Stanford CS224W: Traditional Methods for Machine Learning in Graphs

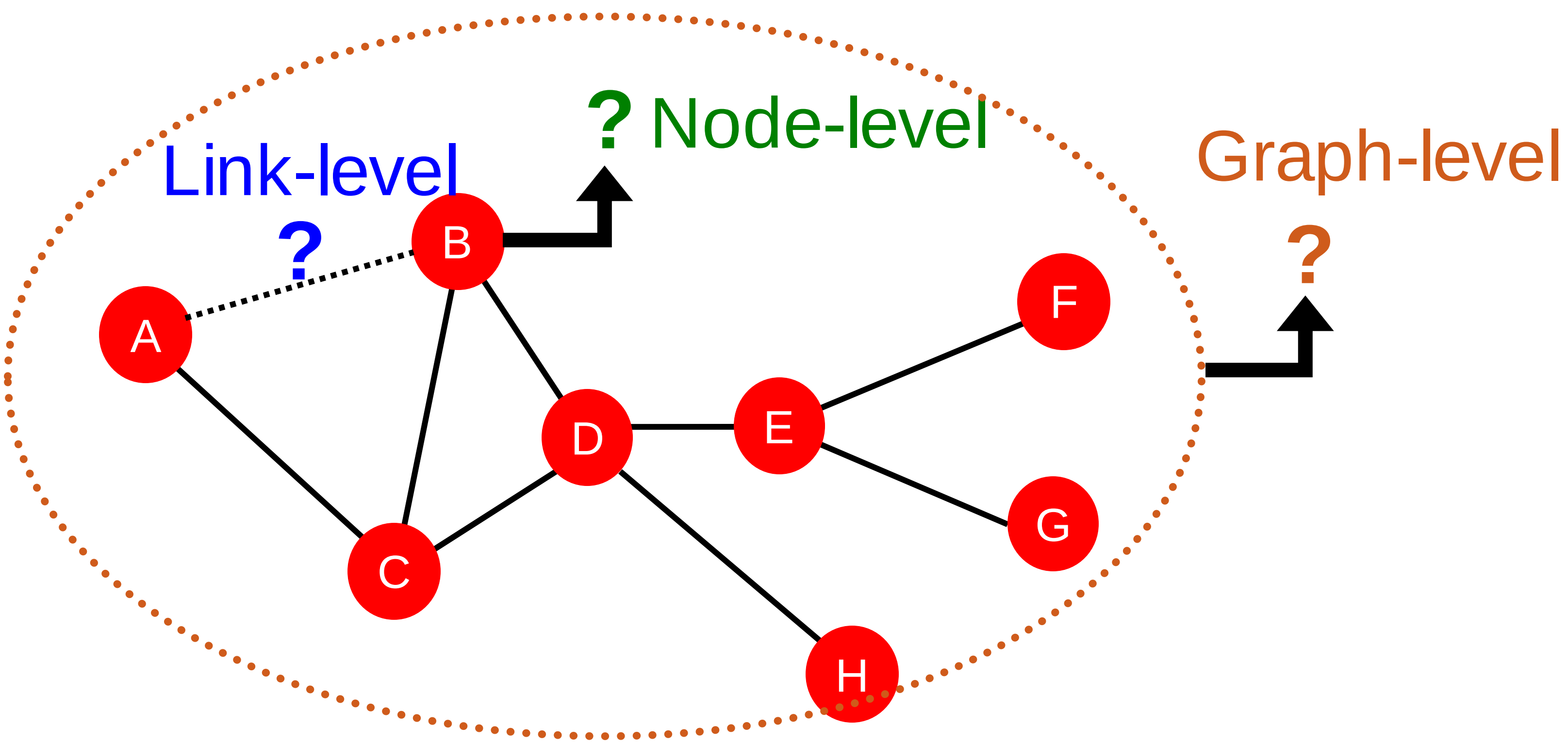
CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

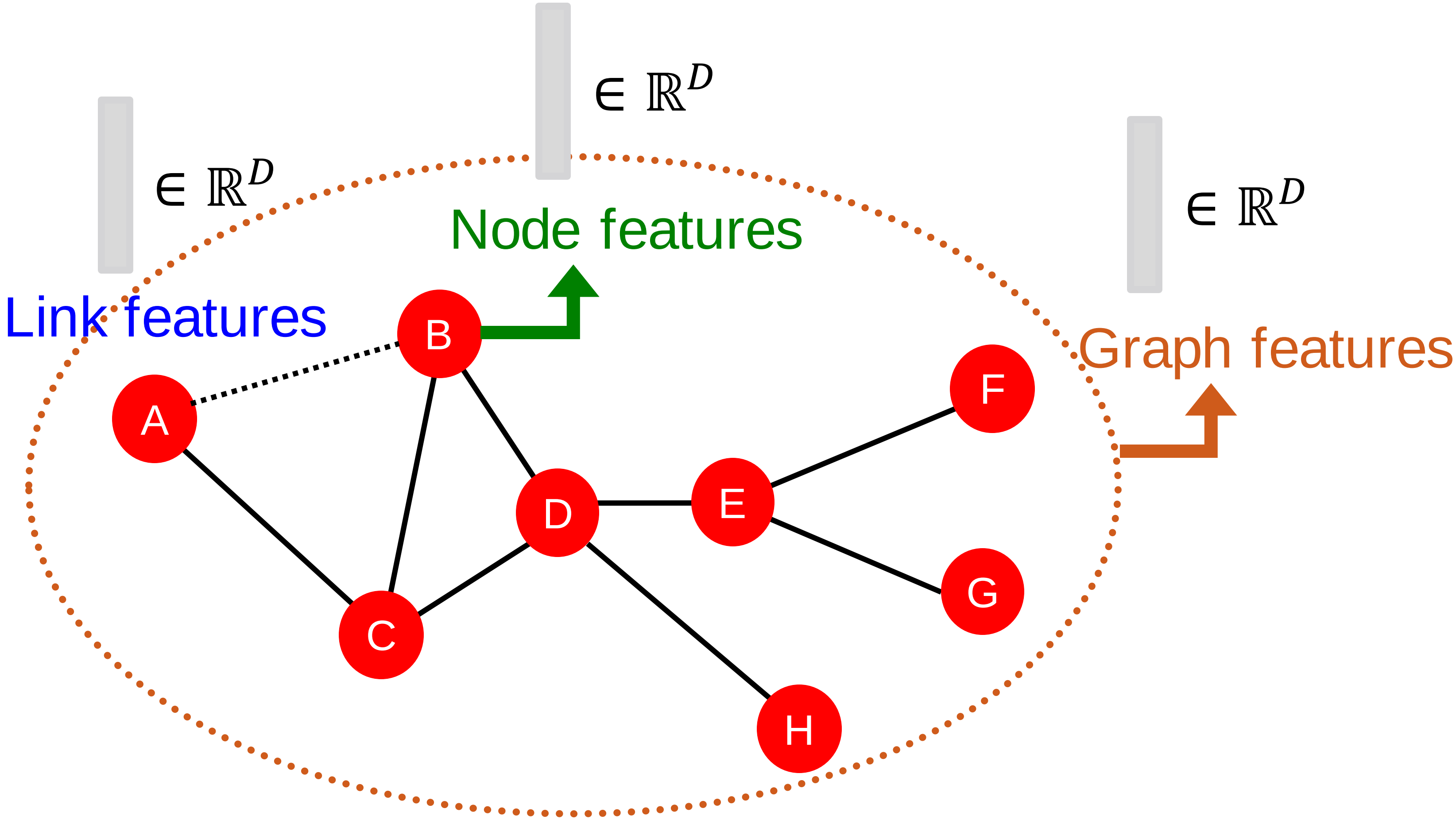
Machine Learning Tasks: Review

- 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.

$$\boldsymbol{x_1} \rightarrow y_1$$

$$\vdots$$

$$\boldsymbol{x_N} \rightarrow y_N$$

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

$$\boldsymbol{x} \rightarrow y$$

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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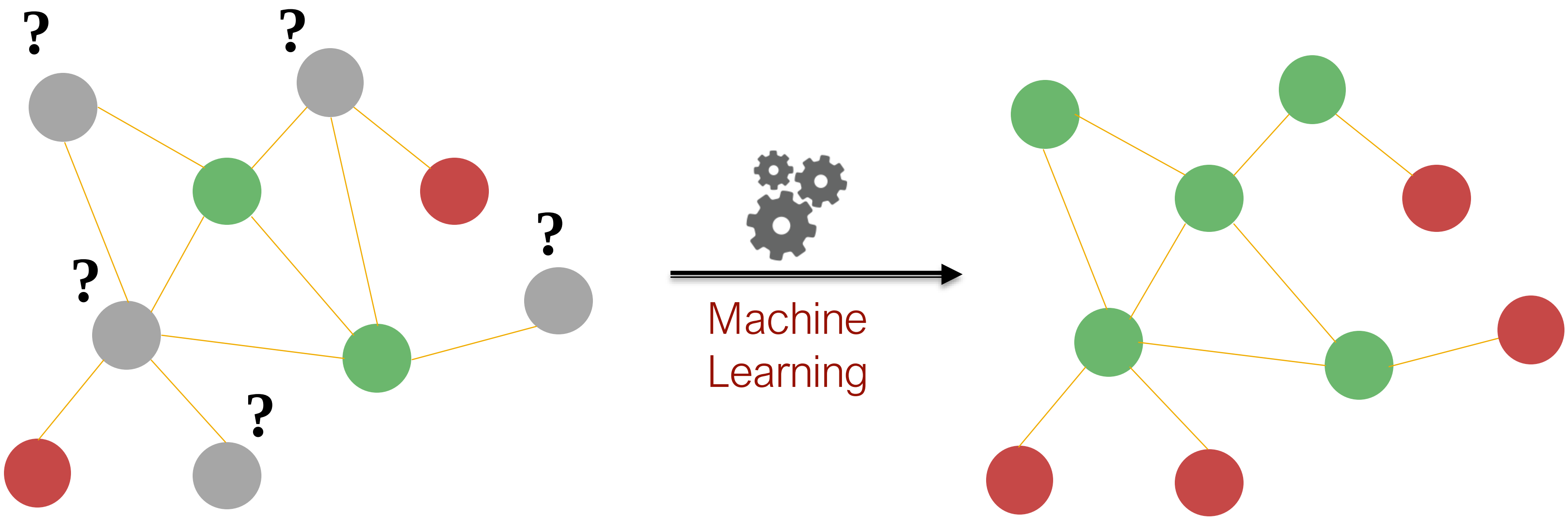
Node-Level Tasks



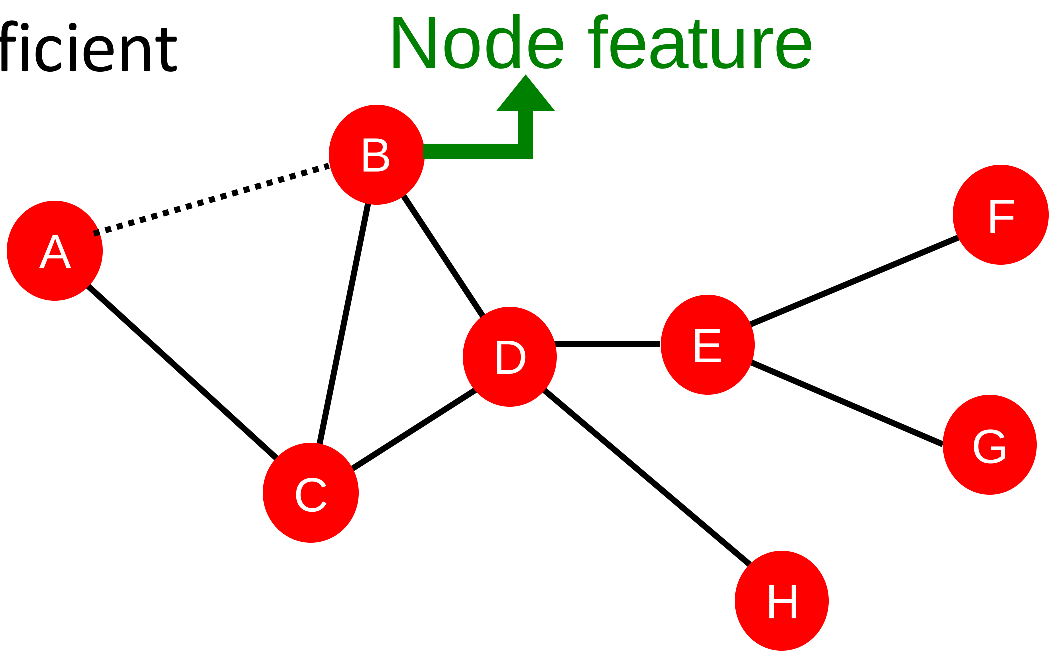
Node classification

ML needs features.

Node-Level Features: Overview

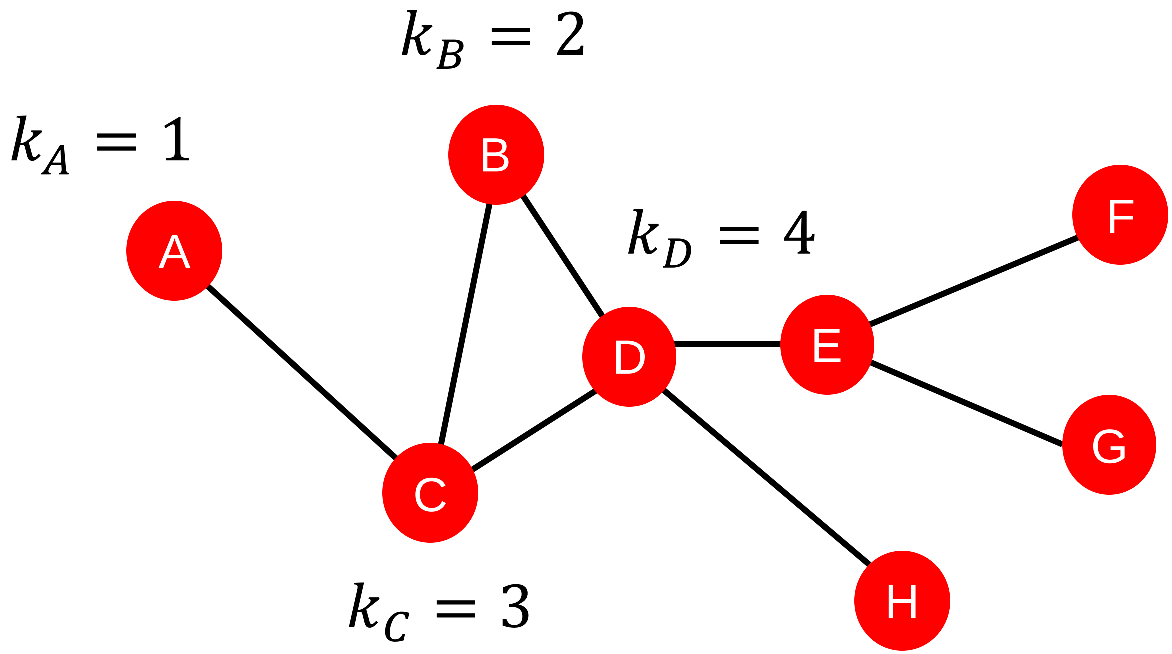
Goal: Characterize the structure and position of a node in the network:

- 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-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

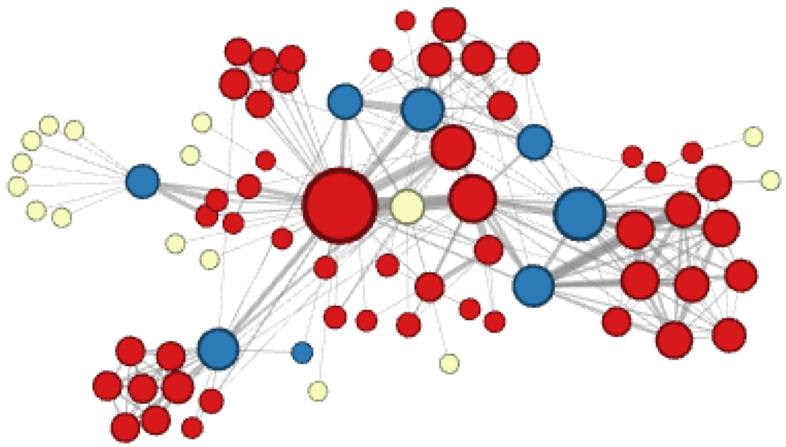
- **Importance-based features**: capture the importance of a node in a graph
  - Node degree:
    - Simply counts the number of neighboring nodes
  - Node centrality:
    - Models importance of neighboring nodes in a graph
    - Different modeling choices: eigenvector centrality, betweenness centrality,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

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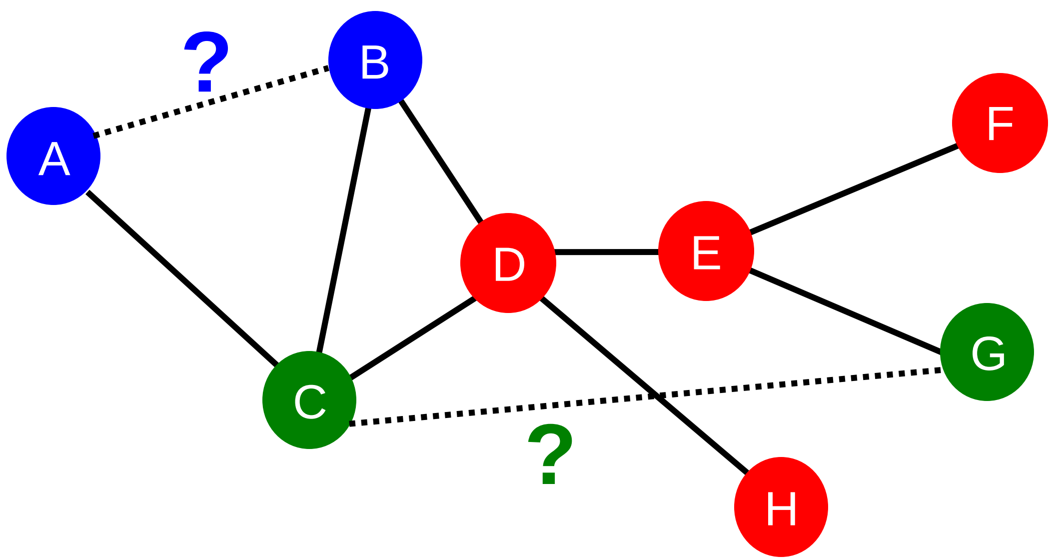
Link-Level Prediction Task: Recap

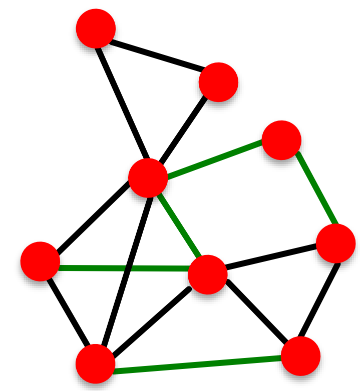
- The task is to predict **new links** based on the existing links.
- At test time, node pairs (with no existing links) are ranked, and top K node pairs are predicted.
- The key is to design features for **a pair of nodes**.



Link Prediction as a Task

Two formulations of the link prediction task:

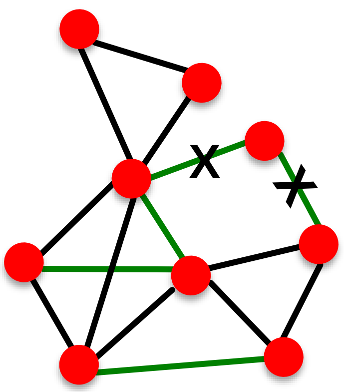
- **1) Links missing at random:**
  - Remove a random set of links and then aim to predict them
- **2) Links over time:**
  - Given $G[t_0, t'_0]$ a graph defined by edges up to time t'_0, **output a ranked list L** of edges (not in $G[t_0, t'_0]$) that are predicted to appear in time $G[t_1, t'_1]$
  - **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



$G[t_0, t'_0]$
$G[t_1, t'_1]$

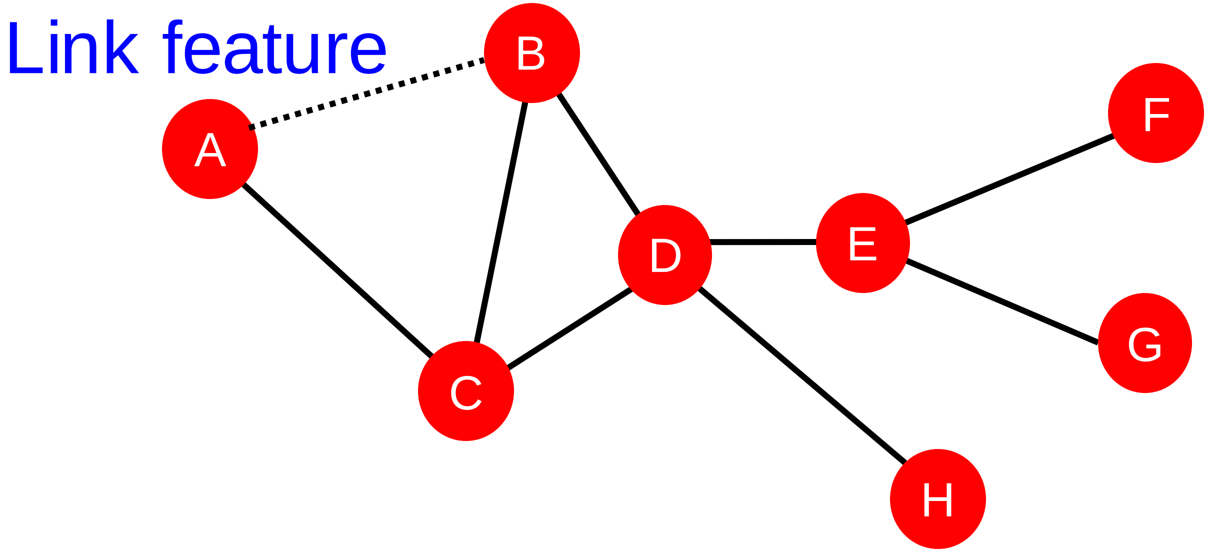
Link Prediction via Proximity

- **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



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

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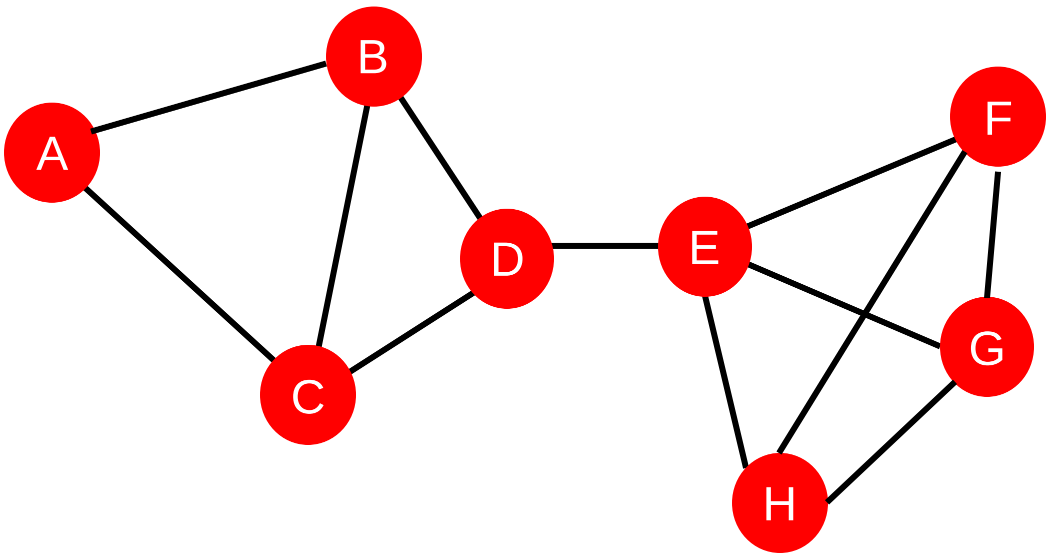
Graph-Level Features

- **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 $\boldsymbol{K} = \left(K(G, G')\right)_{G,G'}$ 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-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