Stanford CS224W: Traditional Methods 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: Q&A

Two ways to ask questions during lecture:

- **In-person (encouraged)**
- **On Ed:**
  - At the beginning of class, we will open a new discussion thread dedicated to this lecture
  - When to ask on Ed?
    - If you are watching the **livestream** remotely
    - If you have a minor clarifying question
    - If we run out of time to get to your question live
    - **Otherwise, try raising your hand first!**
- **Class goes till 3pm (not 2:50pm, sorry)**

Course Logistics: Colab 0

- **Colabs 0 and 1 will be released on our course website at 3pm today (Thu 9/23)**
- **Colab 0:**
  - Does not need to be handed-in
  - TAs will hold two recitations (on Zoom) to walk through Colab 0 with you:
    - Federico – Friday (9/24), 3-5pm PT
    - Yige – Monday (9/27), 10am-12pm PT
    - **Links to Zoom will be posted on Ed**

Course Logistics: Colab 1

- **Colabs 0 and 1 will be released on our course website at 3pm today (Thu 9/23)**
- **Colab 1:**
  - Due on Thursday 10/07 (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!

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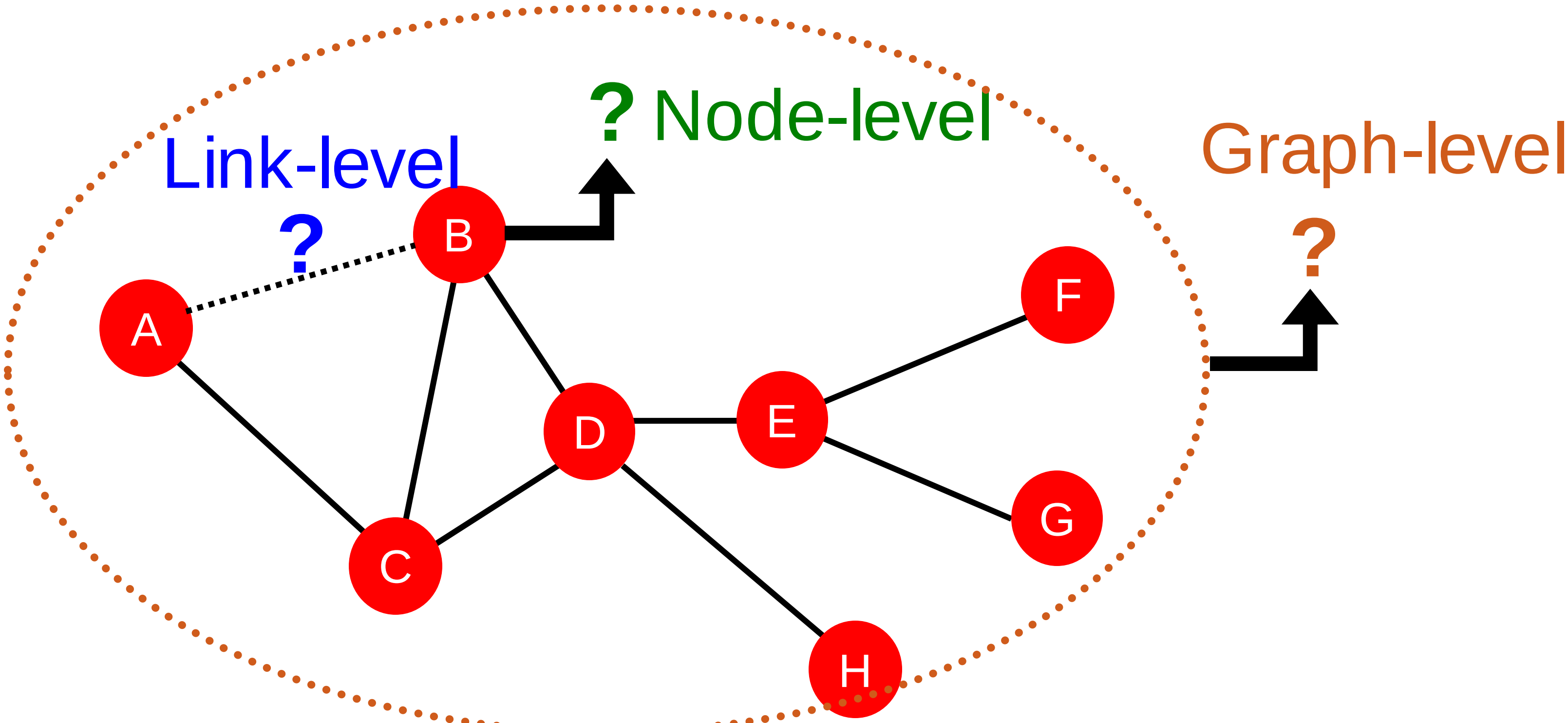
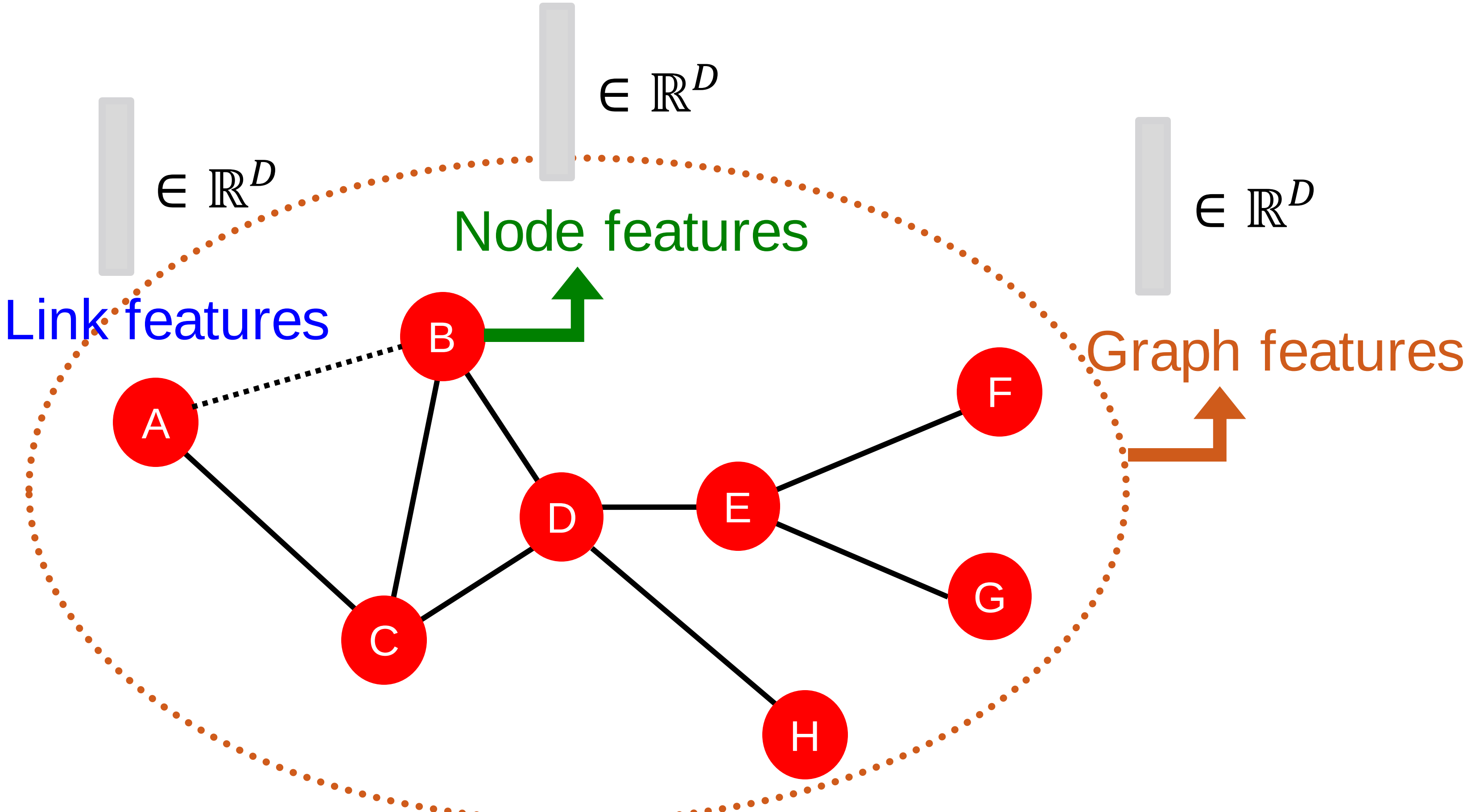
Machine Learning Tasks: Review

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



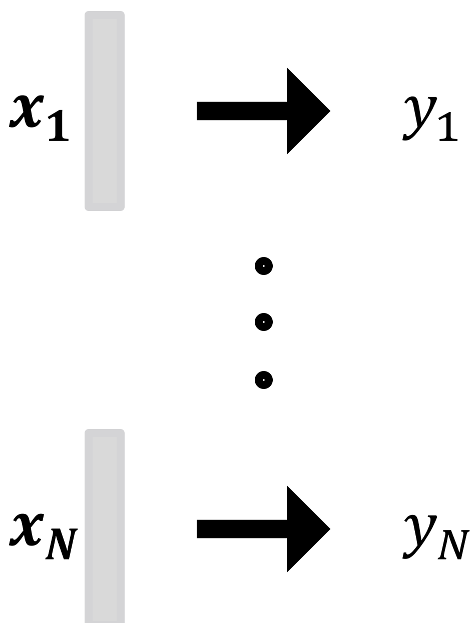
Traditional ML Pipeline

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

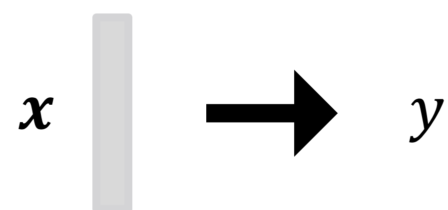


Traditional ML Pipeline

- **Train an ML model:**
  - Random forest
  - SVM
  - Neural network, etc.



- **Apply the model:**
  - Given a new node/link/graph, obtain its features and make a prediction



This Lecture: Feature Design

- **Using effective features 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
- **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: $f : V \to \mathbb{R}$

How do we learn the function?

Stanford CS224W: Node-Level Tasks and Features

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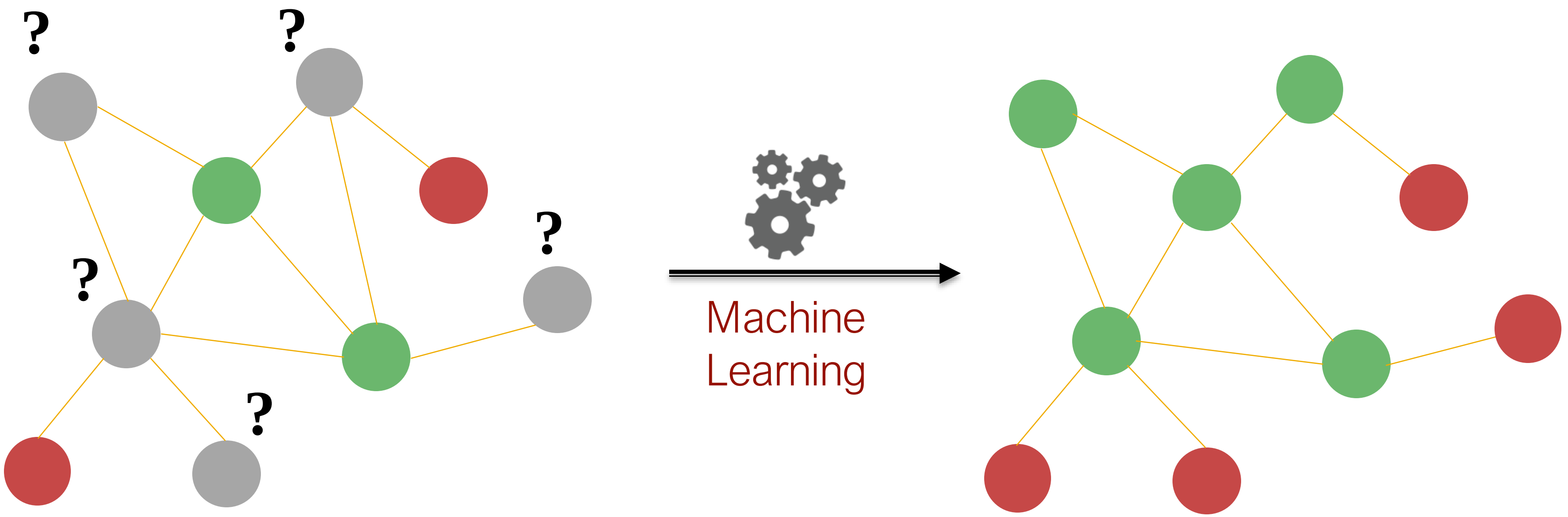
Node-Level Tasks



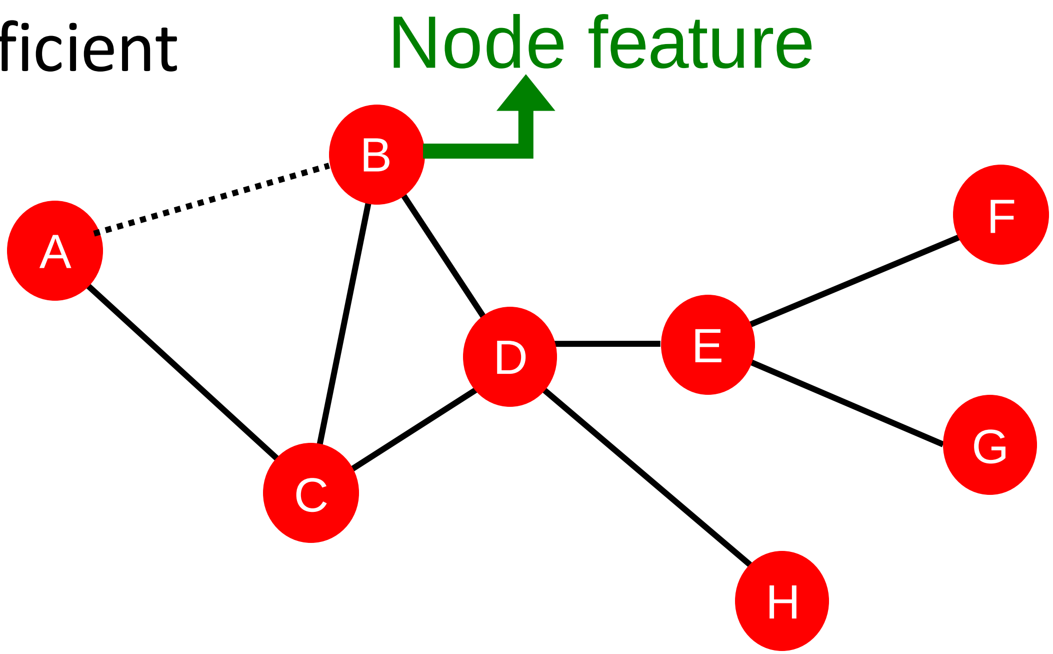
Node classification

ML needs features.

Node-Level Features: Overview

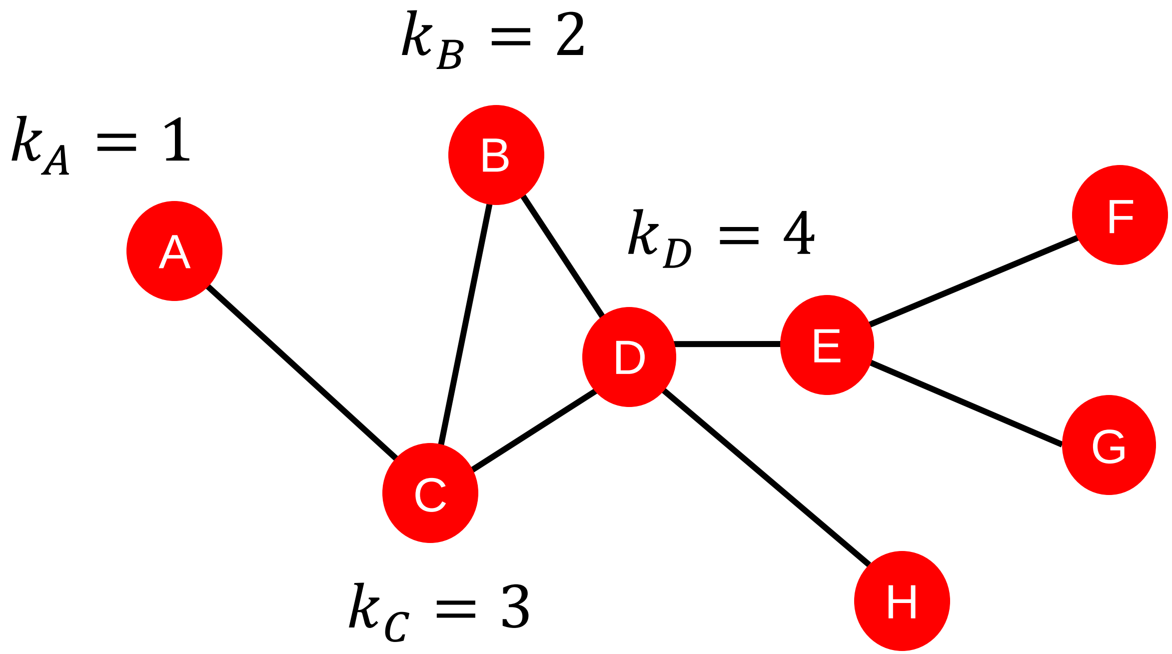
Goal: Characterize the structure and position of a node in the network:

- 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.

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

λ is normalization const (largest eigenvalue of A)

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

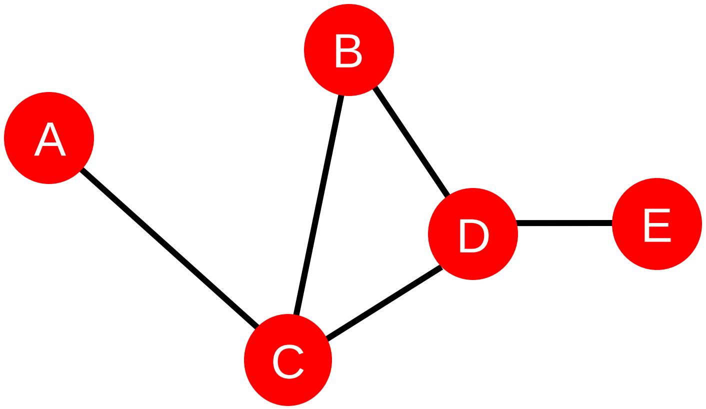
  - We see that centrality c is the **eigenvector of $\boldsymbol{A}$**!
  - The largest eigenvalue λ_{max} is always positive and unique (by Perron-Frobenius Theorem).
  - The eigenvector $\boldsymbol{c}_{max}$ corresponding to λ_{max} is used for centrality.

Node Centrality (2)

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

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

  - **Example:**



$c_A = c_B = c_E = 0$

$c_C = 3$

(A-<u>C</u>-B, A-<u>C</u>-D, A-<u>C</u>-D-E)

$c_D = 3$

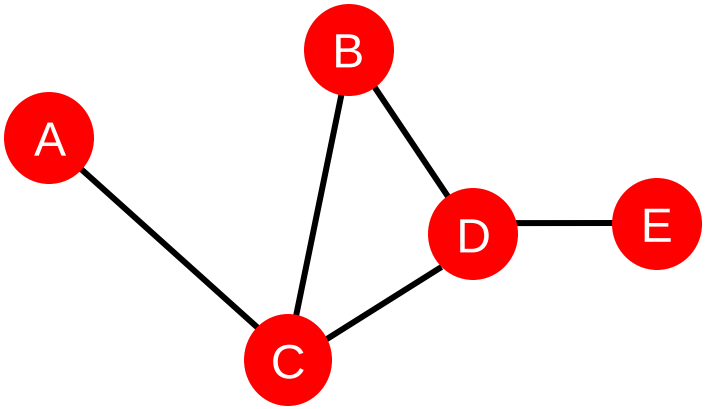
(A-C-<u>D</u>-E, B-<u>D</u>-E, C-<u>D</u>-E)

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)

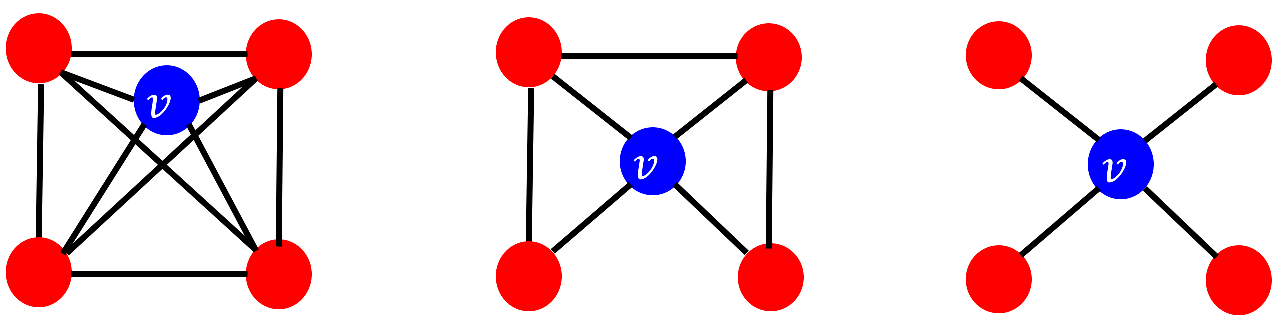
Node Features: Clustering Coefficient

- Measures how connected $v's$ neighboring nodes are:

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

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

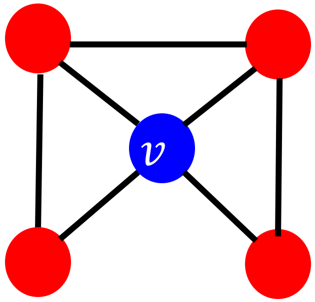
- **Examples:**



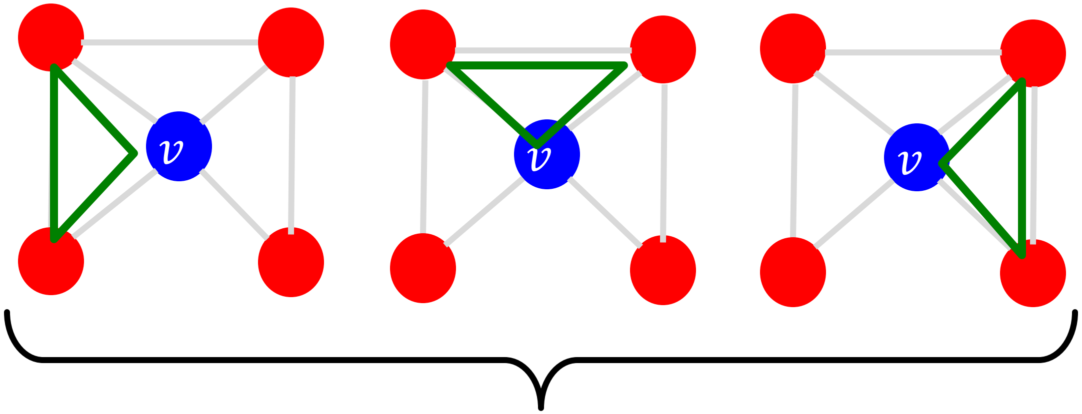
$e_v = 1$ $e_v = 0.5$ $e_v = 0$

Node Features: Graphlets

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



$e_v = 0.5$

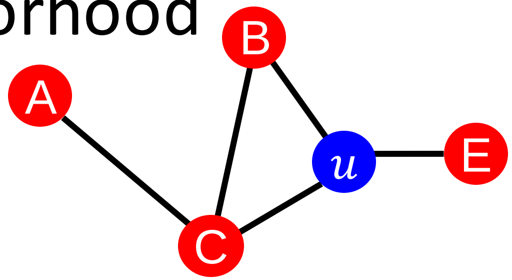


3 triangles (out of 6 node triplets)

- 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

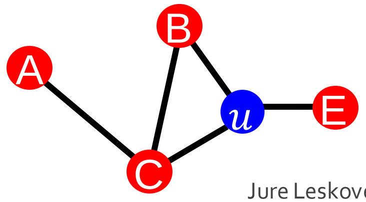


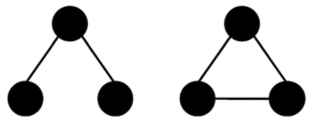
Analogy:

- **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

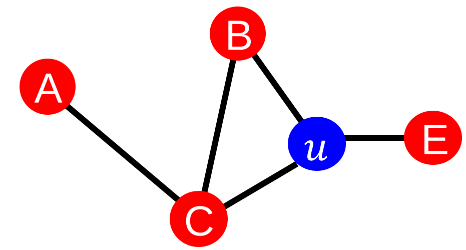
- Considering graphlets of size 2-5 nodes we get:
  - **Vector of 73 coordinates** is a signature of a node that describes the topology of node's neighborhood
- Graphlet degree vector provides a measure of a **node's local network topology**:
  - Comparing vectors of two nodes provides a more detailed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



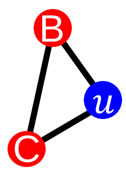


Induced Subgraph & Isomorphism

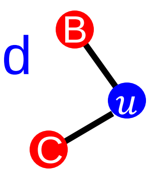
- **Def: Induced subgraph** is another graph, formed from a subset of vertices and *all* of the edges connecting the vertices in that subset.



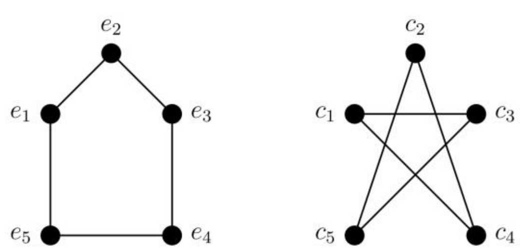
Induced subgraph:



Not induced subgraph:

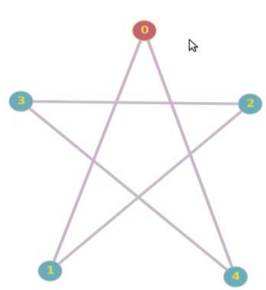


- **Def: Graph Isomorphism**
  - Two graphs which contain the same number of nodes connected in the same way are said to be isomorphic.

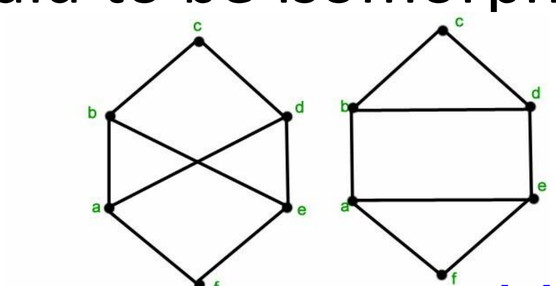


Isomorphic

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



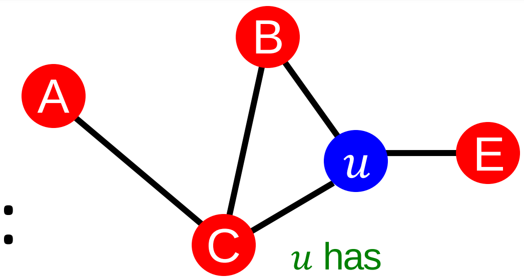
Source: Mathoverflow



Non-Isomorphic

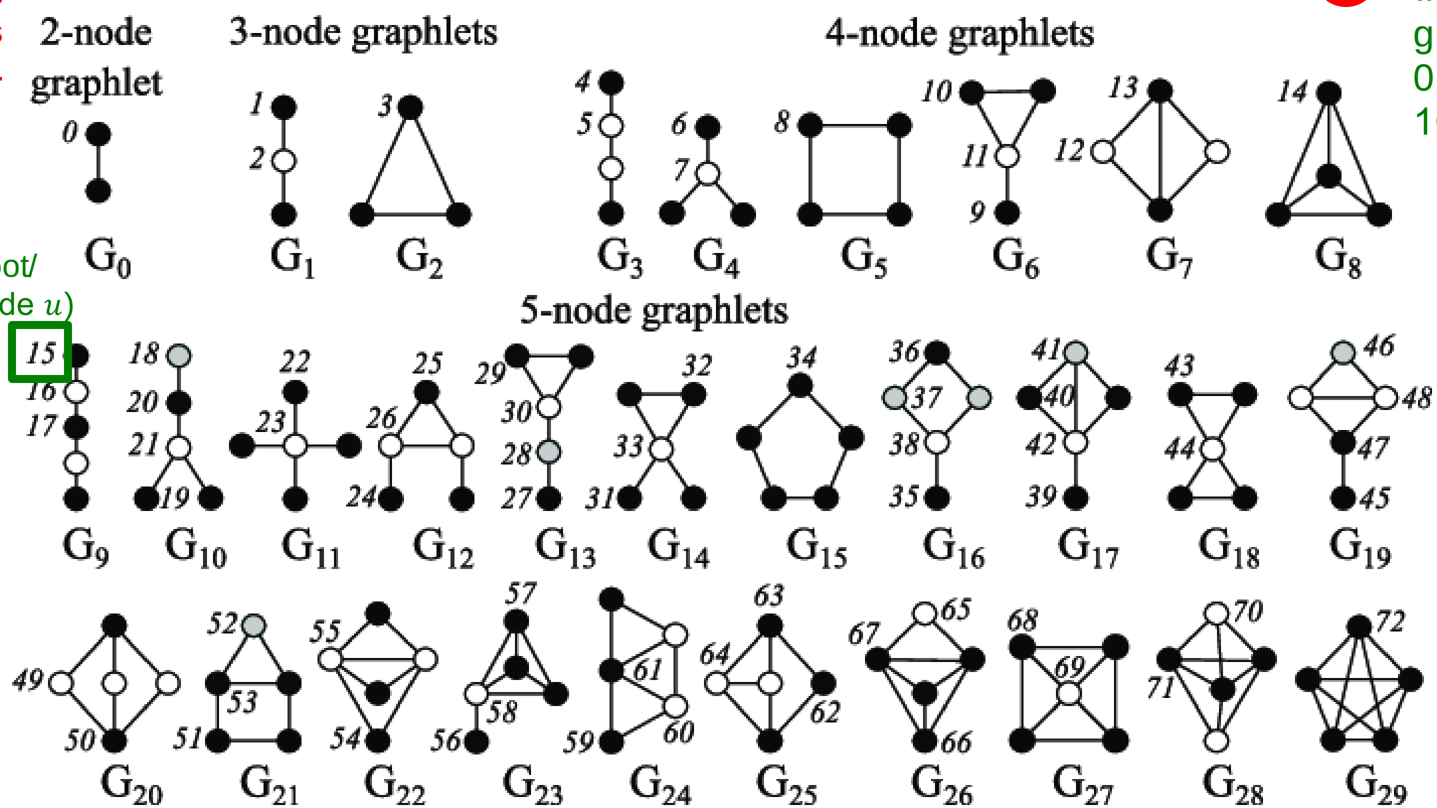
The right graph has cycles of length 3 but he left graph does not, so the graphs cannot be isomorphic.

Node Features: Graphlets



Graphlets: Rooted connected induced **non-isomorphic** subgraphs:

Take some nodes and all the edges between them.



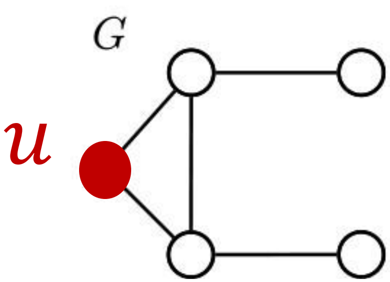
Graphlet id (Root/ "position" of node u)

u has graphlets: 0, 1, 2, 3, 5, 10, 11, …

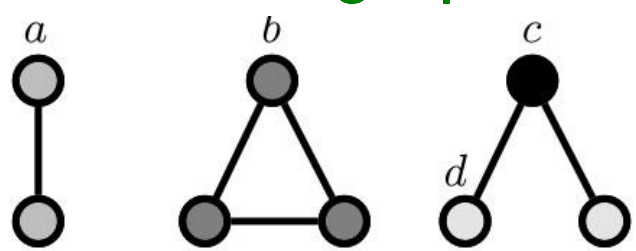
There are 73 different graphlets on up to 5 nodes

Node Features: Graphlets

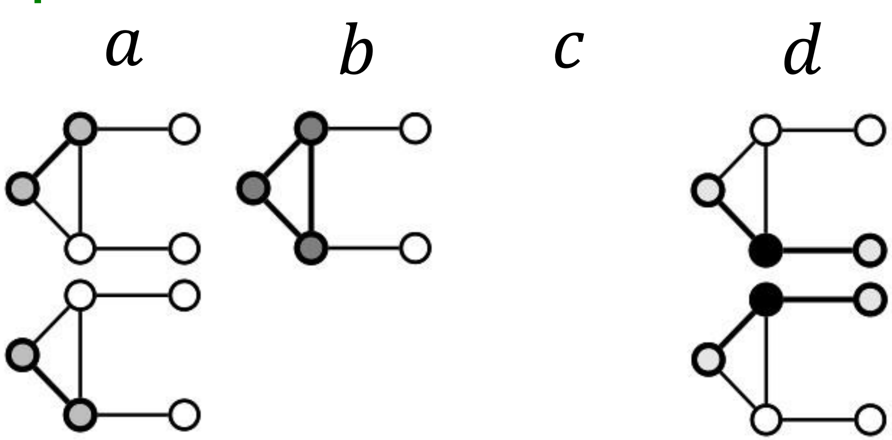
- **Graphlet Degree Vector (GDV):** A count vector of graphlets rooted at a given node.
- **Example:**



Possible graphlets up to size 3



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

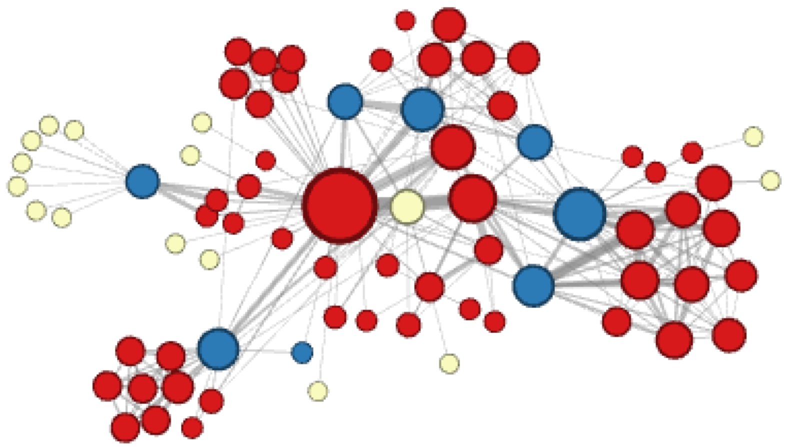
- **Importance-based features**: capture the importance of a node in a graph
  - Node degree:
    - Simply counts the number of neighboring nodes
  - Node centrality:
    - Models importance of neighboring nodes in a graph
    - Different modeling choices: eigenvector centrality, betweenness centrality, 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

Stanford CS224W: Link Prediction Task and Features

CS224W: Machine Learning with Graphs

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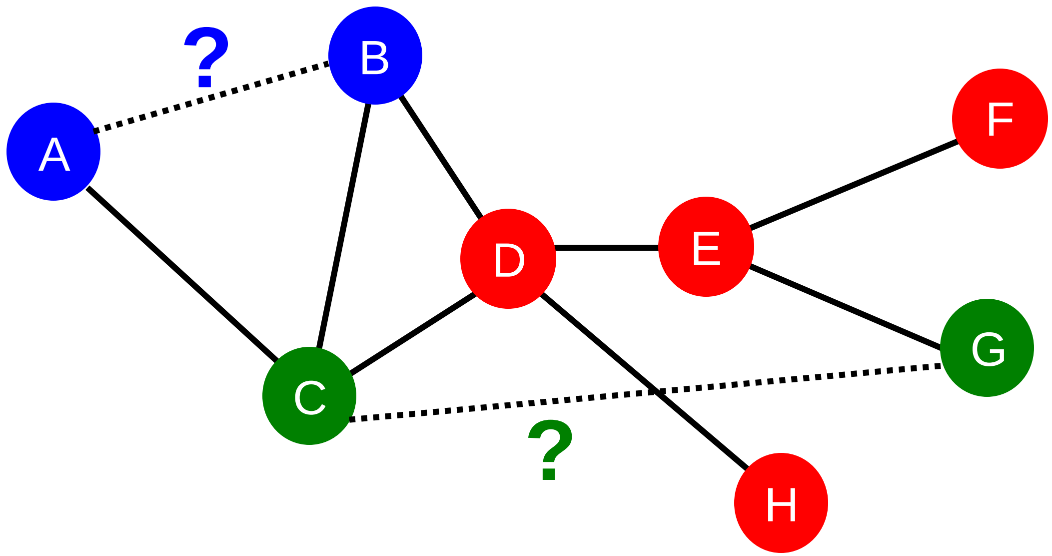
Link-Level Prediction Task: Recap

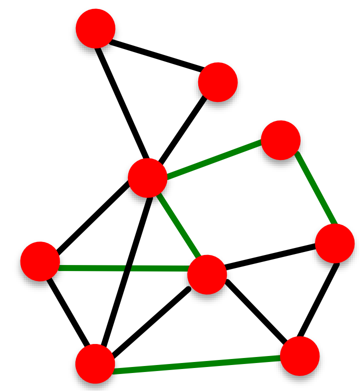
- The task is to predict **new links** based on the existing links.
- At test time, node pairs (with no existing links) are ranked, and top K node pairs are predicted.
- The key is to design features for **a pair of nodes**.



Link Prediction as a Task

Two formulations of the link prediction task:

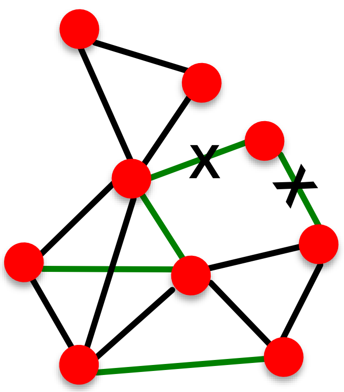
- **1) Links missing at random:**
  - Remove a random set of links and then aim to predict them
- **2) Links over time:**
  - Given $G[t_0, t_0']$ a graph defined by edges up to time t_0', **output a ranked list L** of edges (not in $G[t_0, t_0']$) that are predicted to appear in time $G[t_1, t_1']$
  - **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



$G[t_0, t_0']$
$G[t_1, t_1']$

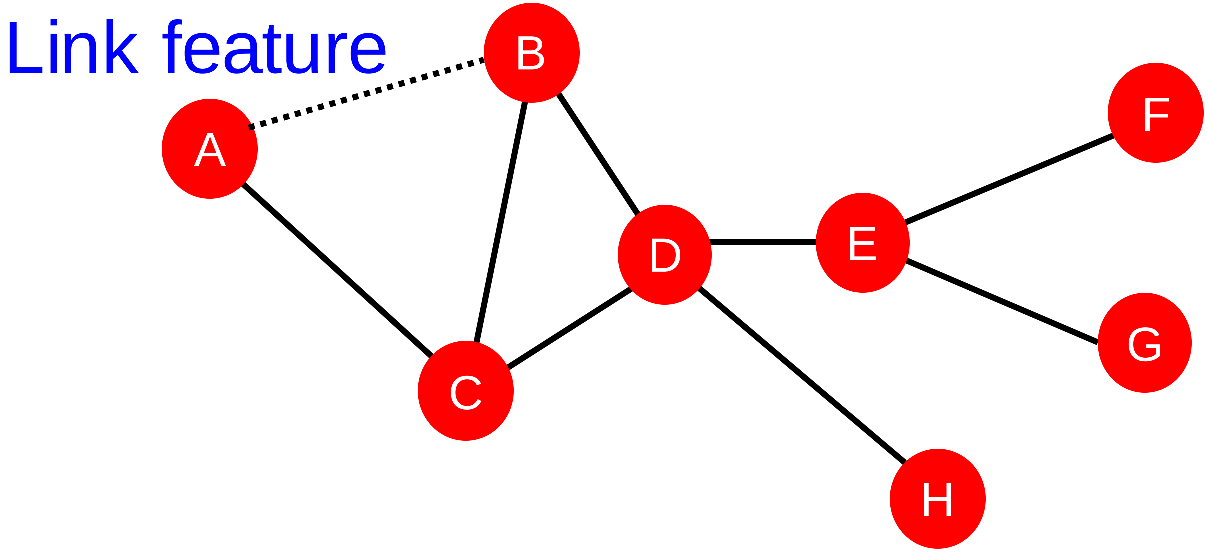
Link Prediction via Proximity

- **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

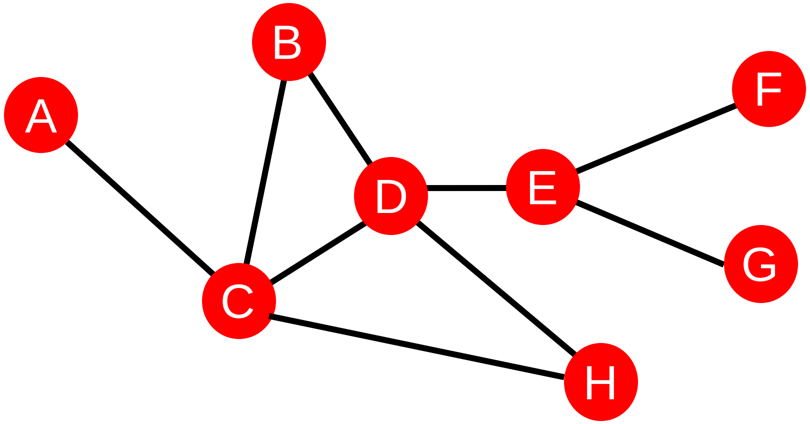
- Distance-based feature
- Local neighborhood overlap
- Global neighborhood overlap



Distance-Based Features

Shortest-path distance between two nodes

- Example:



$$S_{BH} = S_{BE} = S_{AB} = 2$$
$$S_{BG} = S_{BF} = 3$$

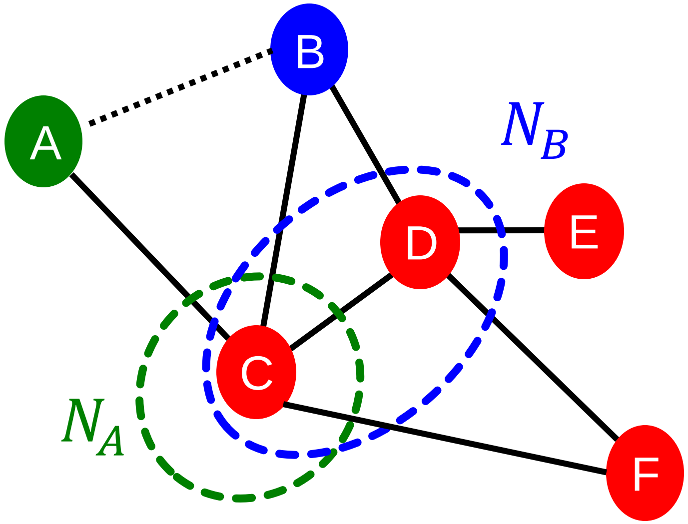
- However, this does not capture the degree of neighborhood overlap:
  - Node pair *(B, H)* has 2 shared neighboring nodes, while pairs *(B, E)* and *(A, B)* only have 1 such node.

Local Neighborhood Overlap

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

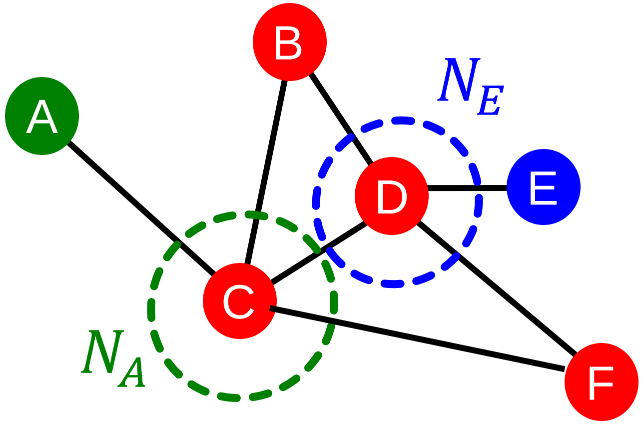
- **Common neighbors:** $|N(v_1) \cap N(v_2)|$
  - Example: $|N(A) \cap N(B)| = |\{C\}| = 1$
- **Jaccard's coefficient:** $\frac{|N(v_1) \cap N(v_2)|}{|N(v_1) \cup N(v_2)|}$
  - Example: $\frac{|N(A) \cap N(B)|}{|N(A) \cup N(B)|} = \frac{|\{C\}|}{|\{C,D\}|} = \frac{1}{2}$
- **Adamic-Adar index:**

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

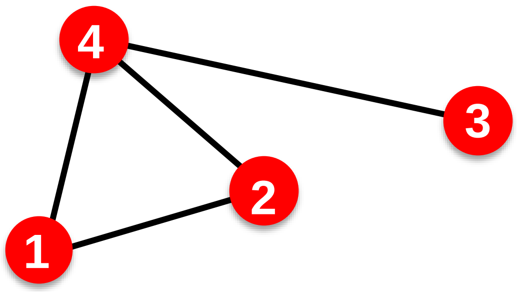
- **Katz index:** count the number of walks of all lengths between a given pair of nodes.

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

$\boldsymbol{P_{12}^{(1)} = A_{12}}$



$$A = \begin{pmatrix} 0 & \boxed{1} & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

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**!
  - $\boldsymbol{A}_{uv}$ specifies #walks of length 1 (direct neighborhood) between u and v.
  - $\boldsymbol{A}_{uv}^{\mathbf{2}}$ specifies #walks of **length 2** (neighbor of neighbor) between u and v.
  - And, $\boldsymbol{A}_{uv}^{\boldsymbol{l}}$ specifies #walks of **length $\boldsymbol{l}$**.

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:

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

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.

Stanford CS224W: Graph-Level Features and Graph Kernels

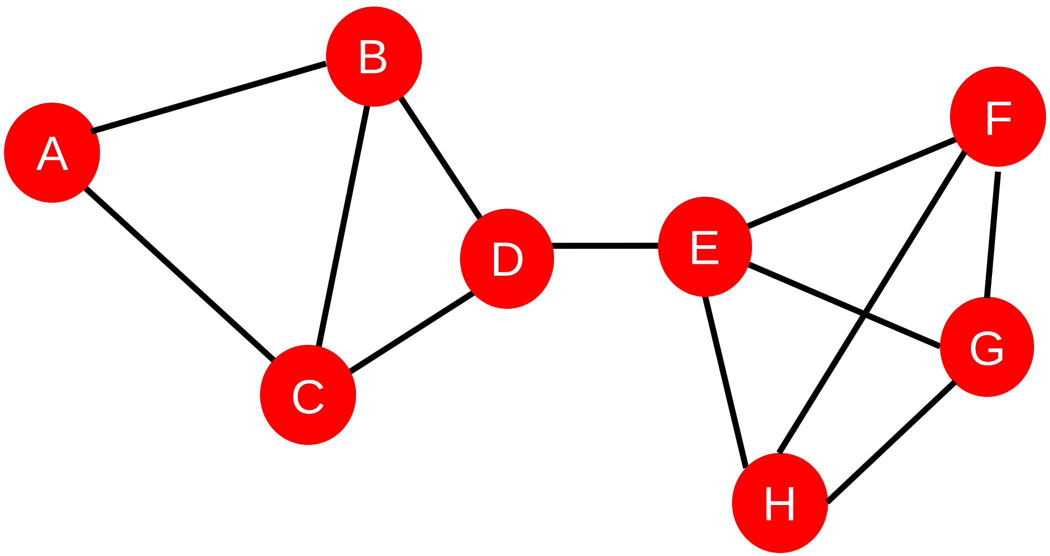
CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

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 $\boldsymbol{K} = \left(K(G, G')\right)_{G,G'}$ must always be positive semidefinite (i.e., has positive eigenvalues)
  - There exists a feature representation $\phi(\cdot)$ such that $K(G, G') = \phi(\mathrm{G})^{\mathrm{T}}\phi(G')$
  - Once the kernel is defined, off-the-shelf ML model, such as kernel SVM, can be used to make predictions.

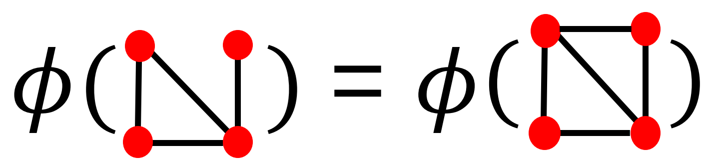
Graph-Level Features: Overview

- **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

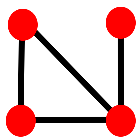
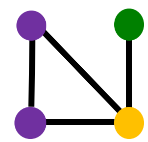
- **Goal**: Design graph feature vector $\phi(G)$
- **Key idea**: Bag-of-Words (BoW) for a graph
  - **Recall:** BoW simply uses the word counts as features for documents (no ordering considered).
  - Naïve extension to a graph: Regard nodes as words.
  - Since both graphs have 4 red nodes, we get the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



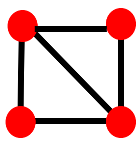
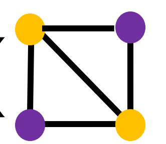
Graph Kernel: Key Idea

What if we use Bag of **node degrees**?

Deg1: ● Deg2: ● Deg3: ●

$\phi($  $)$ = count() = [1, 2, 1]

Obtains different features for different graphs!

$\phi($  $)$ = count() = [0, 2, 2]

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

Graphlet Features

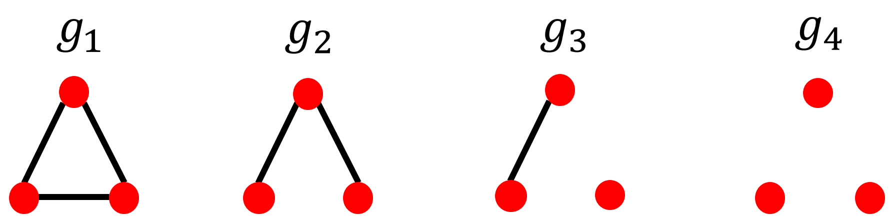
- Key idea: Count the number of different graphlets in a graph.

  - **Note:** Definition of graphlets here is slightly different from 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.

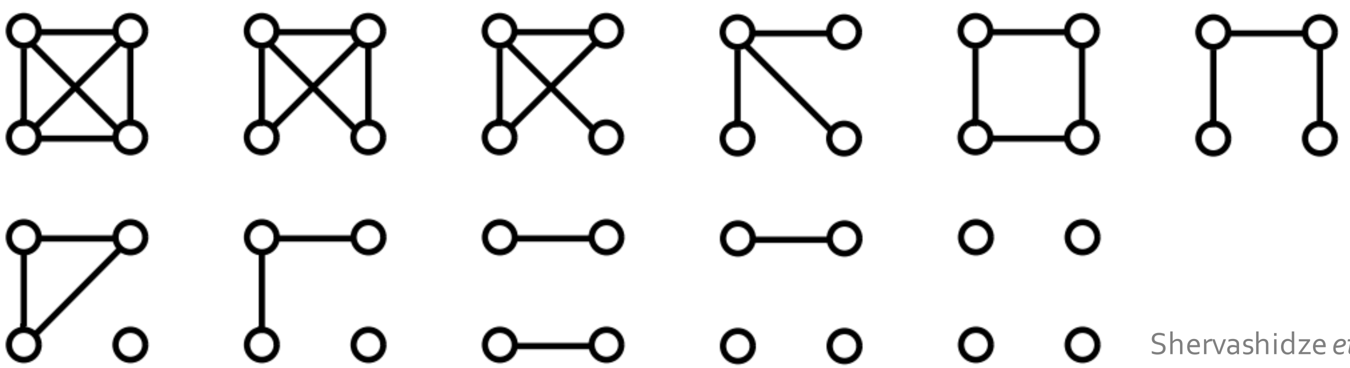
Graphlet Features

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

Graphlet Features

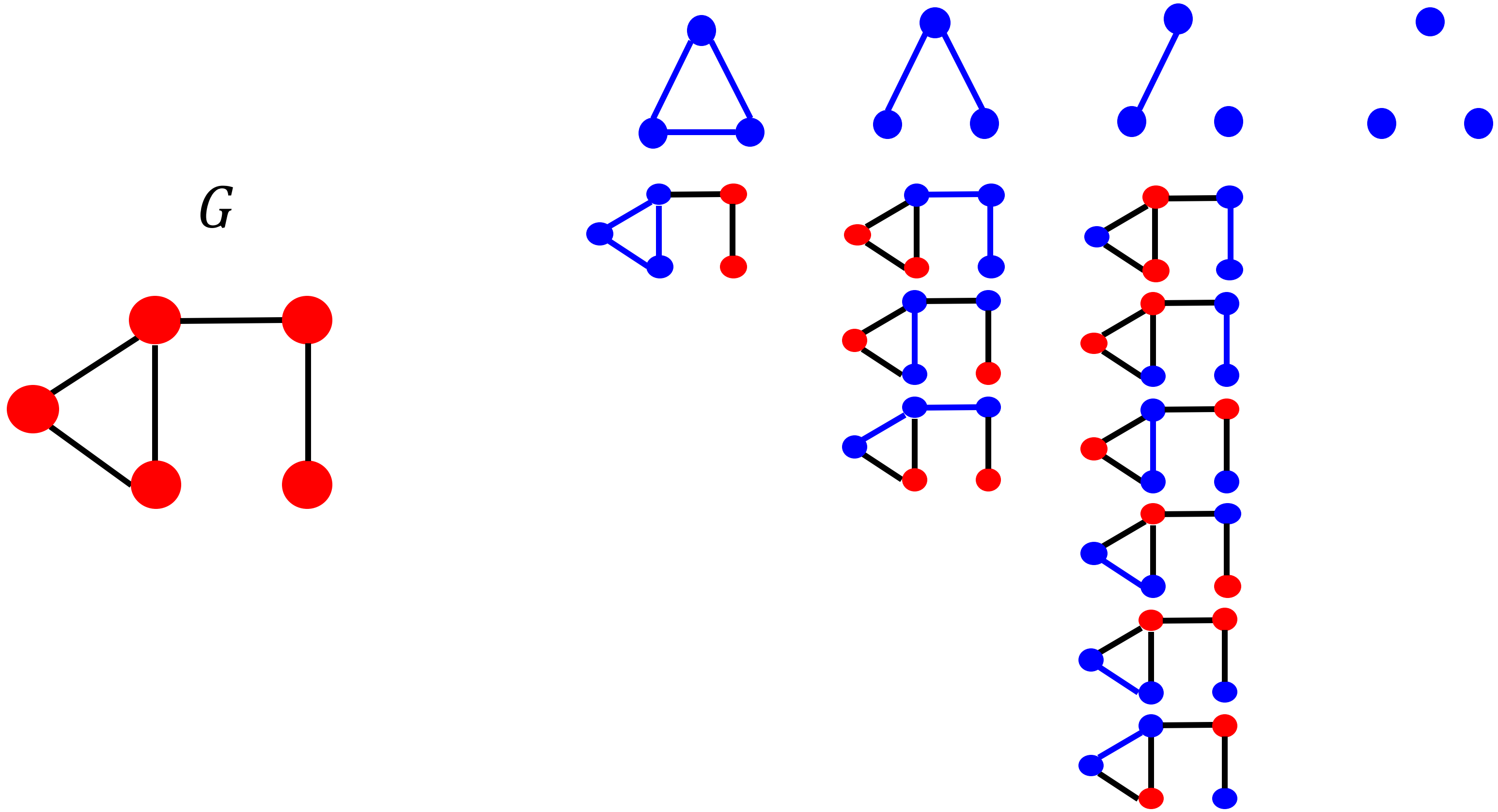
- Given graph G, and a graphlet list $\mathcal{G}_k = (g_{1,} g_2, \dots, g_{n_k})$, define the graphlet count vector $\boldsymbol{f}_G \in \mathbb{R}^{n_k}$ as

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

Graphlet Features

- Example for k = 3.

g_1 g_2 g_3 g_4



$$f_G = (1, \quad 3, \quad 6, \quad 0)^{\mathrm{T}}$$

Graphlet Kernel

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

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

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

$$\boldsymbol{h}_G = \frac{\boldsymbol{f}_G}{\mathrm{Sum}(\boldsymbol{f}_G)} \qquad K(G, G') = \boldsymbol{h}_G{}^{\mathrm{T}} \boldsymbol{h}_{G'}$$

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

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

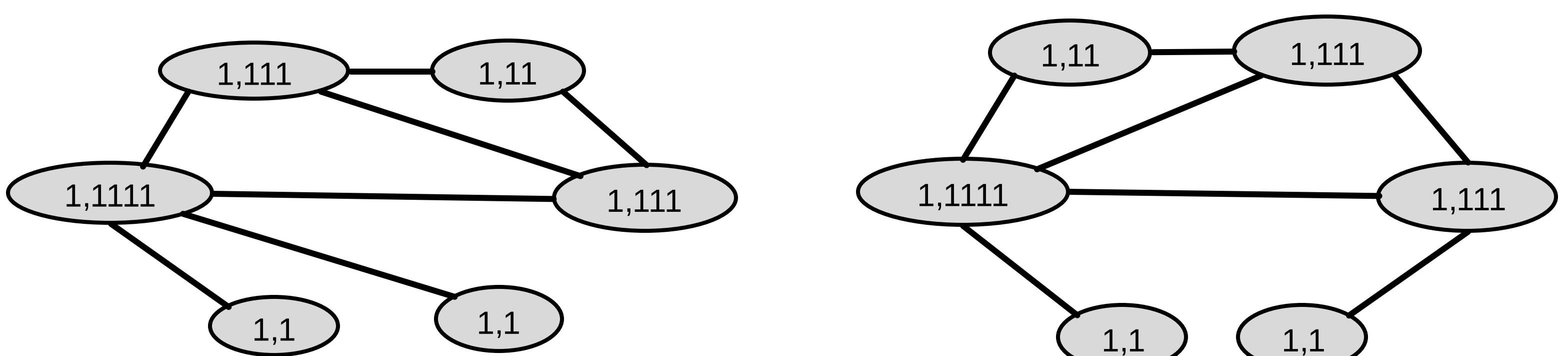
    where HASH maps different inputs to different colors.
  - After K steps of color refinement, $c^{(K)}(v)$ summarizes the structure of K-hop neighborhood

Color Refinement (1)

Example of color refinement given two graphs

- Assign initial colors

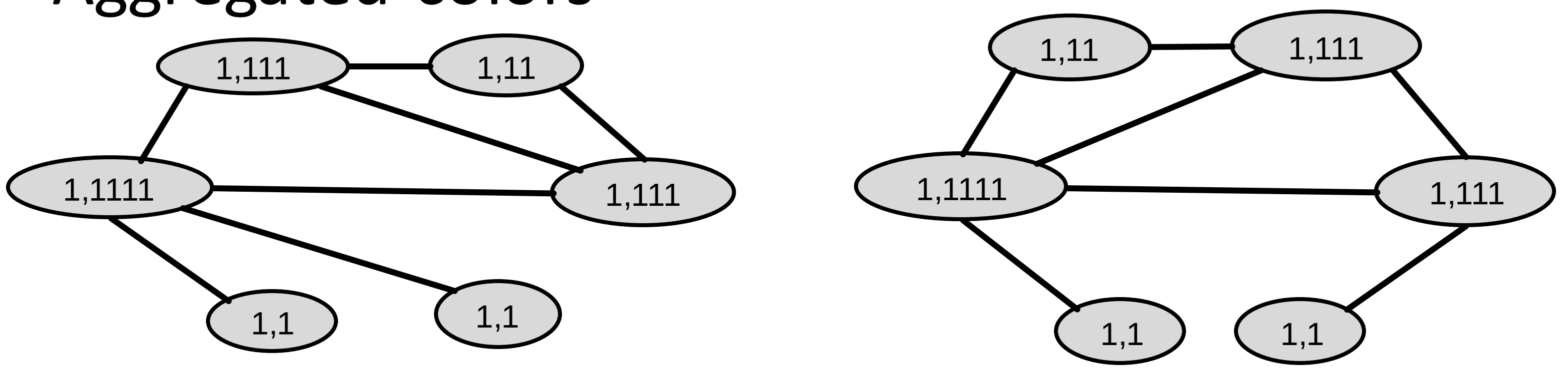
- Aggregate neighboring colors



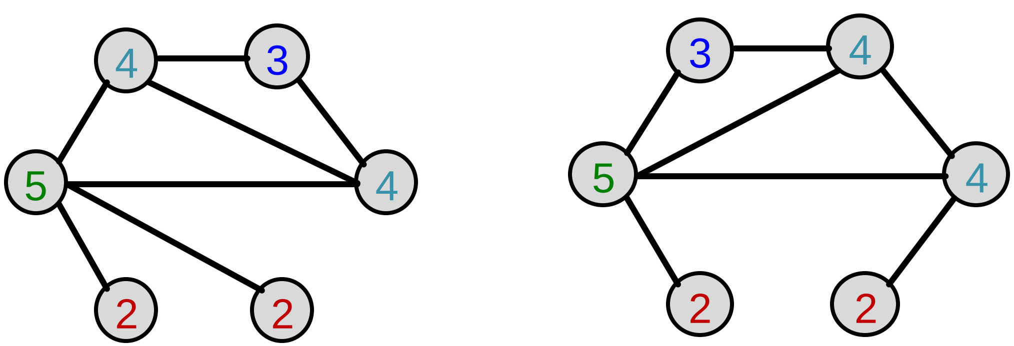
Color Refinement (2)

Example of color refinement given two graphs

- Aggregated colors



- Hash aggregated colors



Hash table

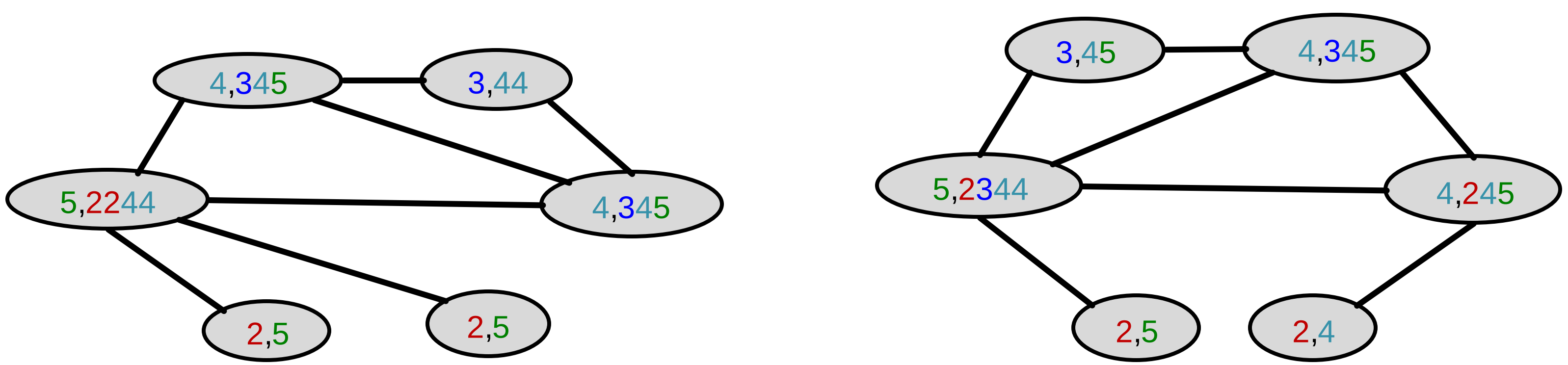
1,1	-->	2
1,11	-->	3
1,111	-->	4
1,1111	-->	5

Color Refinement (3)

Example of color refinement given two graphs

- Aggregated colors

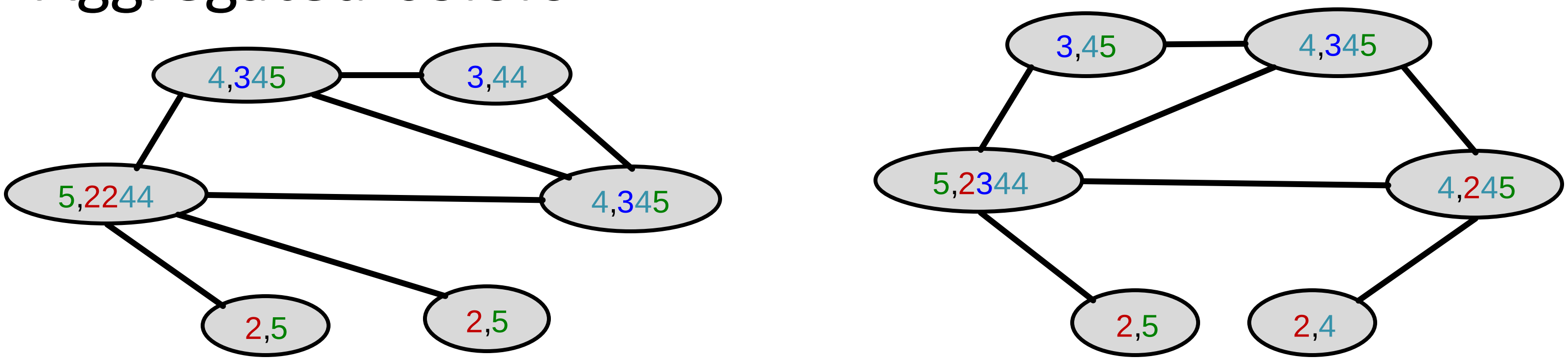
- Hash aggregated colors



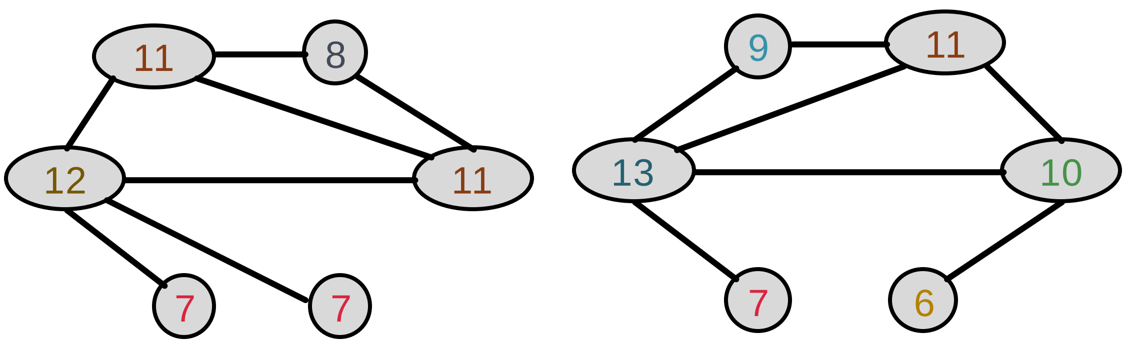
Color Refinement (4)

Example of color refinement given two graphs

- Aggregated colors



- Hash aggregated colors

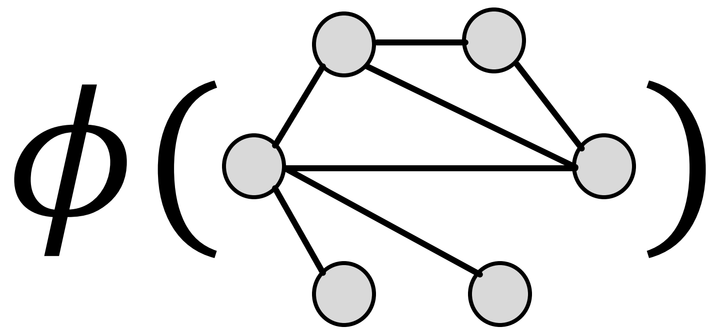


Hash table

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

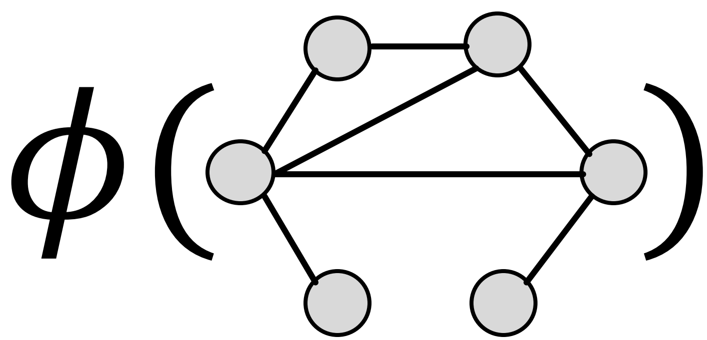
After color refinement, WL kernel counts number of nodes with a given color.



Colors

1,2,3,4,5,6,7,8,9,10,11,12,13
= [6,2,1,2,1,0,2,1,0, 0, 0, 2, 1]

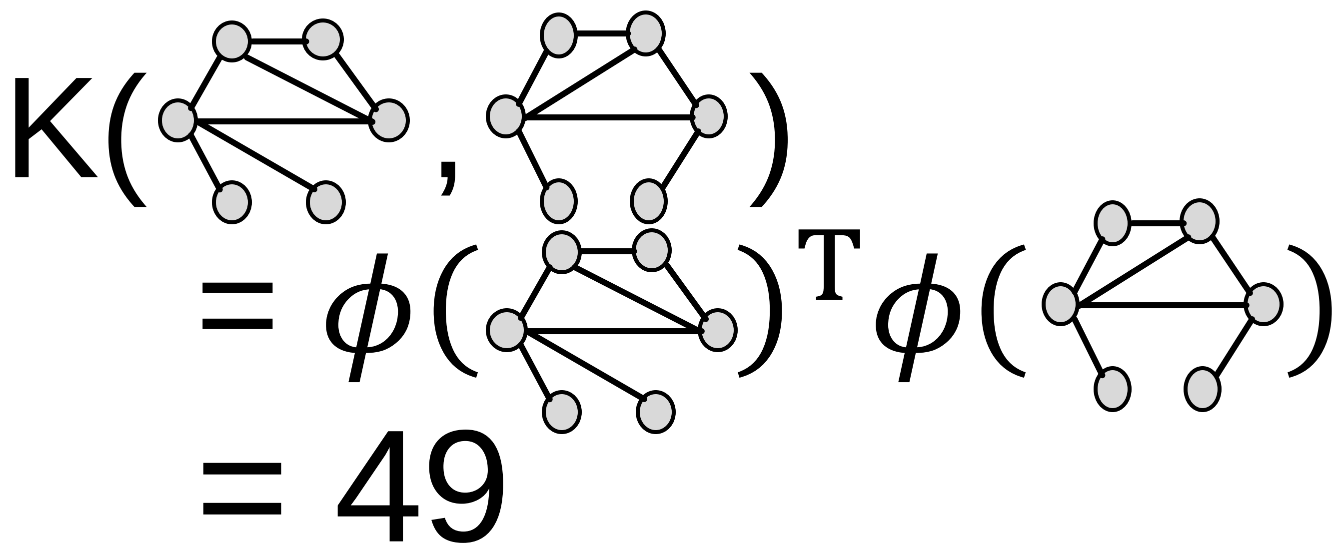
Counts



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]

Weisfeiler-Lehman Kernel

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



Weisfeiler-Lehman Kernel

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