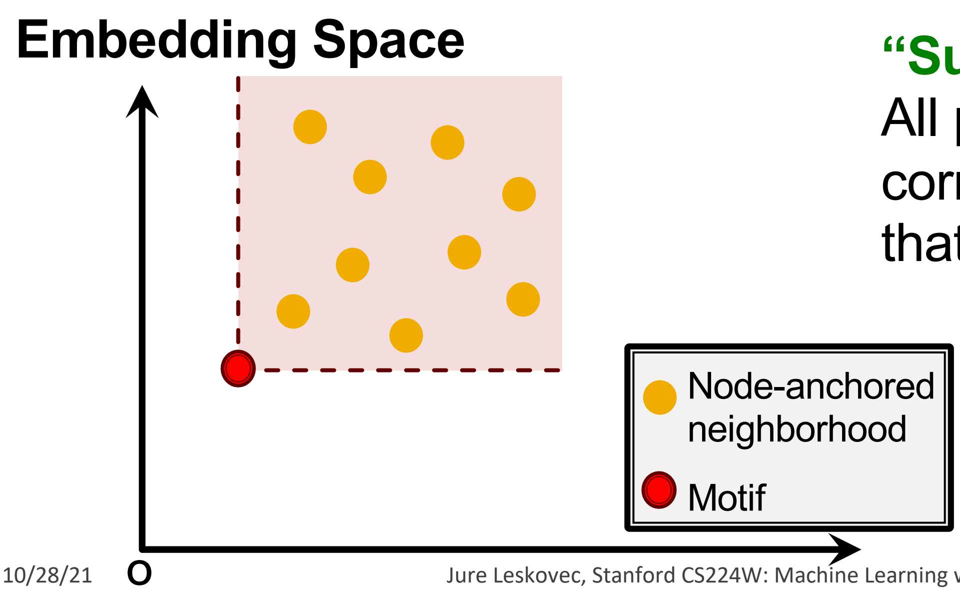
Same as neural subgraph matching

SPMiner: Key Idea

- Decompose input graph G_T into neighborhoods
- Embed neighborhoods into an order embedding space
- **Key benefit of order embedding:** We can quickly "predict" the frequency of a given subgraph G_Q

Motif Frequency Estimation

- **Given:** Set of subgraphs ("node-anchored neighborhoods") G_{N_i} of G_T (sampled randomly)
- **Key idea:** Estimate frequency of G_Q by counting the number of G_{N_i} such that their embeddings z_{N_i} satisfy $z_Q \leq z_{N_i}$
  - This is a consequence of the **order embedding space property**

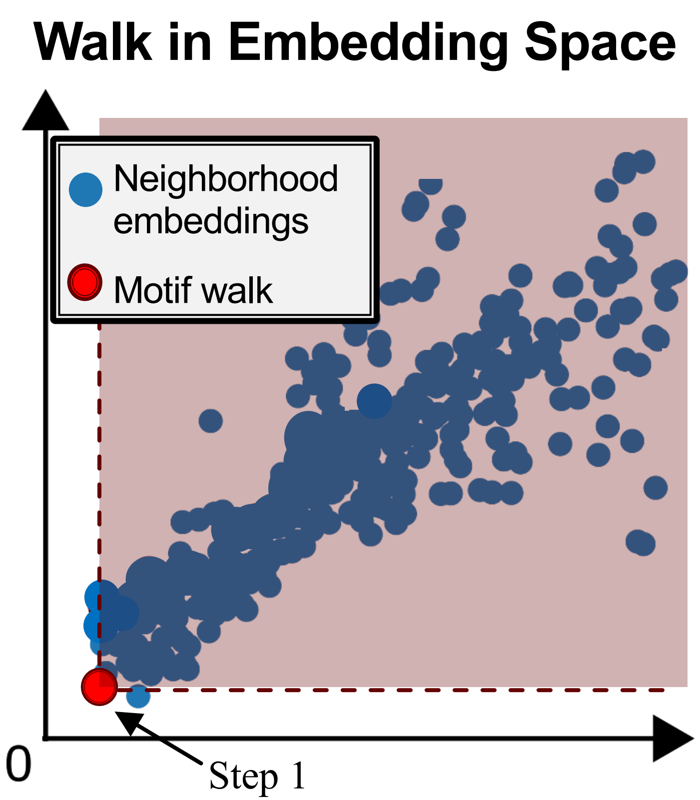


"Super-graph" region:
All points in the red shaded region correspond to neighborhoods in G_T that contain G_Q

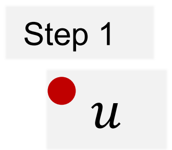
Benefit: Super-fast subgraph frequency counting!

SPMiner Search Procedure (1)

Initial step: Start by randomly picking a starting node u in the target graph G_T. Set $S = \{u\}$.



Each point in the shaded region represents a neighborhood in target graph that contains the motif pattern

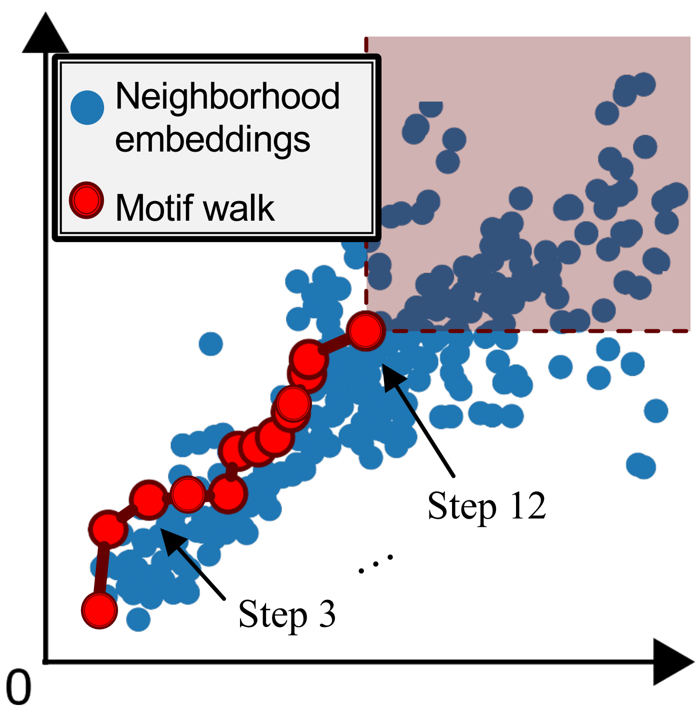


Initially, all neighborhoods contain the trivial subgraph

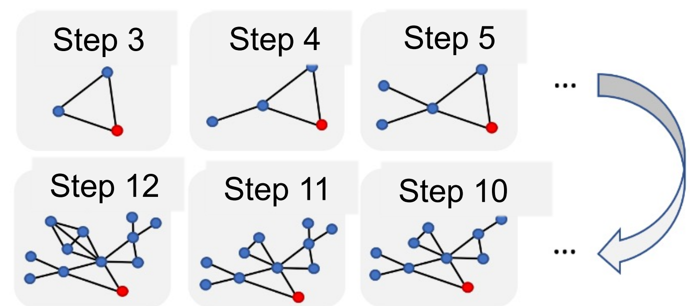
SPMiner Search Procedure (2)

Iteratively: Grow a motif by iteratively choosing a neighbor in G_T of a node in S and add that node to S. We grow the motif S to find **larger frequent** motifs!

Walk in Embedding Space



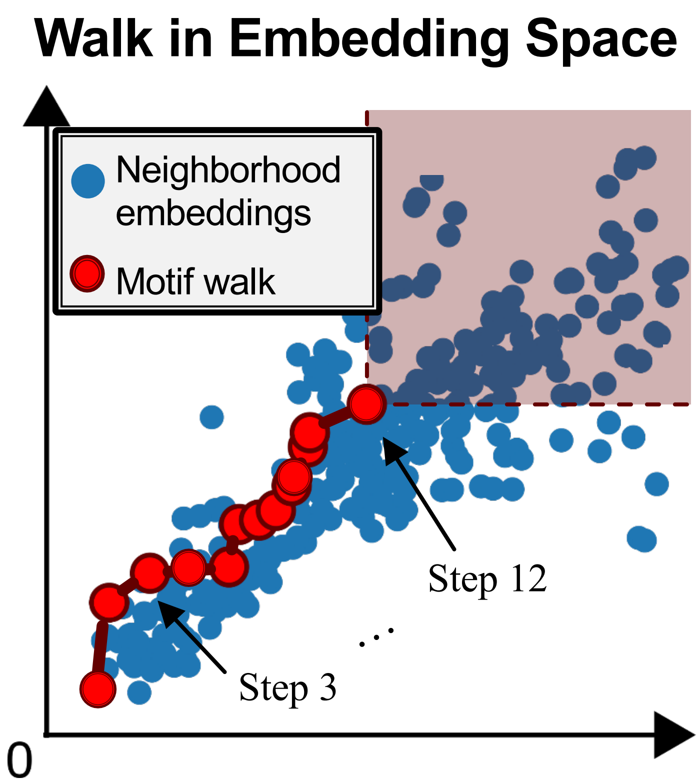
- Small motifs grow by adding neighbors
- Their embeddings correspond to red points on the left

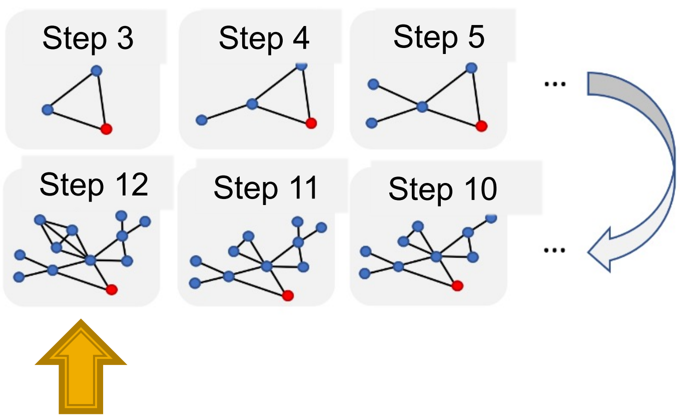


Goal: maximize number of neighborhoods in red shaded area after k step!

SPMiner Search Procedure (3)

Termination: Upon reaching a desired motif size, take the subgraph of the target graph induced by S.





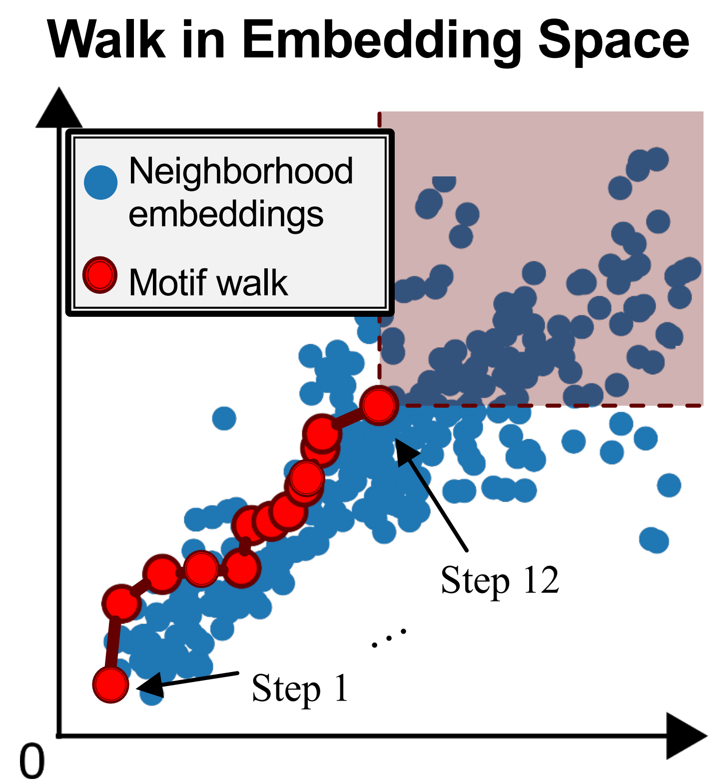
Identified frequent motif of size 12:
It has the largest number of blue points in super-graph region, among all embeddings of possible subgraphs of size 12

SPMiner Search Procedure (4)

How to pick which node to add at each step?

Def: Total violation of a subgraph G:
the number of neighborhoods that do not contain G.

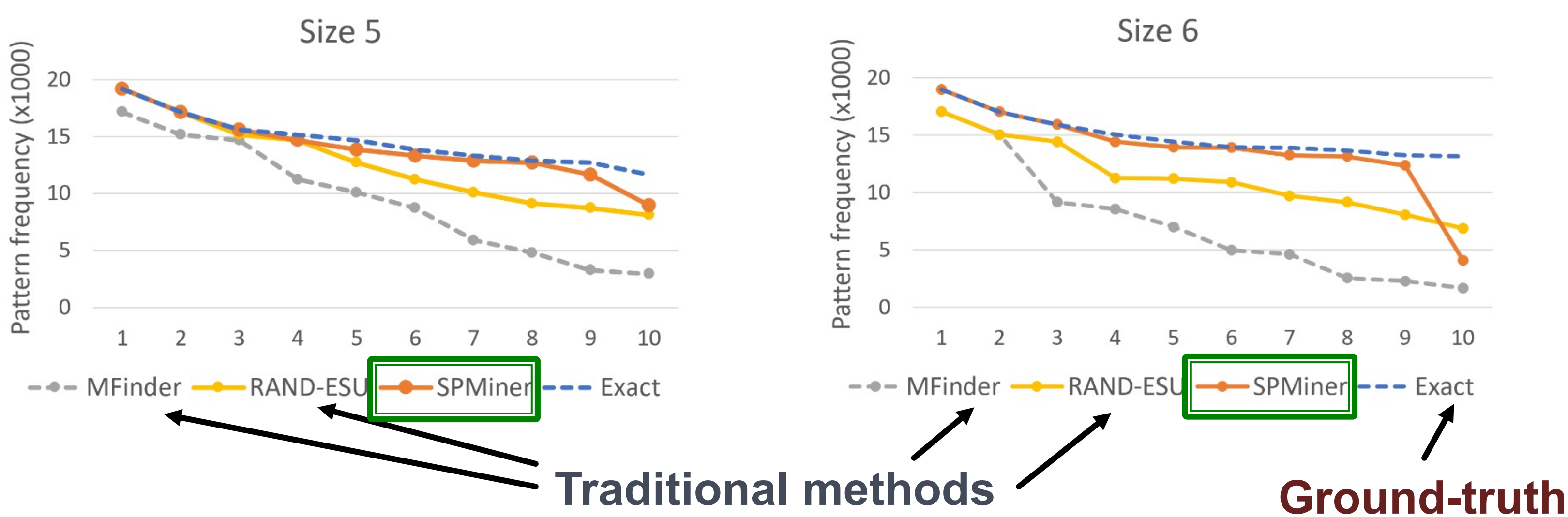
- The number of neighborhoods G_{N_i} that do **not** satisfy $z_Q \preccurlyeq z_{N_i}$
- Minimizing total violation = maximizing frequency



Greedy strategy (heuristic):
At every step, add the node that results in the **smallest total violation**

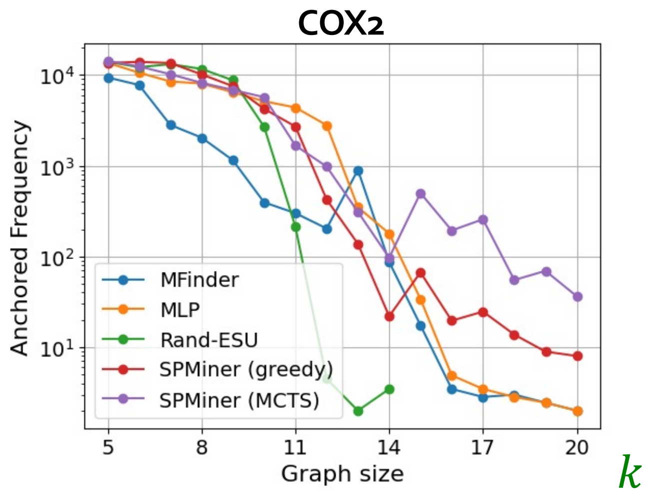
Results: Small Motifs

- **Ground-truth:** Find most frequent 10 motifs in dataset by brute-force exact enumeration (expensive)
- **Question**: Can the model identify frequent motifs?
- **Result**: The model identifies 9 and 8 of the top 10 motifs, respectively.

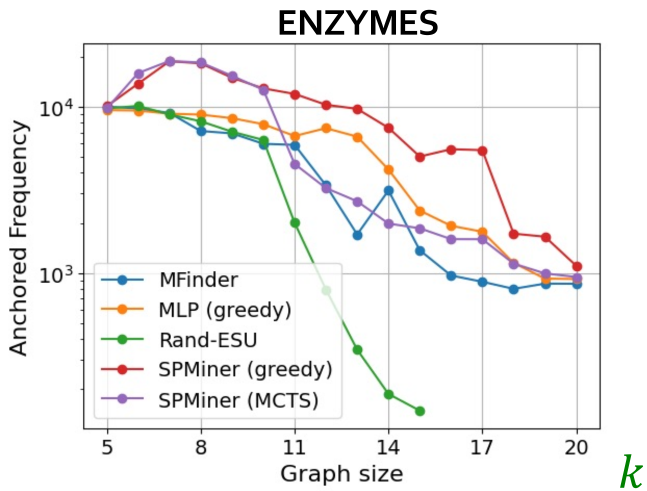


Experiments: Large motifs

- **Question**: How do the frequencies of the identified motif compare?
- **Result**: SPMiner identifies motifs that appear 10-100x more frequently than the baselines



Molecule dataset



Protein dataset

Summary

- **Subgraphs** and **motifs** are important concepts that provide insights into the structure of graphs. Their frequency can be used as features for nodes/graphs.
- We covered **neural approaches** to prediction subgraph isomorphism relationship.
- **Order embeddings** have desirable properties and can be used to encode subgraph relations
- **Neural embedding-guided search** in order embedding space can enable ML model to identify motifs much more frequent than existing methods