

Stanford CS224W: Feature Engineering for Machine Learning in Graphs

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



Stanford CS224W: Further Course Logistics

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Course Logistics: Colab o

- **Colabs 0 and 1 will be released today (Thu 1/12) by 9PM on our course website**
- **Colab 0:**
 - Does not need to be handed in
 - TAs will hold a recitation session to walk you through Colab 0:
 - Time: Friday (1/13), 3-4pm PT
 - Location: Zoom, link will be posted on Ed
 - Session will be recorded

Course Logistics: Colab 1

- Colabs 0 and 1 will be released today (Thu 1/12) by 9PM on our course website
- **Colab 1:**
 - Due on Thursday 1/26 (2 weeks from today)
 - Submit written answers and code on Gradescope
 - Will cover material from Lectures 1-4, but you can get started right away!

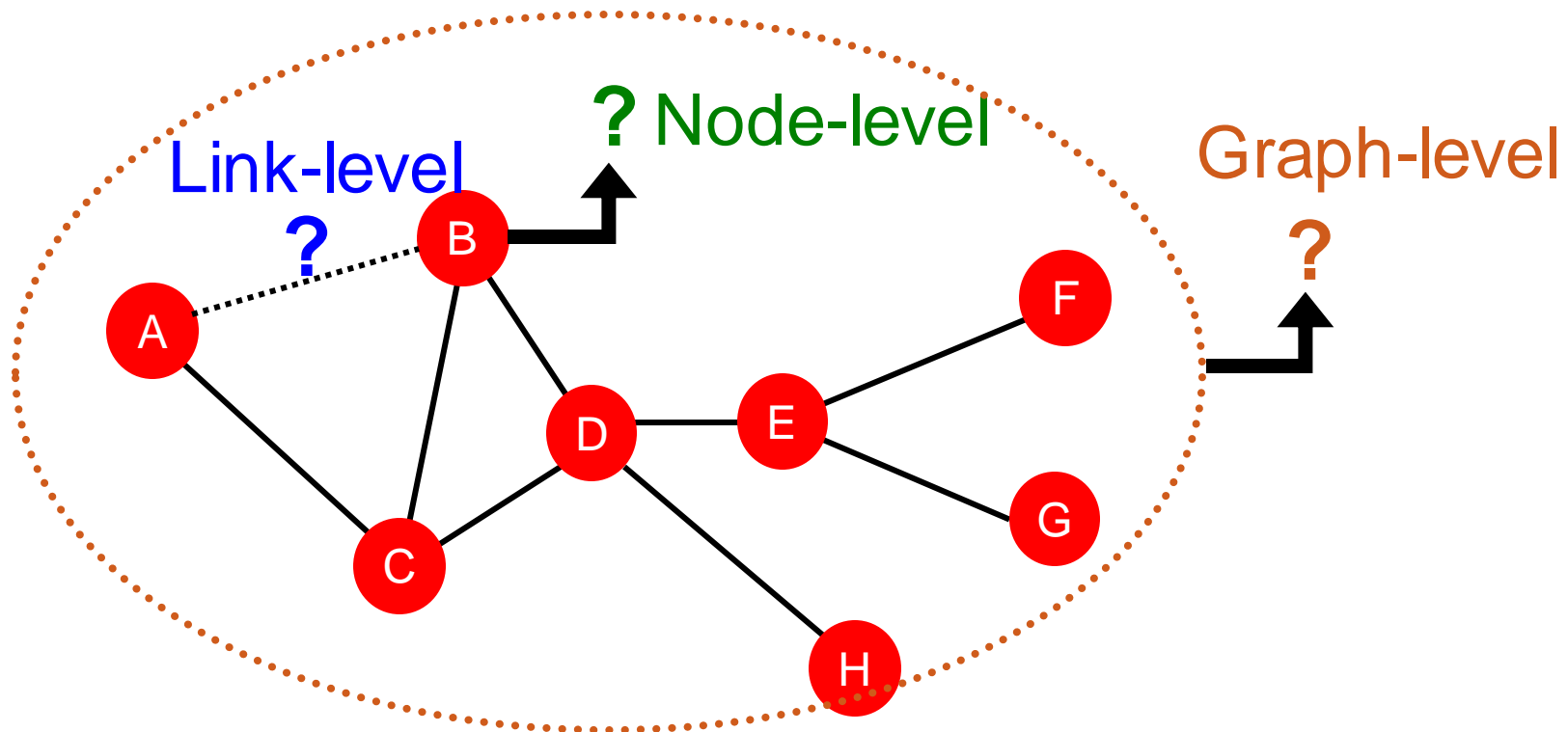
Stanford CS224W: Feature Engineering for Machine Learning in Graphs

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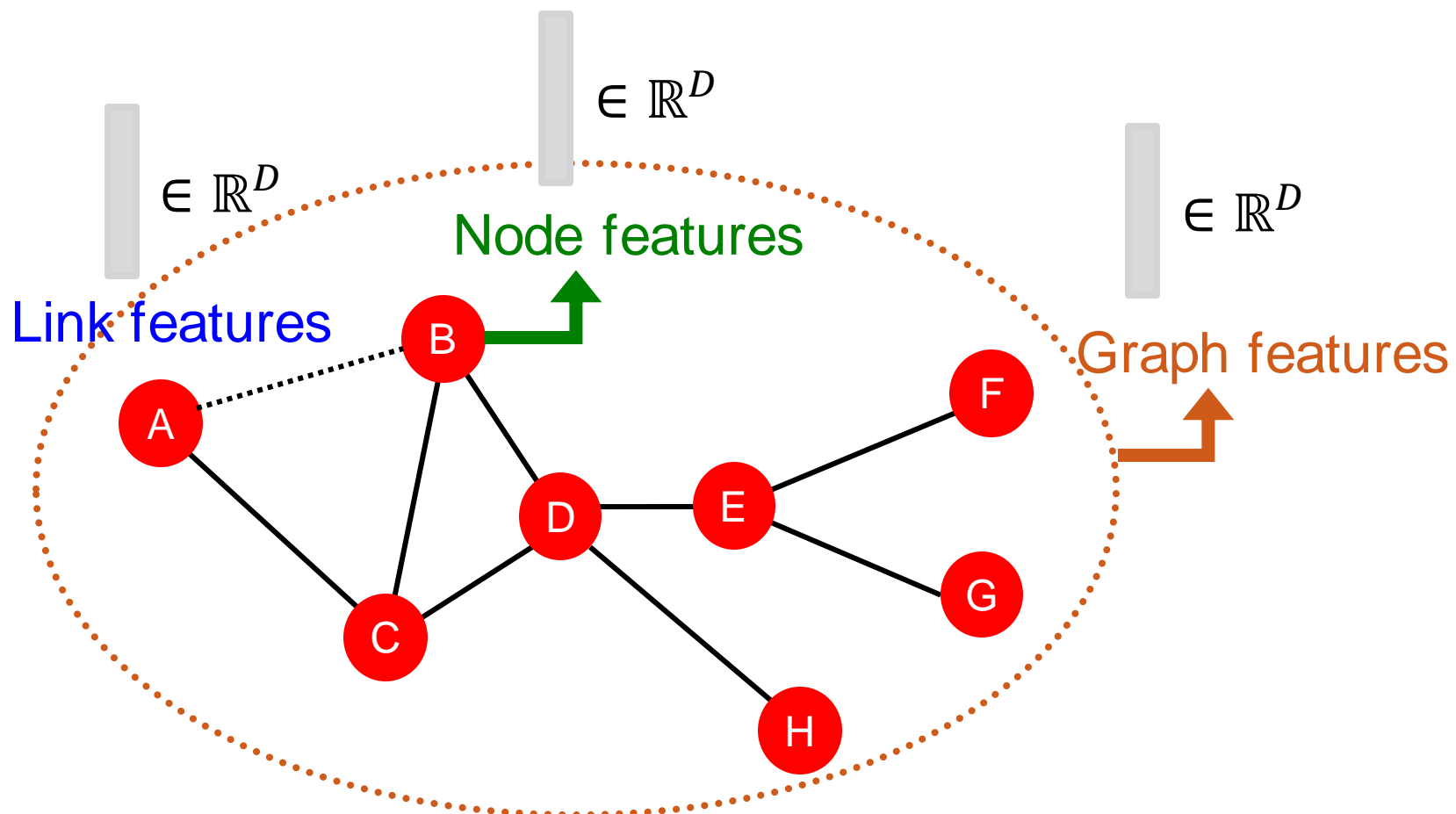
Machine Learning Tasks: Review

- Node-level prediction
- Link-level prediction
- Graph-level prediction



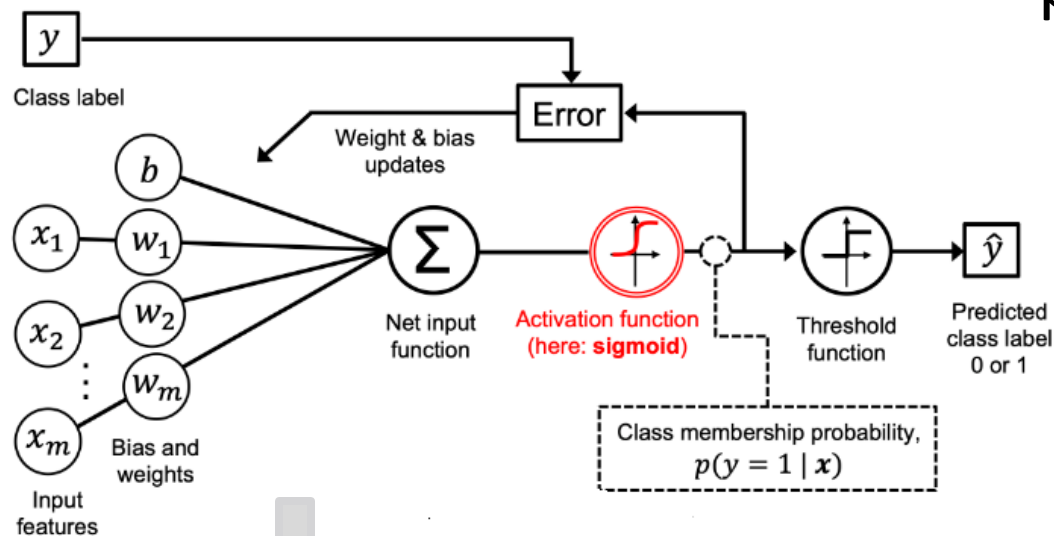
Traditional ML Pipeline

- Design features for nodes/links/graphs
- Obtain features for all training data



Traditional ML Pipeline

- **Train an ML model:**
 - Logistic Regression
 - Random forest
 - Neural network, etc.
- **Apply the model:**
 - Given a new node/link/graph, obtain its features and make a prediction



x_N \rightarrow y_N

x \rightarrow y

This Lecture: Feature Design

- Using effective features \mathbf{x} over graphs is the key to achieving good model performance.
- Traditional ML pipeline uses hand-designed features.
- In this lecture, we overview the traditional features for:
 - Node-level prediction
 - Link-level prediction
 - Graph-level prediction
- For simplicity, we focus on undirected graphs.

Machine Learning in Graphs

Goal: Make predictions for a set of objects

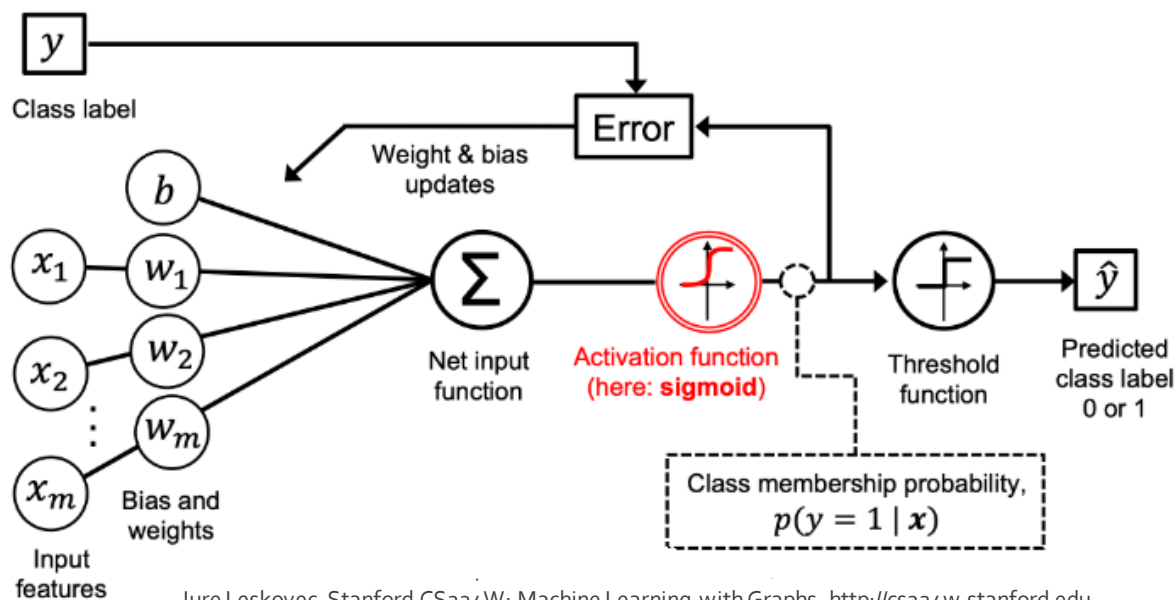
Design choices:

- **Features:** d -dimensional vectors x
- **Objects:** Nodes, edges, sets of nodes, entire graphs
- **Objective function:**
 - What task are we aiming to solve?

Machine Learning in Graphs

Example: Node-level prediction

- Given: $G = (V, E)$
- Learn a function: $f : V \rightarrow \mathbb{R}$

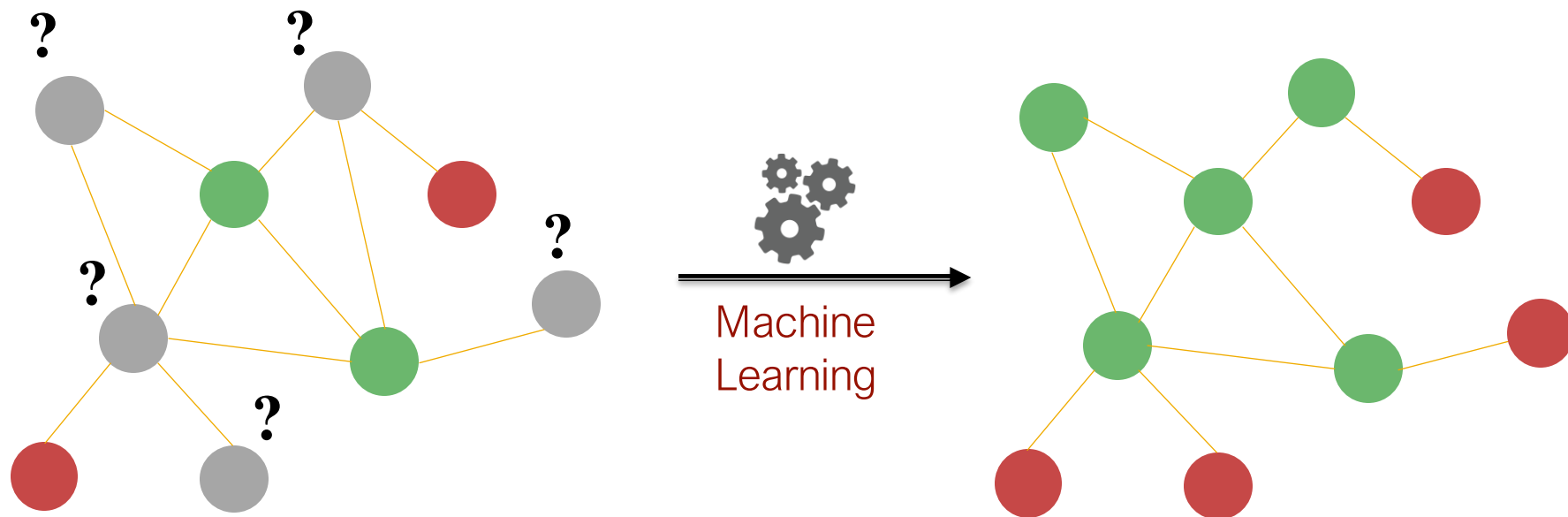


Stanford CS224W: Node-Level Tasks and Features

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Node-Level Tasks



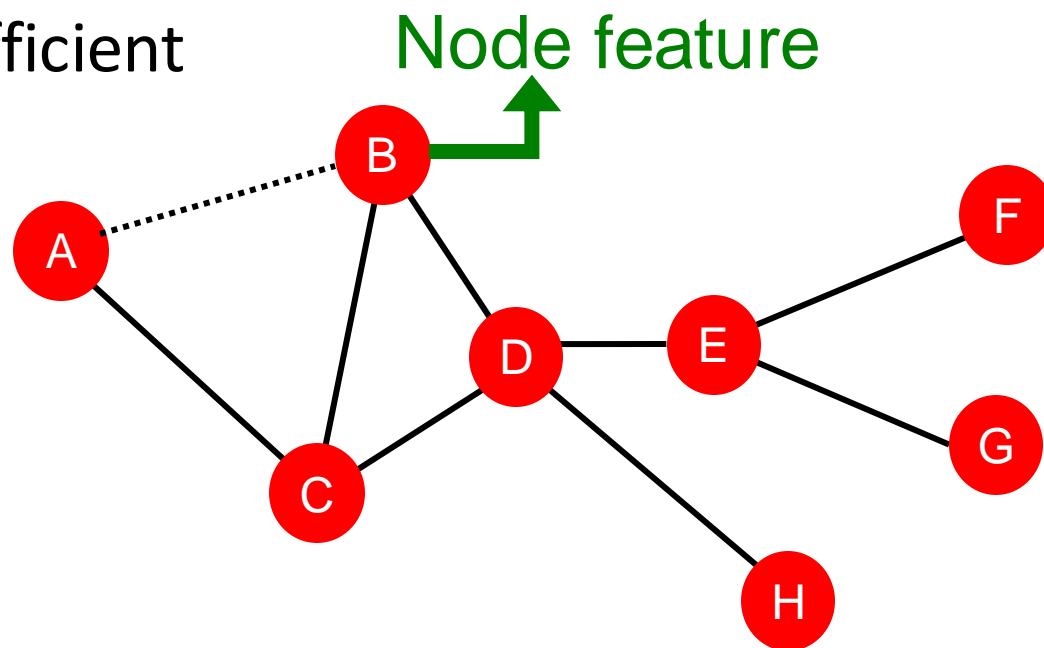
Node classification

ML needs features.

Node-Level Features: Overview

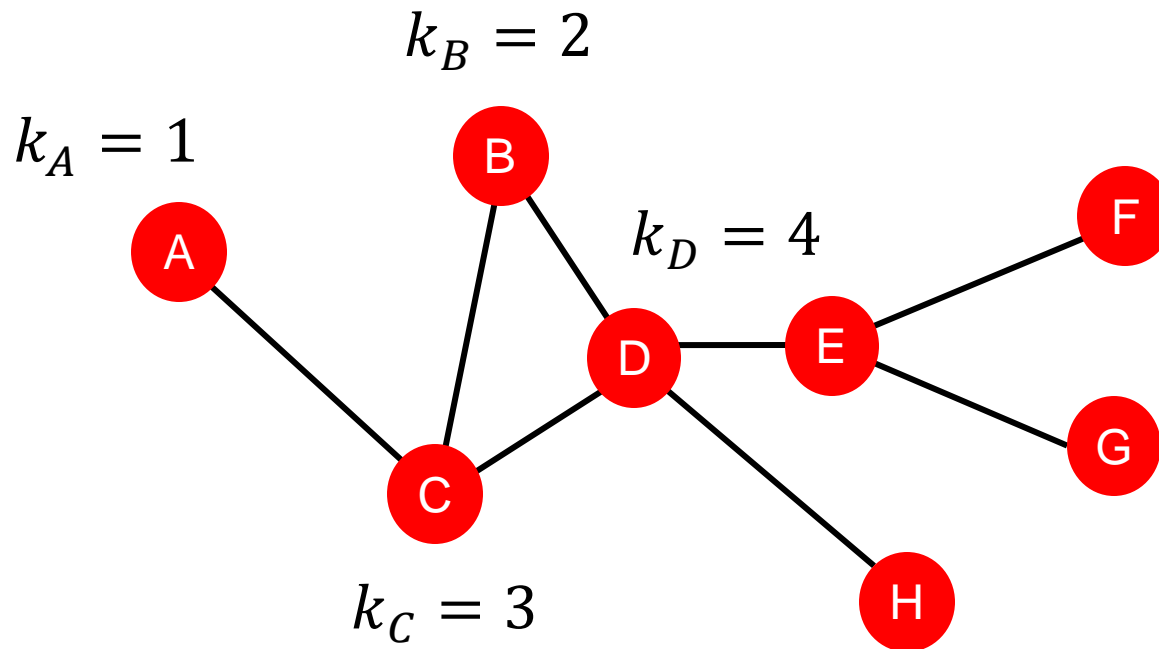
Goal: Characterize the structure and position of a node in the network:

- Node degree
- Node centrality
- Clustering coefficient
- Graphlets



Node Features: Node Degree

- The degree k_v of node v is the number of edges (neighboring nodes) the node has.
- Treats all neighboring nodes equally.



Node Features: Node Centrality

- Node degree counts the neighboring nodes without capturing their importance.
- Node centrality c_v takes the node importance in a graph into account
- **Different ways to model importance:**
 - Eigenvector centrality
 - Betweenness centrality
 - Closeness centrality
 - and many others...

Node Centrality (1)

■ Eigenvector centrality:

- A node v is important if **surrounded by important neighboring nodes** $u \in N(v)$.
- We model the centrality of node v as **the sum of the centrality of neighboring nodes**:

$$c_v = \frac{1}{\lambda} \sum_{u \in N(v)} c_u$$

λ is normalization constant (it will turn out to be the largest eigenvalue of A)

- Notice that the above equation models centrality in a **recursive manner**. **How do we solve it?**

Node Centrality (1)

■ Eigenvector centrality:

- Rewrite the recursive equation in the matrix form.

$$c_v = \frac{1}{\lambda} \sum_{u \in N(v)} c_u \quad \longleftrightarrow \quad \lambda \mathbf{c} = \mathbf{A} \mathbf{c}$$

λ is normalization const
(largest eigenvalue of \mathbf{A})

- \mathbf{A} : Adjacency matrix
 $A_{uv} = 1$ if $u \in N(v)$
- \mathbf{c} : Centrality vector
- λ : Eigenvalue

- We see that centrality \mathbf{c} is the **eigenvector of \mathbf{A} !**
- The largest eigenvalue λ_{max} is always positive and unique (by Perron-Frobenius Theorem).
- The eigenvector \mathbf{c}_{max} corresponding to λ_{max} is used for centrality.

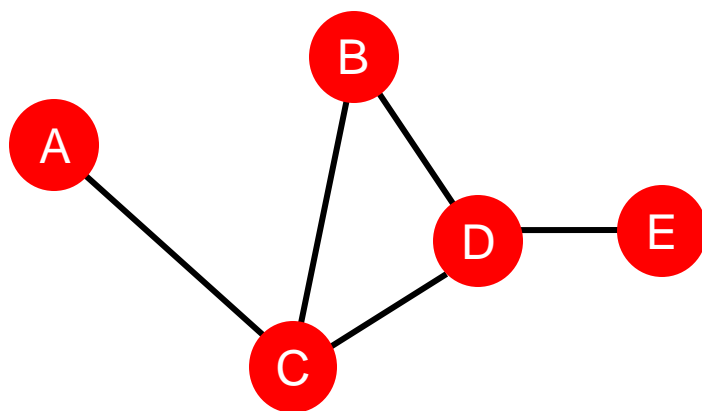
Node Centrality (2)

■ Betweenness centrality:

- A node is important if it lies on many shortest paths between other nodes.

$$c_v = \sum_{s \neq v \neq t} \frac{\#(\text{shortest paths between } s \text{ and } t \text{ that contain } v)}{\#(\text{shortest paths between } s \text{ and } t)}$$

■ Example:



$$c_A = c_B = c_E = 0$$
$$c_C = 3$$

(A-C-B, A-C-D, A-C-D-E)

$$c_D = 3$$

(A-C-D-E, B-D-E, C-D-E)

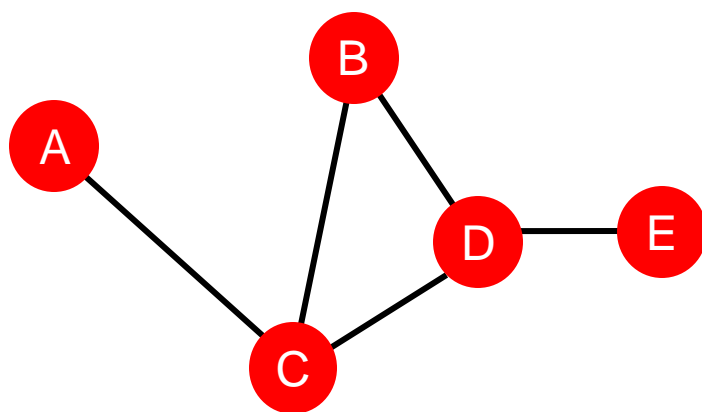
Node Centrality (3)

■ Closeness centrality:

- A node is important if it has small shortest path lengths to all other nodes.

$$c_v = \frac{1}{\sum_{u \neq v} \text{shortest path length between } u \text{ and } v}$$

■ Example:



$$c_A = 1/(2 + 1 + 2 + 3) = 1/8$$

(A-C-B, A-C, A-C-D, A-C-D-E)

$$c_D = 1/(2 + 1 + 1 + 1) = 1/5$$

(D-C-A, D-B, D-C, D-E)

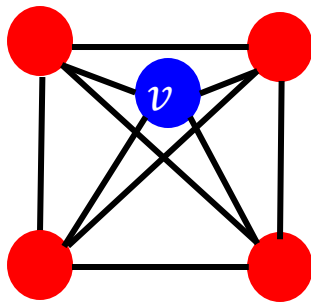
Node Features: Clustering Coefficient

- Measures how connected v 's neighboring nodes are:

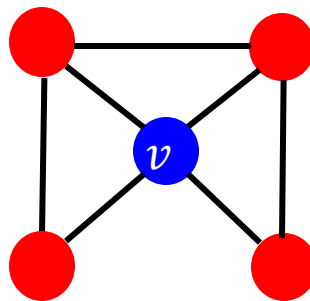
$$e_v = \frac{\#(\text{edges among neighboring nodes})}{\binom{k_v}{2}} \in [0,1]$$

$\#(\text{node pairs among } k_v \text{ neighboring nodes})$
In our examples below the denominator is 6 (4 choose 2).

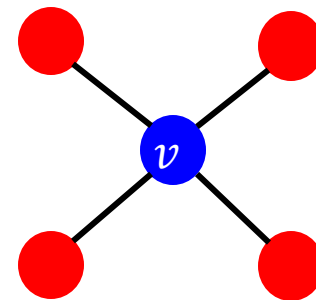
- Examples:**



$$e_v = 1$$



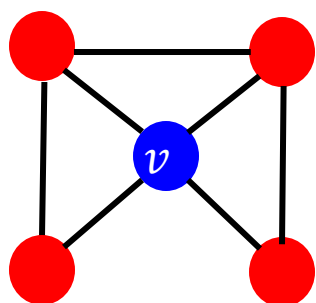
$$e_v = 0.5$$



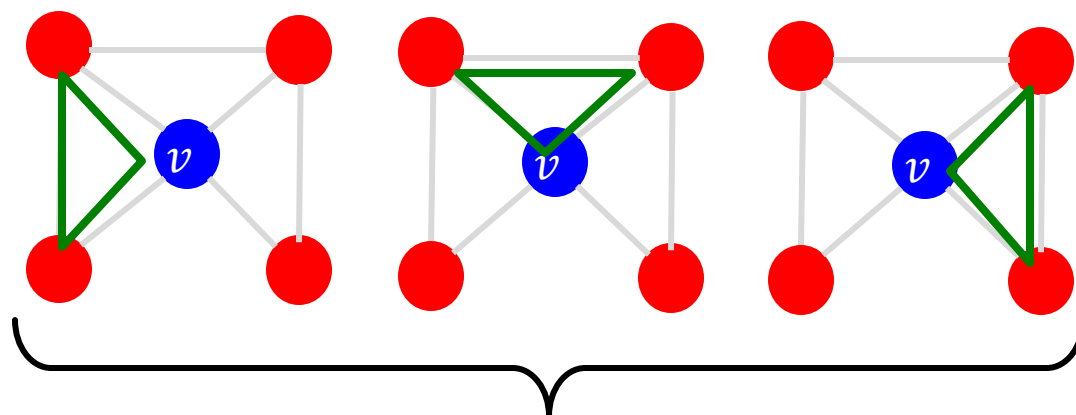
$$e_v = 0$$

Node Features: Graphlets

- **Observation:** Clustering coefficient counts the #(triangles) in the **ego-network**



$$e_v = 0.5$$

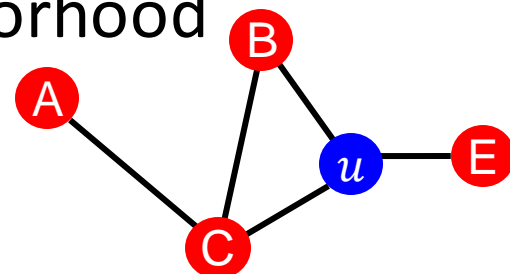


3 triangles (out of 6 node triplets)

- We can generalize the above by counting #(pre-specified subgraphs, i.e., **graphlets**).

Node Features: Graphlets

- **Goal:** Describe network structure around node u
 - **Graphlets** are small subgraphs that describe the structure of node u 's network neighborhood

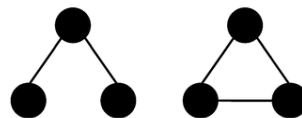
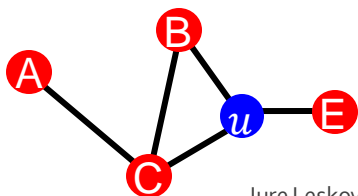


Analogy:

- **Degree** counts **#(edges)** that a node touches
- **Clustering coefficient** counts **#(triangles)** that a node touches.
- **Graphlet Degree Vector (GDV):** Graphlet-base features for nodes
 - **GDV** counts **#(graphlets)** that a node touches

Node Features: Graphlets

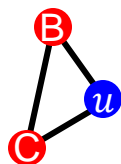
- Considering graphlets of size 2-5 nodes we get:
 - **Vector of 73 coordinates** is a signature of a node that describes the topology of node's neighborhood
- Graphlet degree vector provides a measure of a **node's local network topology**:
 - Comparing vectors of two nodes provides a more detailed measure of local topological similarity than node degrees or clustering coefficient.



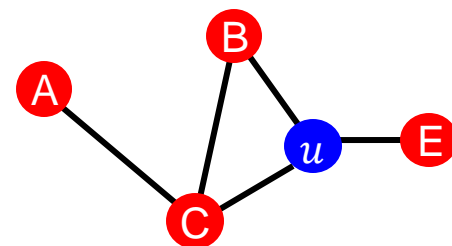
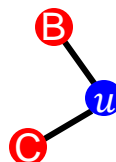
Induced Subgraph & Isomorphism

- **Def: Induced subgraph** is another graph, formed from a subset of vertices and *all* of the edges connecting the vertices in the subset.

Induced subgraph:

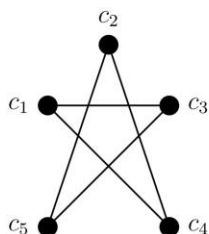
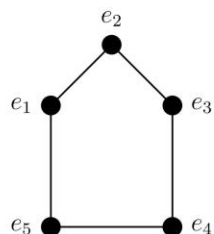


Not an induced subgraph:



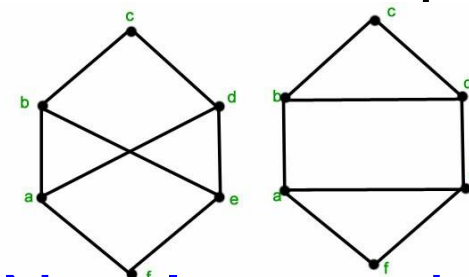
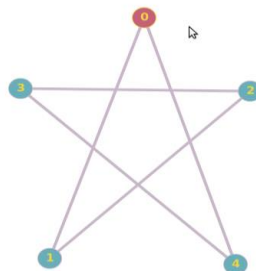
- **Def: Graph Isomorphism**

- Two graphs which contain the same number of nodes connected in the same way are said to be isomorphic.



Isomorphic

Node mapping: (e2,c2), (e1, c5), (e3,c4), (e5,c3), (e4,c1)



Non-Isomorphic

The right graph has cycles of length 3 but the left graph does not, so the graphs cannot be isomorphic.

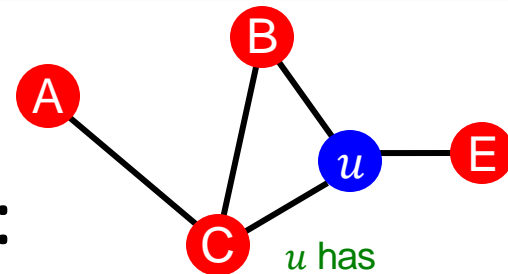
Source: Mathoverflow

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Node Features: Graphlets

Graphlets: Rooted connected induced non-isomorphic subgraphs:

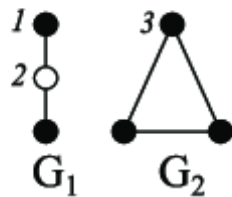
Take some nodes and all the edges between them.



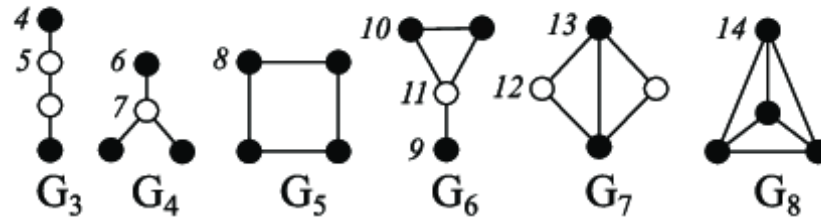
2-node graphlet



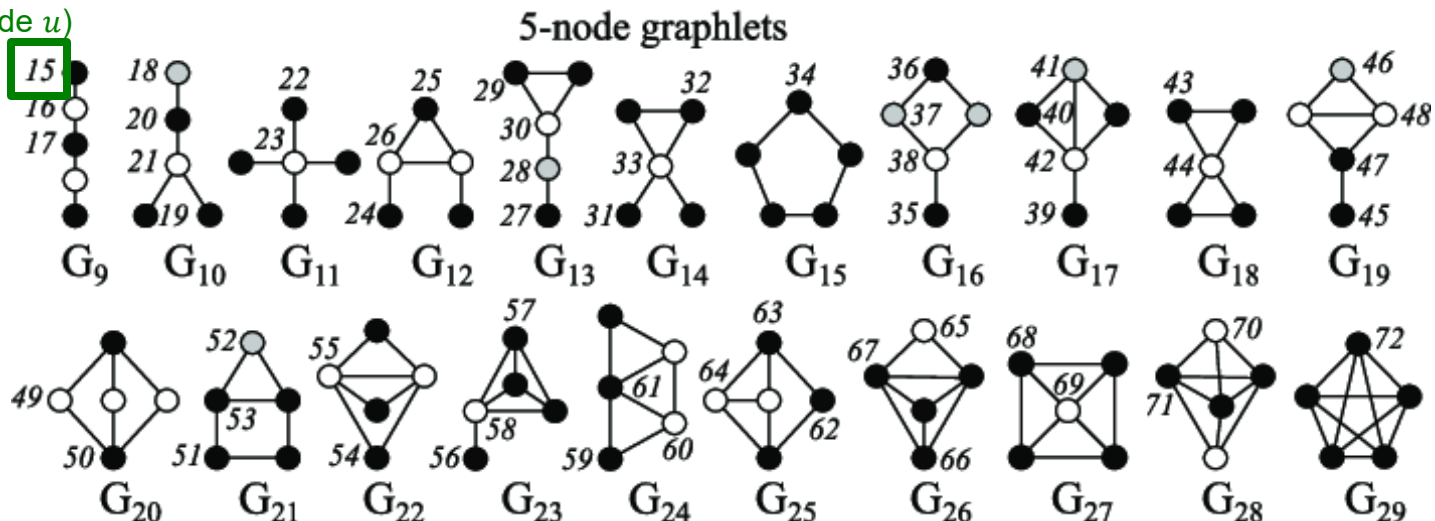
3-node graphlets



4-node graphlets



Graphlet ID (Root/ "position" of node u)



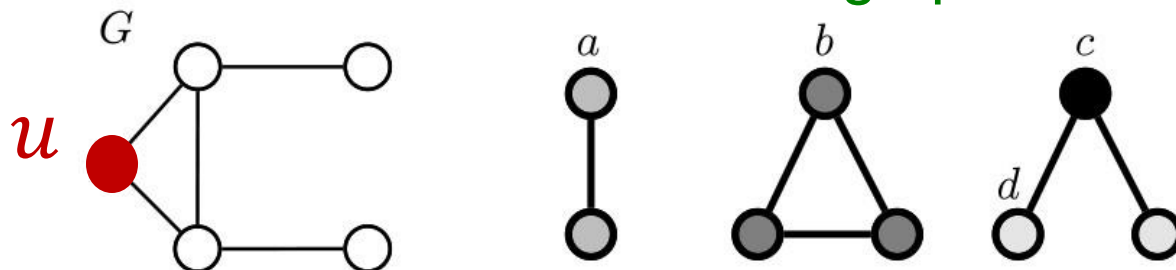
There are 73 different graphlets on up to 5 nodes

Node Features: Graphlets

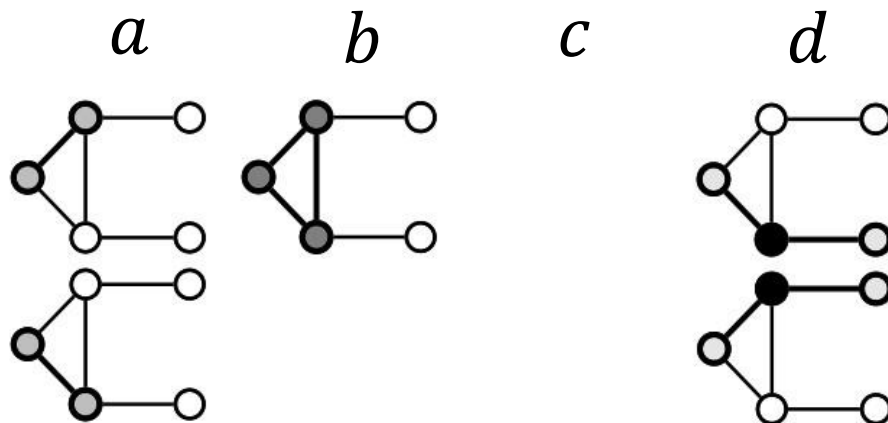
- **Graphlet Degree Vector (GDV):** A count vector of graphlets rooted at a given node.

- **Example:**

Possible graphlets on up to 3 nodes



Graphlet instances of node u :



GDV of node u :
 a, b, c, d
 $[2, 1, 0, 2]$

Node-Level Feature: Summary

- We have introduced different ways to obtain node features.
- They can be categorized as:
 - Importance-based features:
 - Node degree
 - Different node centrality measures
 - Structure-based features:
 - Node degree
 - Clustering coefficient
 - Graphlet count vector

Node-Level Feature: Summary

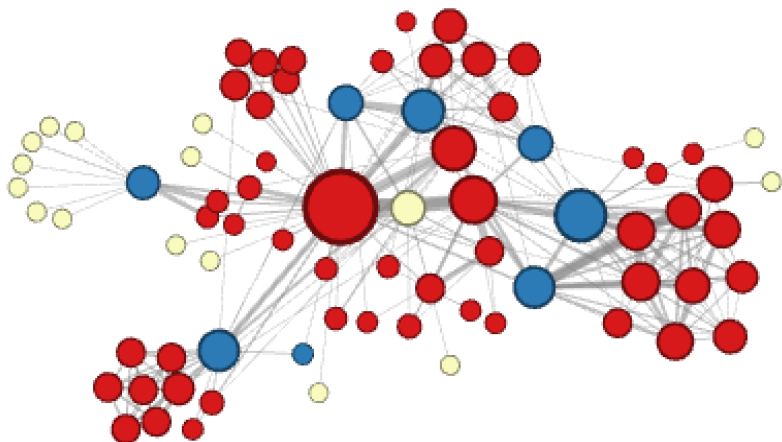
- **Importance-based features:** capture the importance of a node in a graph
 - Node degree:
 - Simply counts the number of neighboring nodes
 - Node centrality:
 - Models **importance of neighboring nodes** in a graph
 - Different modeling choices: eigenvector centrality, betweenness centrality, closeness centrality
- Useful for predicting influential nodes in a graph
 - **Example:** predicting celebrity users in a social network

Node-Level Feature: Summary

- **Structure-based features:** Capture topological properties of local neighborhood around a node.
 - **Node degree:**
 - Counts the number of neighboring nodes
 - **Clustering coefficient:**
 - Measures how connected neighboring nodes are
 - **Graphlet degree vector:**
 - Counts the occurrences of different graphlets
- **Useful for predicting a particular role a node plays in a graph:**
 - **Example:** Predicting protein functionality in a protein-protein interaction network.

Discussion

Different ways to label nodes of the network:



Node features defined so far would allow to distinguish nodes in the above example



However, the features defines so far would not allow for distinguishing the above node labelling

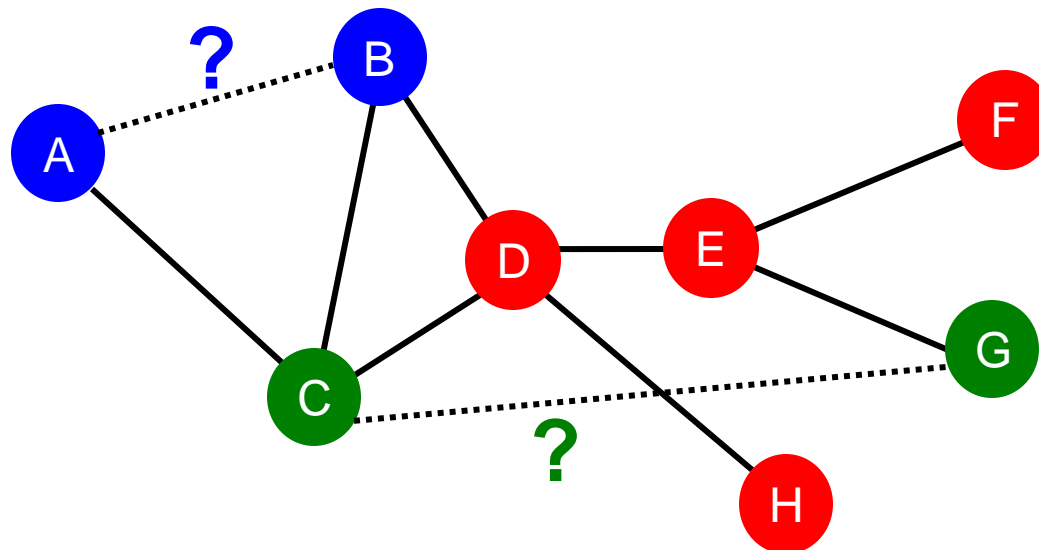
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Link-Level Prediction Task: Recap

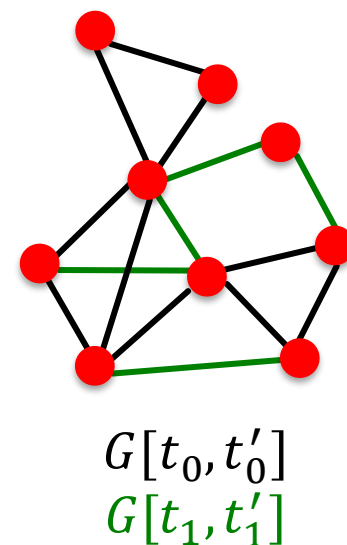
- The task is to predict **new links** based on the existing links.
- At test time, node pairs (with no existing links) are ranked, and top K node pairs are predicted.
- The key is to design features for a **pair of nodes**.



Link Prediction as a Task

Two formulations of the link prediction task:

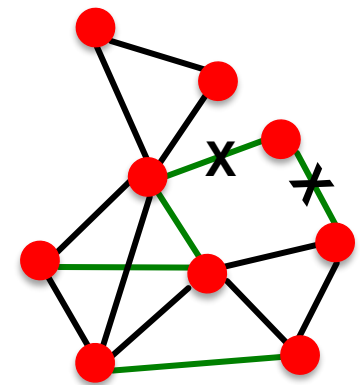
- **1) Links missing at random:**
 - Remove a random set of links and then aim to predict them
- **2) Links over time:**
 - Given $G[t_0, t'_0]$ a graph defined by edges up to time t'_0 , **output a ranked list L** of edges (not in $G[t_0, t'_0]$) that are predicted to appear in time $G[t_1, t'_1]$
 - **Evaluation:**
 - $n = |E_{new}|$: # new edges that appear during the test period $[t_1, t'_1]$
 - Take top n elements of L and count correct edges



Link Prediction via Proximity

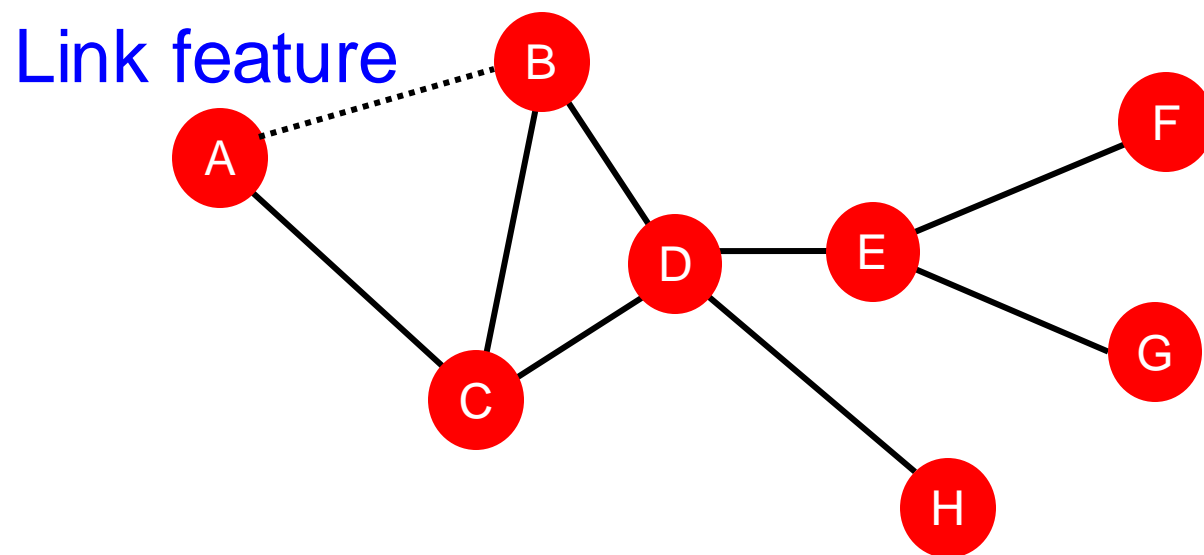
■ Methodology:

- For each pair of nodes (x,y) compute score $c(x,y)$
 - For example, $c(x,y)$ could be the # of common neighbors of x and y
- Sort pairs (x,y) by the decreasing score $c(x,y)$
- **Predict top n pairs as new links**
- **See which of these links actually appear in $G[t_1, t'_1]$**



Link-Level Features: Overview

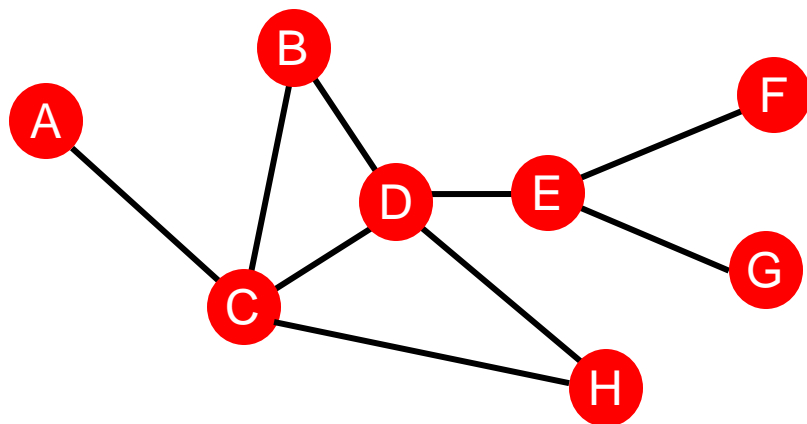
- Distance-based feature
- Local neighborhood overlap
- Global neighborhood overlap



Distance-Based Features

Shortest-path distance between two nodes

■ Example:



- However, this does not capture the degree of neighborhood overlap:
 - Node pair (B, H) has 2 shared neighboring nodes, while pairs (B, E) and (A, B) only have 1 such node.

Local Neighborhood Overlap

Captures # neighboring nodes shared between two nodes v_1 and v_2 :

- **Common neighbors:** $|N(v_1) \cap N(v_2)|$

- Example: $|N(A) \cap N(B)| = |\{C\}| = 1$

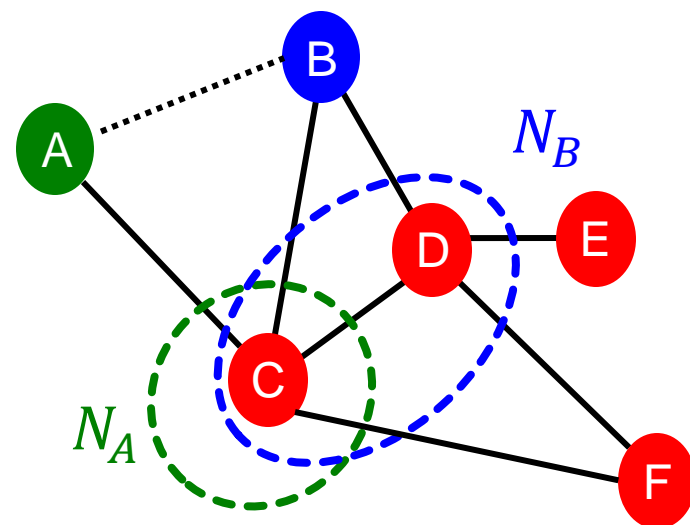
- **Jaccard's coefficient:** $\frac{|N(v_1) \cap N(v_2)|}{|N(v_1) \cup N(v_2)|}$

- Example: $\frac{|N(A) \cap N(B)|}{|N(A) \cup N(B)|} = \frac{|\{C\}|}{|\{C, D\}|} = \frac{1}{2}$

- **Adamic-Adar index:**

$$\sum_{u \in N(v_1) \cap N(v_2)} \frac{1}{\log(k_u)}$$

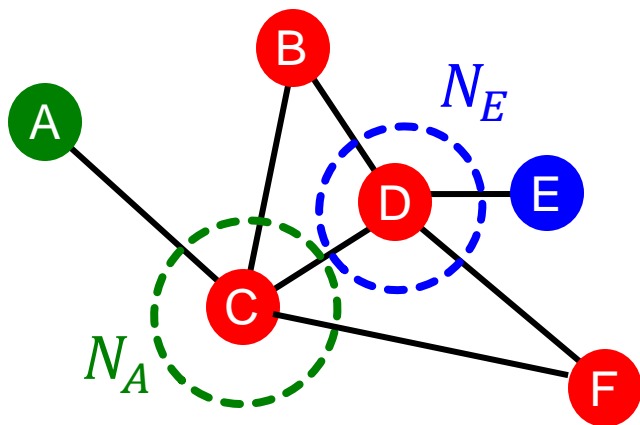
- Example: $\frac{1}{\log(k_C)} = \frac{1}{\log 4}$



Global Neighborhood Overlap

- **Limitation of local neighborhood features:**

- Metric is always zero if the two nodes do not have any neighbors in common.



$$N_A \cap N_E = \phi$$
$$|N_A \cap N_E| = 0$$

- However, the two nodes may still potentially be connected in the future.
- **Global neighborhood overlap** metrics resolve the limitation by considering the entire graph.

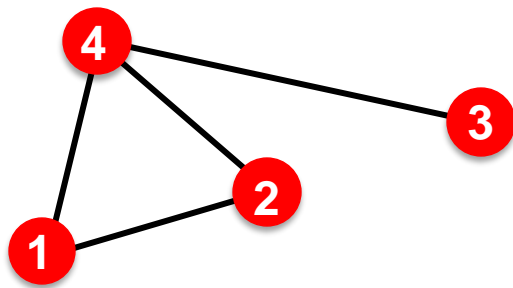
Global Neighborhood Overlap

- **Katz index:** count the number of walks of all lengths between a given pair of nodes.
- **Q: How to compute #walks between two nodes?**
- Use **powers of the graph adjacency matrix!**

Intuition: Powers of Adj Matrices

■ Computing #walks between two nodes

- Recall: $A_{uv} = 1$ if $u \in N(v)$
- Let $P_{uv}^{(K)} = \text{\#walks of length } K \text{ between } u \text{ and } v$
- We will show $P^{(K)} = A^k$
- $P_{uv}^{(1)} = \text{\#walks of length 1 (direct neighborhood) between } u \text{ and } v = A_{uv}$



$$P_{12}^{(1)} = A_{12}$$
$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Intuition: Powers of Adj Matrices

- How to compute $P_{uv}^{(2)}$?
 - Step 1: Compute **#walks** of length 1 **between each of u 's neighbor and v**
 - Step 2: **Sum up** these #walks across u 's neighbors
 - $P_{uv}^{(2)} = \sum_i A_{ui} * P_{iv}^{(1)} = \sum_i A_{ui} * A_{iv} = A_{uv}^2$

Node 1's neighbors

#walks of length 1 between
Node 1's neighbors and Node 2

$$P_{12}^{(2)} = A_{12}^2$$

$$A^2 = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \times \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 3 \end{pmatrix}$$

Power of adjacency

Global Neighborhood Overlap

- **Katz index:** count the number of walks of all lengths between a pair of nodes.
- How to compute #walks between two nodes?
- Use **adjacency matrix powers!**
 - A_{uv} specifies #walks of length 1 (direct neighborhood) between u and v .
 - A_{uv}^2 specifies #walks of **length 2** (neighbor of neighbor) between u and v .
 - And, A_{uv}^l specifies #walks of **length l** .

Global Neighborhood Overlap

- **Katz index** between v_1 and v_2 is calculated as

Sum over *all walk lengths*

$$S_{v_1 v_2} = \sum_{l=1}^{\infty} \boxed{\beta^l} \boxed{A_{v_1 v_2}^l}$$

#walks of length l between v_1 and v_2

$0 < \beta < 1$: discount factor

- Katz index matrix is computed in closed-form:

$$S = \sum_{i=1}^{\infty} \beta^i A^i = \underbrace{(I - \beta A)^{-1} - I}_{= \sum_{i=0}^{\infty} \beta^i A^i}$$

by geometric series of matrices

Link-Level Features: Summary

- **Distance-based features:**
 - Uses the shortest path length between two nodes but does not capture how neighborhood overlaps.
- **Local neighborhood overlap:**
 - Captures how many neighboring nodes are shared by two nodes.
 - Becomes zero when no neighbor nodes are shared.
- **Global neighborhood overlap:**
 - Uses global graph structure to score two nodes.
 - Katz index counts #walks of all lengths between two nodes.

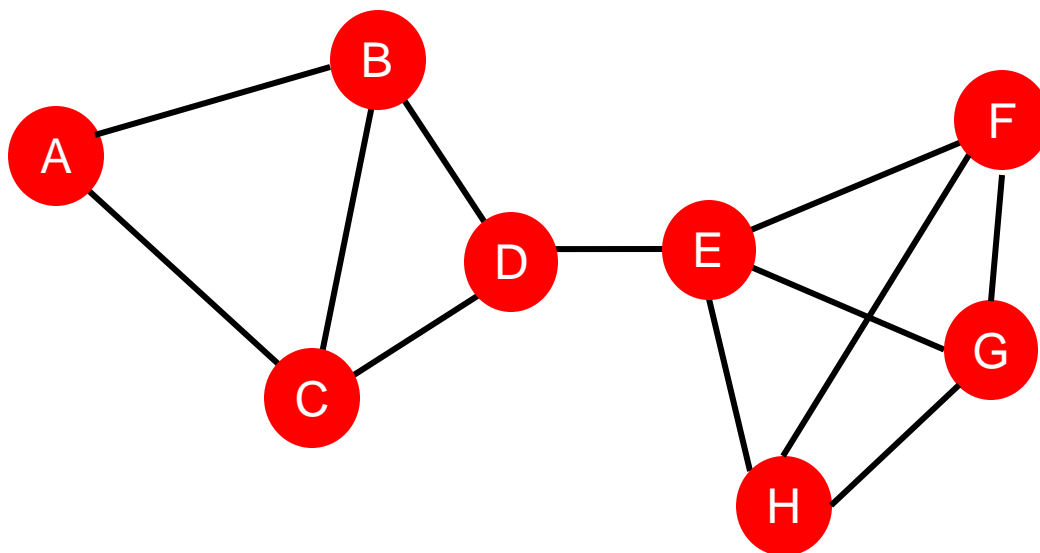
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Graph-Level Features

- **Goal:** We want features that characterize the structure of an entire graph.
- **For example:**



Background: Kernel Methods

- **Kernel methods** are widely-used for traditional ML for graph-level prediction.
- **Idea: Design kernels instead of feature vectors.**
- **A quick introduction to Kernels:**
 - Kernel $K(G, G') \in \mathbb{R}$ measures similarity b/w data
 - Kernel matrix $\mathbf{K} = (K(G, G'))_{G, G'}$ must always be positive semidefinite (i.e., has positive eigenvalues)
 - There exists a feature representation $\phi(\cdot)$ such that $K(G, G') = \phi(G)^T \phi(G')$
 - Once the kernel is defined, off-the-shelf ML model, such as **kernel SVM**, can be used to make predictions.

Graph-Level Features: Overview

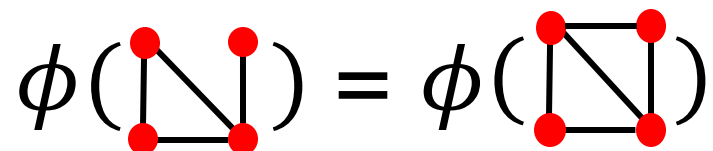
- **Graph Kernels:** Measure similarity between two graphs:
 - Graphlet Kernel [1]
 - Weisfeiler-Lehman Kernel [2]
 - Other kernels are also proposed in the literature (beyond the scope of this lecture)
 - Random-walk kernel
 - Shortest-path graph kernel
 - And many more...

[1] Shervashidze, Nino, et al. "Efficient graphlet kernels for large graph comparison." Artificial Intelligence and Statistics. 2009.

[2] Shervashidze, Nino, et al. "Weisfeiler-lehman graph kernels." Journal of Machine Learning Research 12.9 (2011).

Graph Kernel: Key Idea

- **Goal:** Design graph feature vector $\phi(G)$
- **Key idea:** **Bag-of-Words (BoW)** for a graph
 - **Recall:** BoW simply uses the word counts as features for documents (no ordering considered).
 - Naïve extension to a graph: **Regard nodes as words.**
 - Since both graphs have **4 red nodes**, we get the same feature vector for two different graphs...

$$\phi(\text{Graph 1}) = \phi(\text{Graph 2})$$


Graph Kernel: Key Idea

What if we use Bag of node degrees?

Deg1: ● Deg2: ● Deg3: ●

$$\phi(\text{triangle}) = \text{count}(\text{triangle with colored nodes}) = [1, 2, 1]$$



Obtains different features for different graphs!

$$\phi(\text{square}) = \text{count}(\text{square with colored nodes}) = [0, 2, 2]$$

- Both Graphlet Kernel and Weisfeiler-Lehman (WL) Kernel use **Bag-of-*** representation of graph, where * is more sophisticated than node degrees!

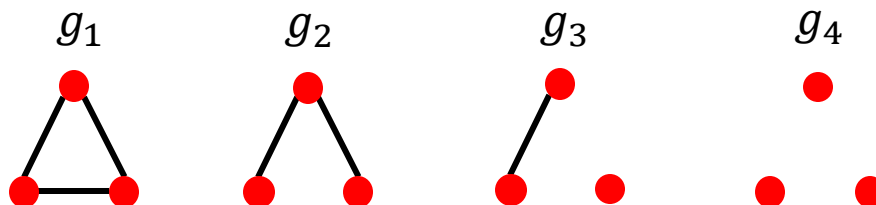
Graph-Level Graphlet Features

- **Key idea:** Count the number of **different graphlets** in a graph.
- **Note:** Definition of graphlets here is slightly different from the node-level features.
- The two differences are:
 - Nodes in graphlets here do **not need to be connected** (allows for isolated nodes)
 - The graphlets here are not rooted.
 - Examples in the next slide illustrate this.

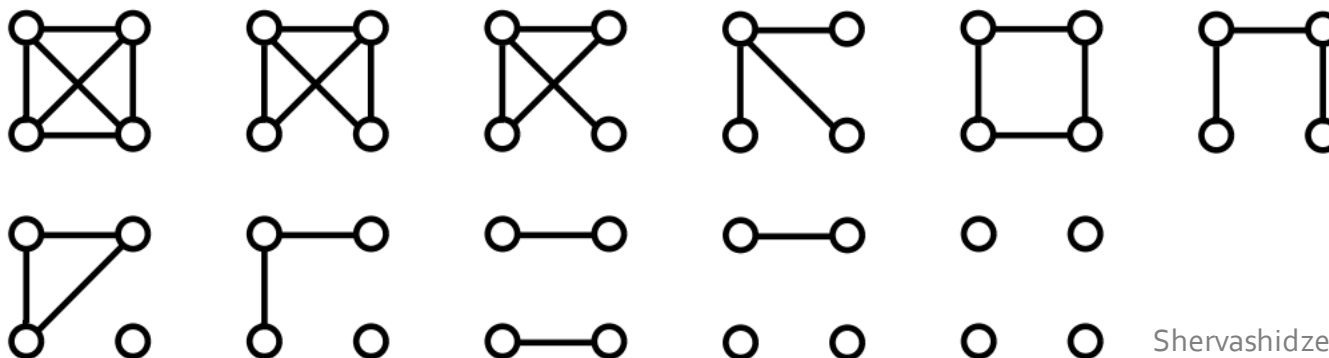
Graph-Level Graphlet Features

Let $\mathcal{G}_k = (g_1, g_2, \dots, g_{n_k})$ be a list of graphlets of size k .

- For $k = 3$, there are 4 graphlets.



- For $k = 4$, there are 11 graphlets.



Shervashidze *et al.*, AISTATS 2011

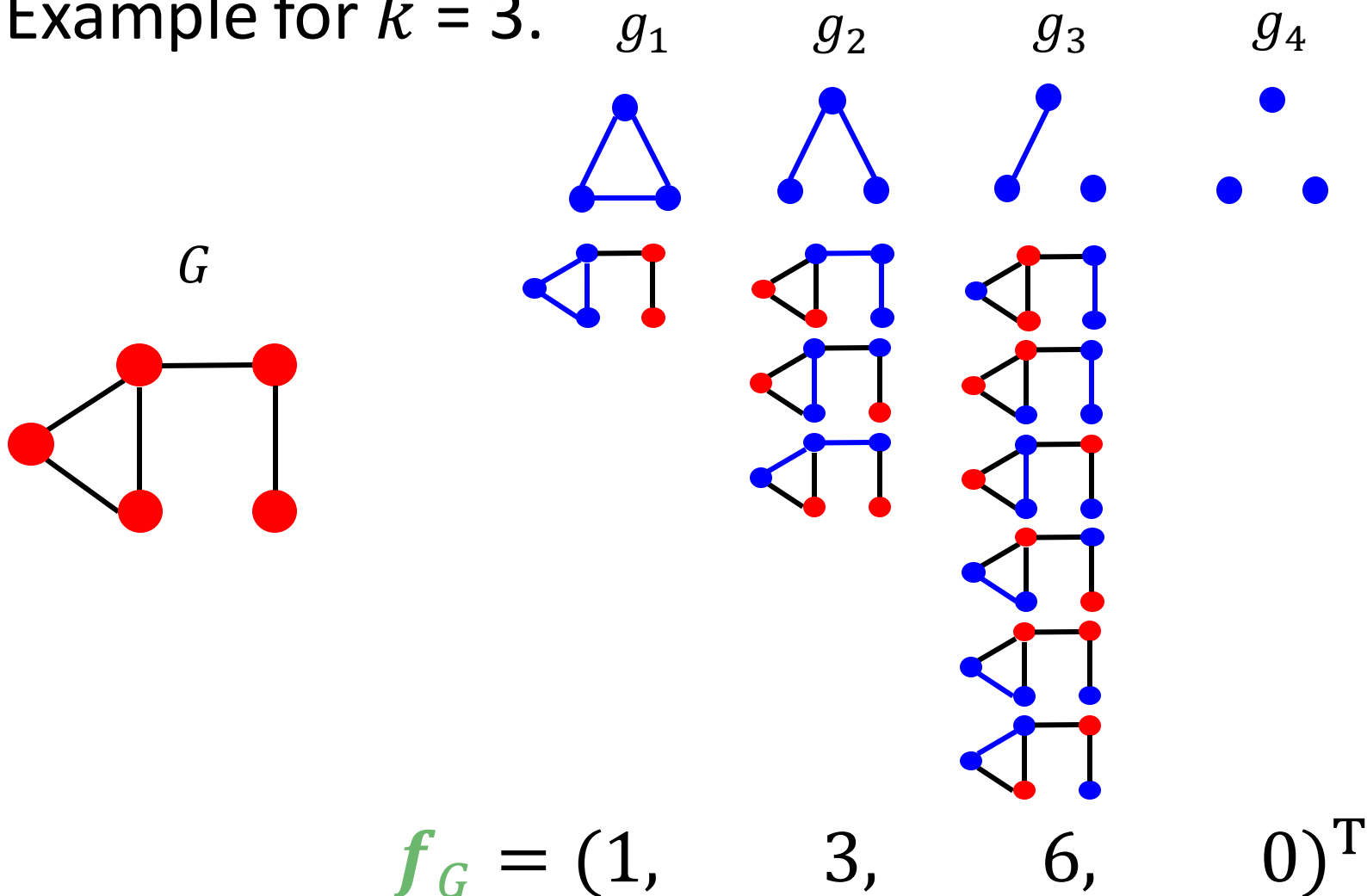
Graph-Level Graphlet Features

- Given graph G , and a graphlet list $\mathcal{G}_k = (g_1, g_2, \dots, g_{n_k})$, define the graphlet count vector $f_G \in \mathbb{R}^{n_k}$ as

$$(f_G)_i = \#(g_i \subseteq G) \text{ for } i = 1, 2, \dots, n_k.$$

Graph-Level Graphlet Features

- Example for $k = 3$.



Graph-Level Graphlet Kernel

- Given two graphs, G and G' , graphlet kernel is computed as

$$K(G, G') = \mathbf{f}_G^T \mathbf{f}_{G'}$$

- **Problem:** if G and G' have different sizes, that will greatly skew the value.
- **Solution:** normalize each feature vector

$$\mathbf{h}_G = \frac{\mathbf{f}_G}{\text{Sum}(\mathbf{f}_G)} \quad K(G, G') = \mathbf{h}_G^T \mathbf{h}_{G'}$$

The Graphlet Kernel

Limitations: Counting graphlets is **expensive!**

- Counting size- k graphlets for a graph with size n by enumeration takes n^k .
- This is unavoidable in the worst-case since **subgraph isomorphism test** (judging whether a graph is a subgraph of another graph) is **NP-hard**.
- If a graph's node degree is bounded by d , an $O(nd^{k-1})$ algorithm exists to count all the graphlets of size k .

Can we design a more efficient graph kernel?

Weisfeiler-Lehman Kernel

- **Goal:** Design an efficient graph feature descriptor $\phi(G)$
- **Idea:** Use neighborhood structure to iteratively enrich node vocabulary.
 - Generalized version of **Bag of node degrees** since node degrees are one-hop neighborhood information.
- **Algorithm to achieve this:**

Color refinement

Color Refinement

- **Given:** A graph G with a set of nodes V .
 - Assign an initial color $c^{(0)}(v)$ to each node v .
 - Iteratively refine node colors by

$$c^{(k+1)}(v) = \text{HASH} \left(\left\{ c^{(k)}(v), \{c^{(k)}(u)\}_{u \in N(v)} \right\} \right),$$

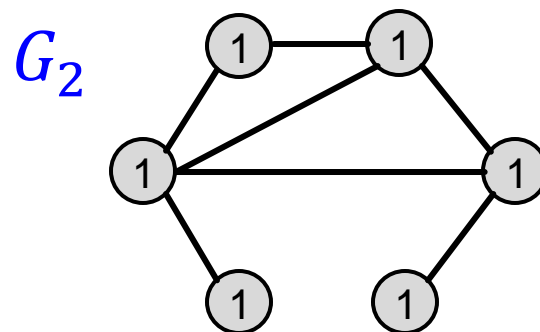
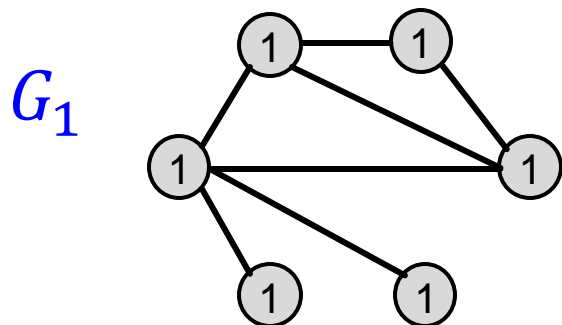
where **HASH** maps different inputs to different colors.

- After K steps of color refinement, $c^{(K)}(v)$ summarizes the structure of K -hop neighborhood

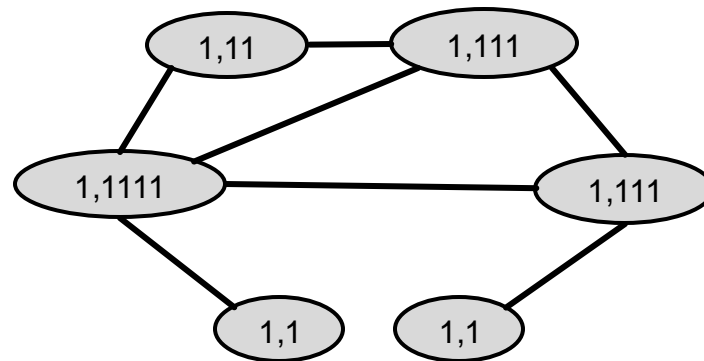
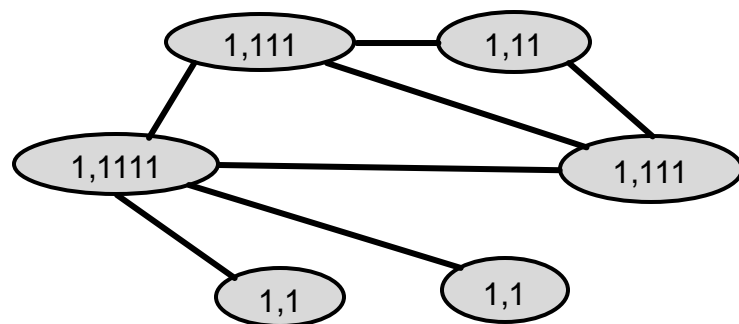
Color Refinement (1)

Example of color refinement given two graphs

- Assign initial colors



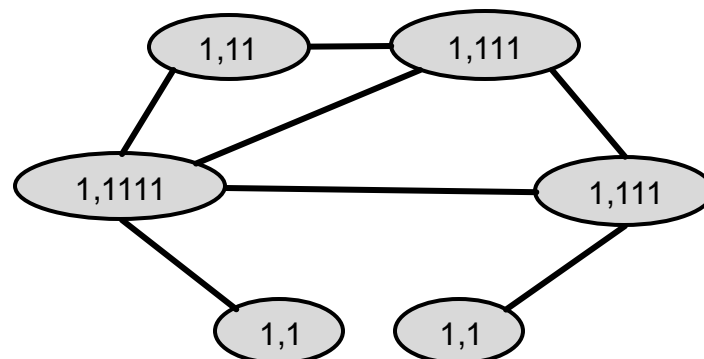
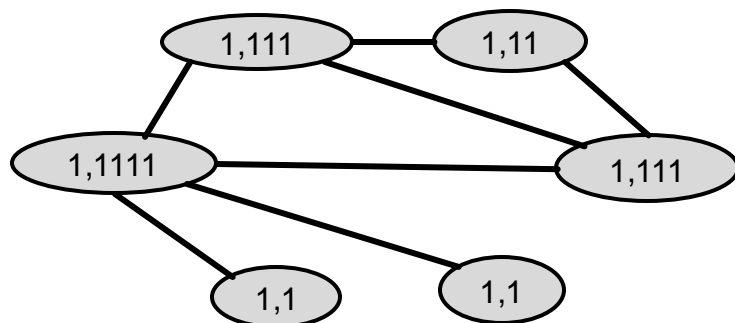
- Aggregate neighboring colors



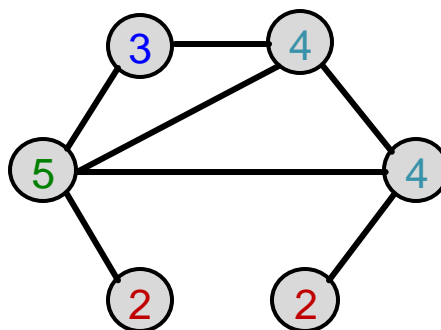
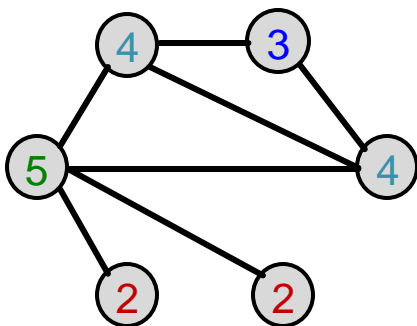
Color Refinement (2)

Example of color refinement given two graphs

- Aggregated colors



- Hash aggregated colors



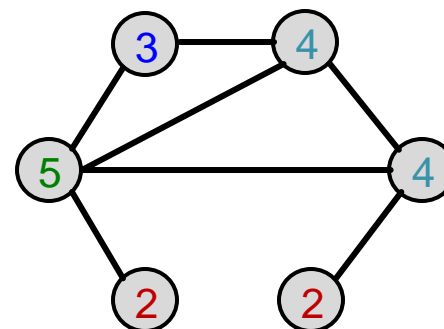
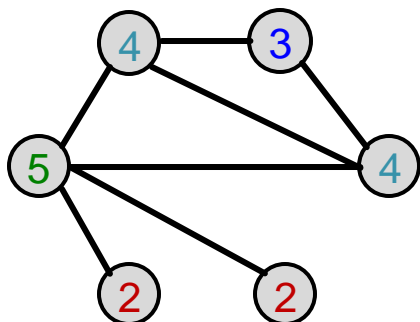
Hash table

1,1	-->	2
1,11	-->	3
1,111	-->	4
1,1111	-->	5

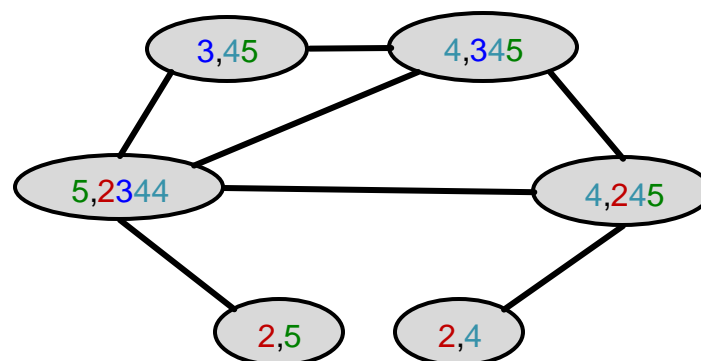
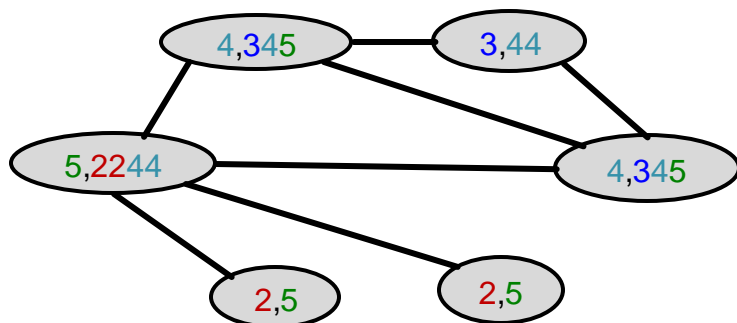
Color Refinement (3)

Example of color refinement given two graphs

- Aggregated colors



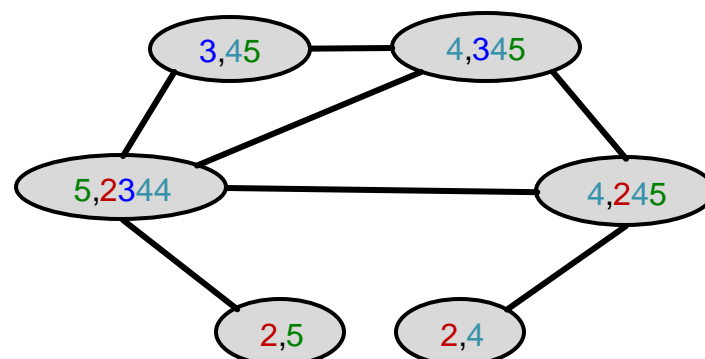
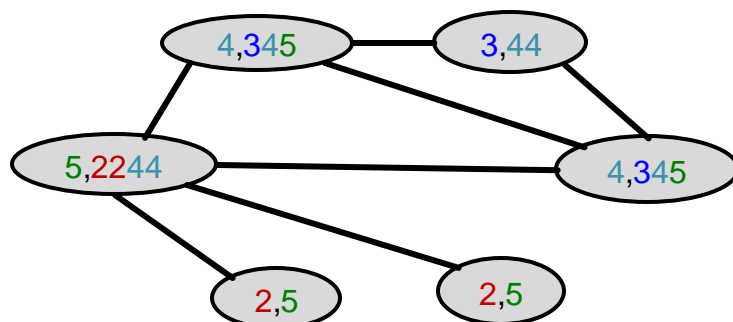
- Hash aggregated colors



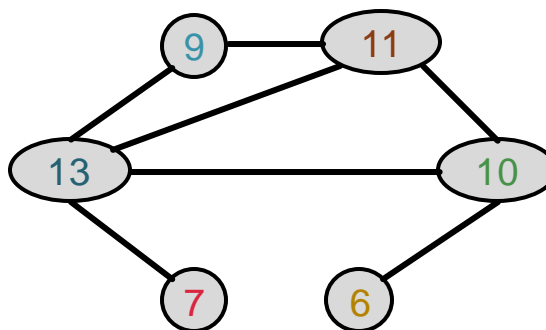
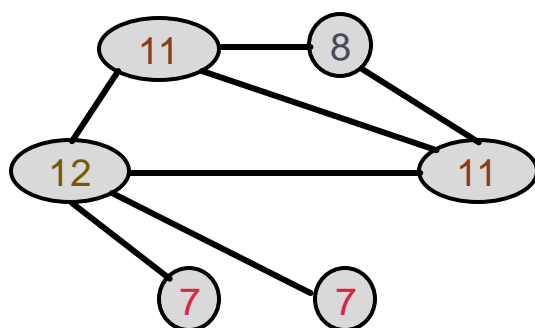
Color Refinement (4)

Example of color refinement given two graphs

■ Aggregated colors



■ Hash aggregated colors

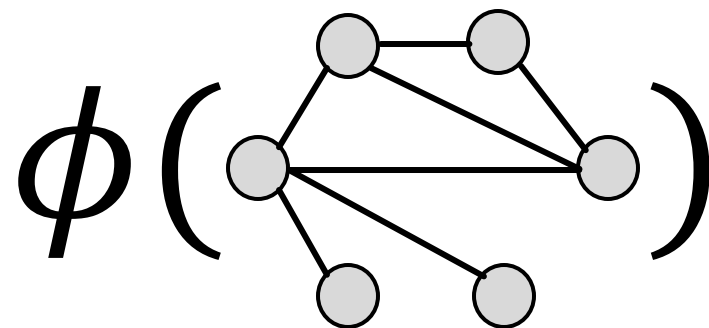


Hash table

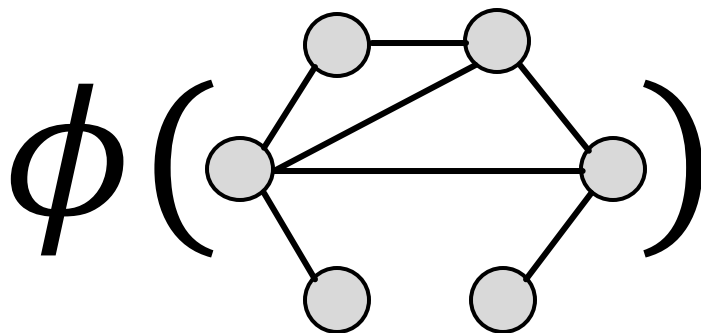
2,4	-->	6
2,5	-->	7
3,44	-->	8
3,45	-->	9
4,245	-->	10
4,345	-->	11
5,2244	-->	12
5,2344	-->	13

Weisfeiler-Lehman Graph Features

After color refinement, WL kernel counts number of nodes with a given color.



$$\begin{array}{c} \text{Colors} \\ 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13 \\ = [6, 2, 1, 2, 1, 0, 2, 1, 0, 0, 2, 1, 0] \\ \text{Counts} \end{array}$$



$$\begin{array}{c} 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13 \\ = [6, 2, 1, 2, 1, 1, 1, 0, 1, 1, 1, 0, 1] \end{array}$$

Weisfeiler-Lehman Kernel

The WL kernel value is computed by the inner product of the color count vectors:

$$\begin{aligned} K(\text{graph}_1, \text{graph}_2) &= \phi(\text{graph}_1)^T \phi(\text{graph}_2) \\ &= 49 \end{aligned}$$

Weisfeiler-Lehman Kernel

- WL kernel is **computationally efficient**
 - The time complexity for color refinement at each step is linear in $\#(\text{edges})$, since it involves aggregating neighboring colors.
- When computing a kernel value, only colors appeared in the two graphs need to be tracked.
 - Thus, $\#(\text{colors})$ is at most the total number of nodes.
- Counting colors takes linear-time w.r.t. $\#(\text{nodes})$.
- In total, time complexity is **linear in $\#(\text{edges})$** .

Graph-Level Features: Summary

■ Graphlet Kernel

- Graph is represented as **Bag-of-graphlets**
- **Computationally expensive**

■ Weisfeiler-Lehman Kernel

- Apply K -step color refinement algorithm to enrich node colors
 - Different colors capture different K -hop neighborhood structures
- Graph is represented as **Bag-of-colors**
- **Computationally efficient**
- Closely related to Graph Neural Networks (as we will see!)

Today's Summary

- **Traditional ML Pipeline**
 - Hand-crafted (structural) features + ML model
- **Hand-crafted features for graph data**
 - **Node-level:**
 - Node degree, centrality, clustering coefficient, graphlets
 - **Link-level:**
 - Distance-based feature
 - local/global neighborhood overlap
 - **Graph-level:**
 - Graphlet kernel, WL kernel
- However, we only considered featurizing the graph structure (but not the attribute of nodes and their neighbors)