Graph-level Tasks

Prof. O-Joun Lee

Dept. of Artificial Intelligence,
The Catholic University of Korea
ojlee@catholic.ac.kr

네트워크 과학 연구실
NETWORK SCIENCE LAB

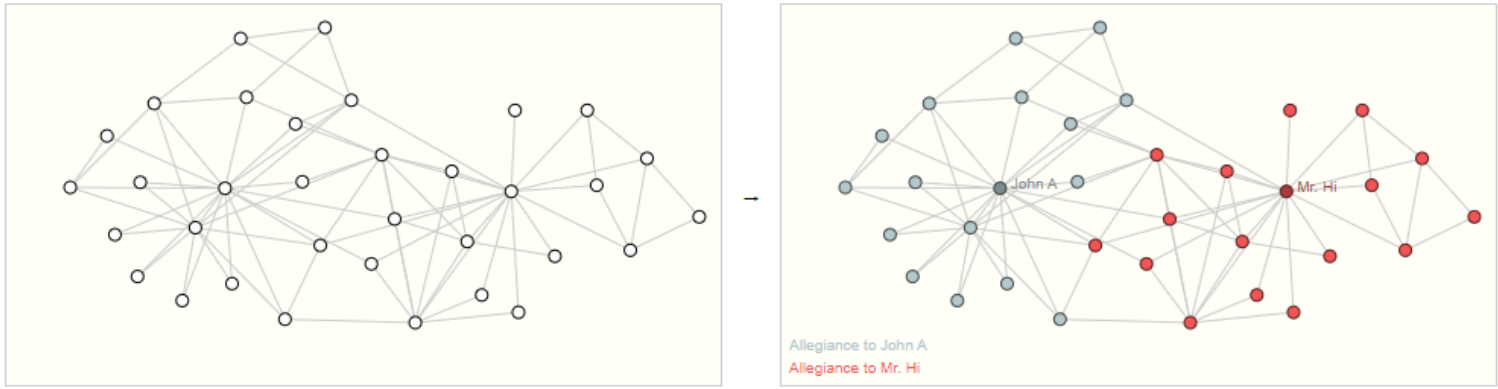
가톨릭대학교
THE CATHOLIC UNIVERSITY OF KOREA

Contents

- Graph-level Overview.
- Feature Extraction Methods.
  - Local Features: graph size, density, connectivity, average degree, centrality measurement, diameter, average clustering coefficient, average shortest path length.
  - Global features: motif counts, subgraph, kernel-based, graph spectrum, Community structure.
- Graph-level Tasks:
  - Graph regression, classification, generation, clustering, similarity, and embedding.
- Applications of Graph-level representation learning.

Machine Learning Tasks on Graphs

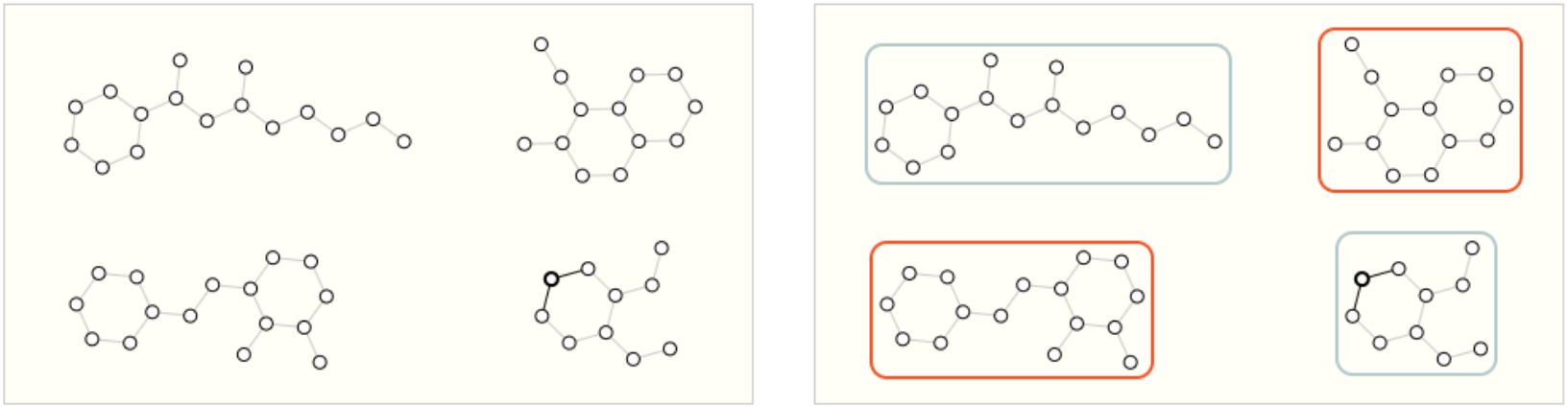
- **Node classification**: given a graph with labels on some nodes, provide a high-quality labeling for the rest of the nodes.



Input: graph with unlabled nodes

Output: graph node labels

- **Graph classification**: given a set of graphs with known class labels for some of them, decide to which class the rest of the graphs belong.

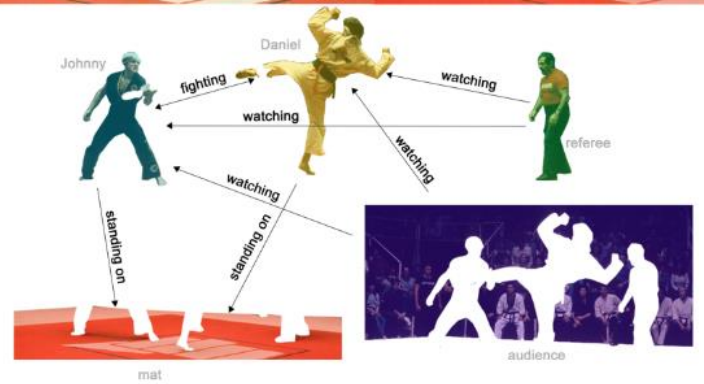


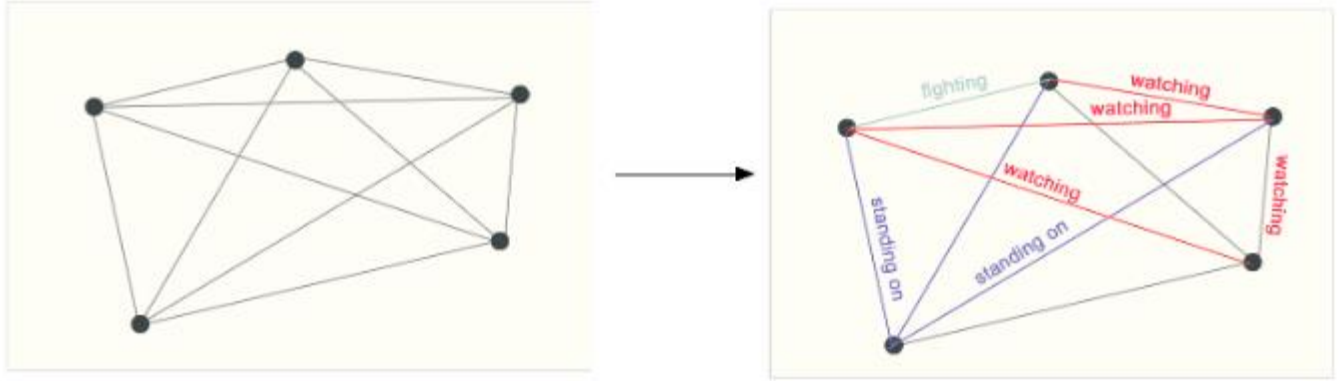
Input: graphs

Output: labels for each graph, (e.g., "does the graph contain two rings?")

Machine Learning Tasks on Graphs

- Edge/Link prediction: given a pair of vertices, predict if they should be linked with an edge.





Input: fully connected graph, unlabeled edges

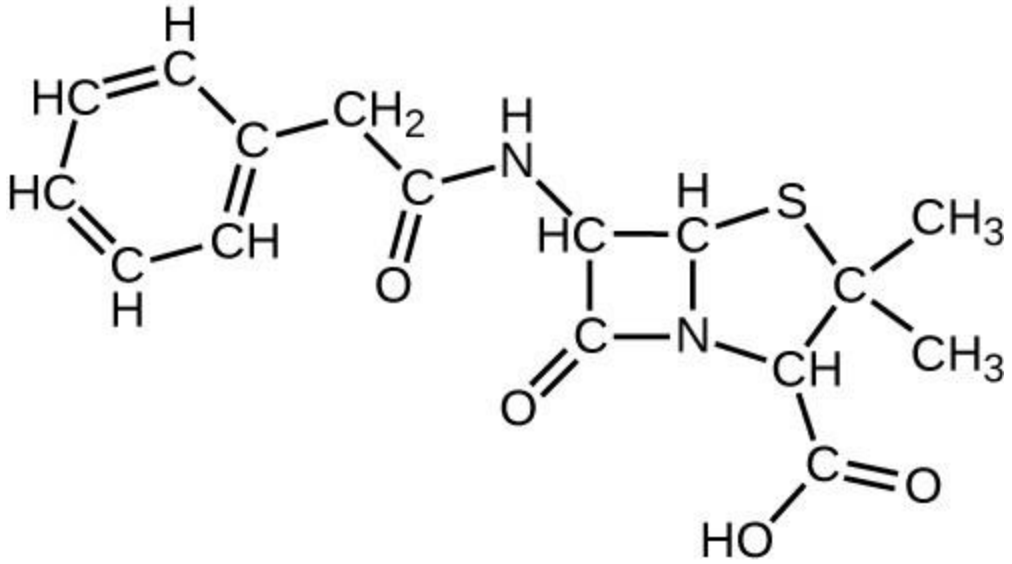
Output: labels for edges

From Node-level to Graph-level Tasks

- Intuition:
  - Node-level tasks involve making predictions or performing computations at the level of individual nodes within a graph.
    - Each node in the graph is treated as a separate entity, and the task focuses on understanding or predicting properties or behaviors specific to each node.
  - Graph-level tasks involve making predictions or performing computations based on the entire graph structure.
    - The entire graph structure is considered as a whole, and the task typically involves understanding or predicting global properties or behaviors of the entire graph.

Motivation – Protein Function Prediction

- For each protein, create a graph that contains information about its:
  - Structure
  - Sequence
  - Chemical properties



- Use graph features to:
  - measure structural similarity between proteins/molecules
  - predict the function of proteins/molecules

Borgwardt et al. “Protein function prediction via graph kernels”. Bioinformatics 21

Motivation – Chemical Compound Classification (Cont.)

- Represent each chemical compound as a graph

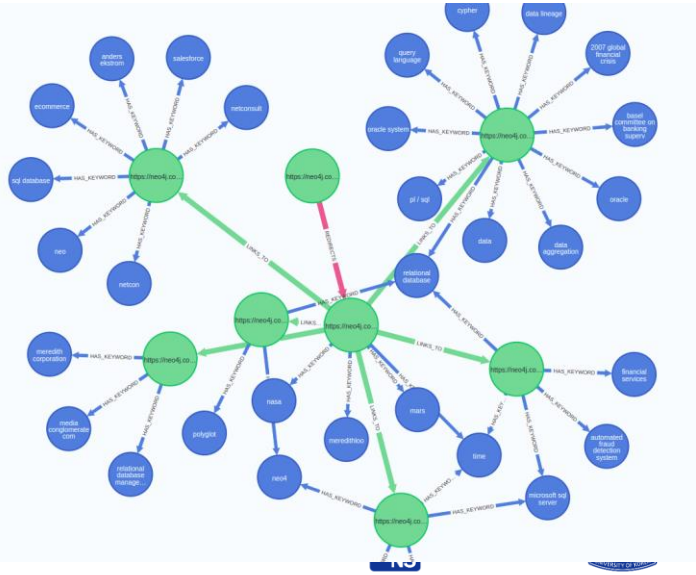
- Use a frequent subgraph discovery algorithm to discover the substructures that occur above a certain support constraint.
- Perform feature selection.
- Use the remaining substructures as features for classification.

Deshpande et al. "Frequent substructure-based approaches for classifying chemical compounds". TKDE 17(8)

Motivation – Anomaly Detection for the Web Graph

- Search engines create snapshots of the web → Web graphs.
- These are necessary for
  - monitoring the evolution of the web.
  - Computing global properties such as PageRank.

- Identify anomalies in a single snapshot by comparing it with previous snapshots.
- Employed similarity measures:
  - Node/edge overlap.
  - Node ranking.
  - Node/edge vector similarity.
  - etc.



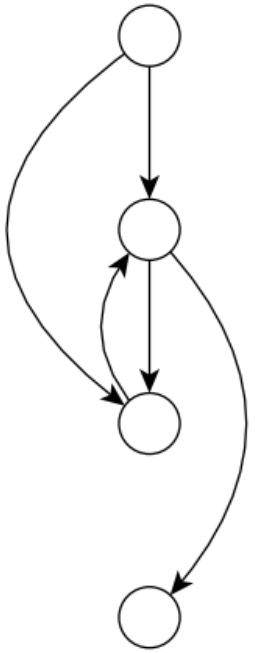
Papadimitriou et al. “Web graph similarity for anomaly detection”. JISA 1(1)

Motivation – Malware Detection

- Given a computer program, create its control flow graph:

```
            processed_pages.append(processed_page)
            visited += 1
            links = extract_links(html_code)
            for link in links:
                if link not in visited_links:
                    links_to_visit.append(link)

    return create_vocabulary(processed_pages)


def parse_page(html_code):
    punct = re.compile(r'([^A-Za-z0-9])')
    soup = BeautifulSoup(html_code, 'html.parser')
    text = soup.get_text()
    processed_text = punct.sub(" ", text)
    tokens = processed_text.split()
    tokens = [token.lower() for token in tokens]
    return tokens


def create_vocabulary(processed_pages):
    vocabulary = {}
    for processed_page in processed_pages:
        for token in processed_page:
            if token in vocabulary:
                vocabulary[token] += 1
            else:
                vocabulary[token] = 1

    return vocabulary
```

→

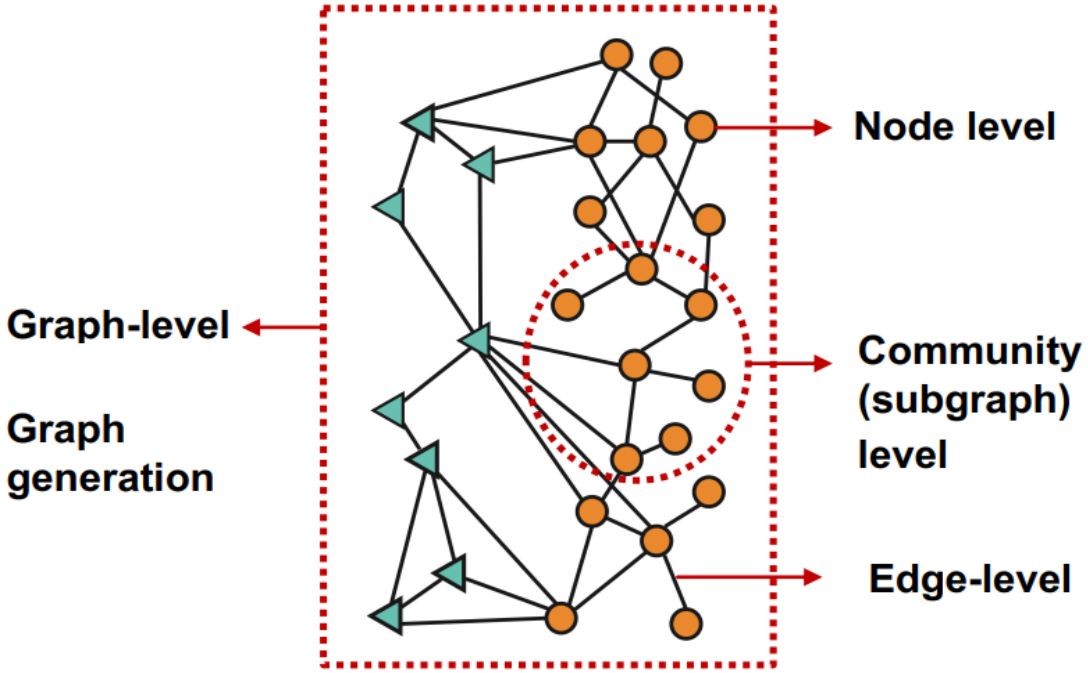


- Compare the control flow graph of the problem against the set of control flow graphs of known malware.
- If it contains a subgraph isomorphic to these graphs → malicious code inside the program

Gascon et al. “Structural detection of android malware using embedded call graphs”. In AISec’13

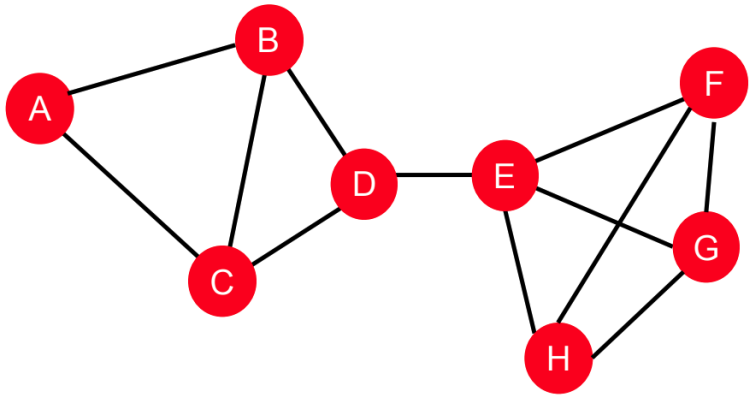
Feature Extraction Approaches

- Three main types of graph components:
  1. Node-level features (Previous week).
  2. Edge-level features (Previous week).
  3. Graph-level features (**This week**).



Graph-level Features Overview

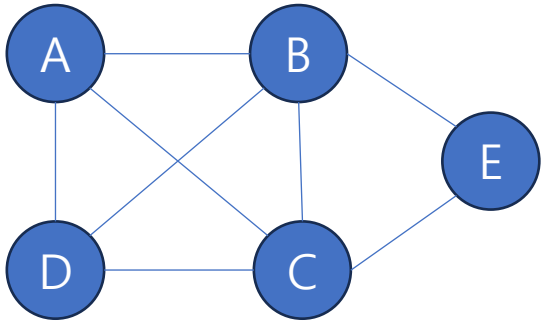
- **Goal**: We want features that characterize the structure of an entire graph.
  - Similar graphs has similar features.
- **Idea**: extract structural information within graphs as graph features.
- **Methods**:
  - Local features: graph size, density, connectivity, degree, centrality, average clustering coefficient, diameter, average shortest path length.
  - Global features: motif/subgraph, kernel, spectral, community.



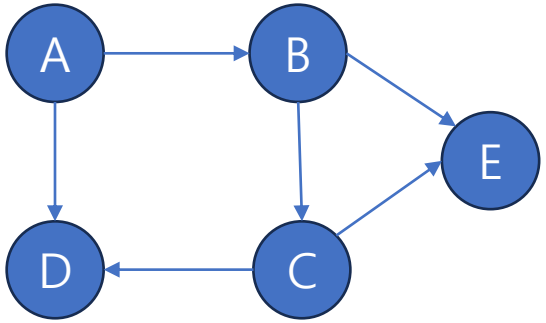
f(graph) = ?

Local Features: Graph Size

- Graph size provide fundamental information about the graph's scale and complexity:
  - Order of a graph is the number of vertices in the graph
    - denotes as $|V|$.
  - Size of a graph is the number of edges in the graph
    - denotes as $|E|$.



- $|V| = 5, |E| = 8$

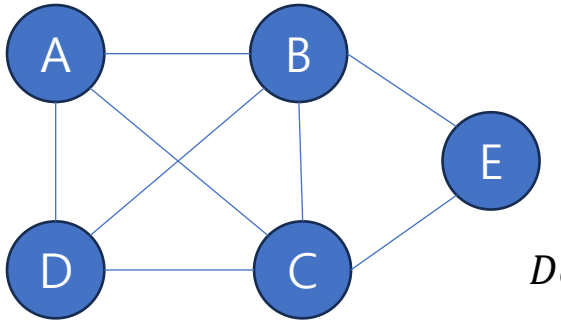


- $|V| = 5, |E| = 6$

Local Features: Graph Density

- Graph Density represents the ratio between the edges present in a graph and the maximum number of edges that the graph can contain.
  - edge connectivity is key to find dense.
- In undirected graph:
  - calculate the maximum number of edges:

$$Max_{EG} = \frac{|V|(|V|-1)}{2}$$



$$Den_G = \frac{2 * 8}{5(5-1)} = 0.8$$

  - the edges are divided by the maximum number of edges that the graph can contain. Density graph is defined

$$Den_G = \frac{|E|}{\frac{|V|(|V|-1)}{2}} = \frac{2|E|}{|V|(|V|-1)}$$

Where $|V|$ is number of nodes.

$|E|$ is number of edges.

Local Features: Graph Density

- Similarly, in directed graph: replace each undirected edge with two bidirectional edges in a directed graph
  - the maximum number of edges:

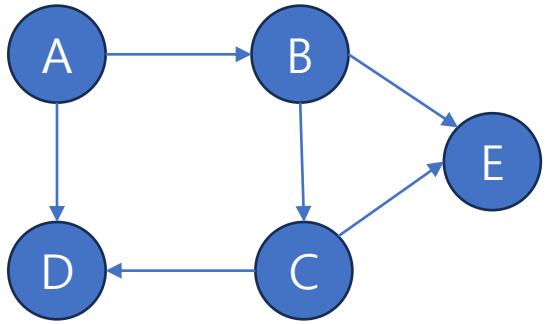
$$Max_{EG} = |V|(|V| - 1)$$

  - the edges are divided by the maximum number of edges that the graph can contain. Density graph is defined

$$Den_G = \frac{|E|}{|V|(|V| - 1)}$$

Where $|V|$ is number of nodes.

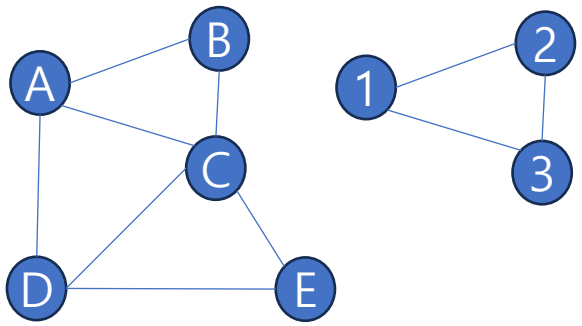
$|E|$ is number of edges.



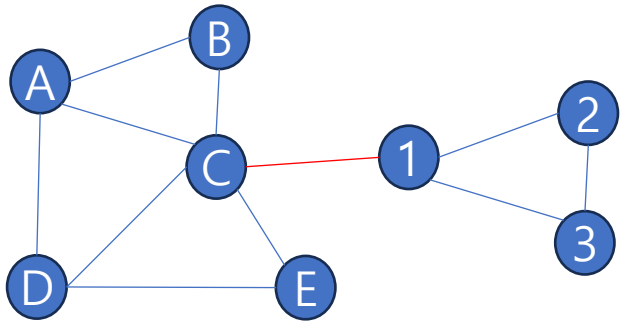
$$Den_{DG} = \frac{6}{5(5-1)} = 0.3$$

Local Features: Graph Connectivity

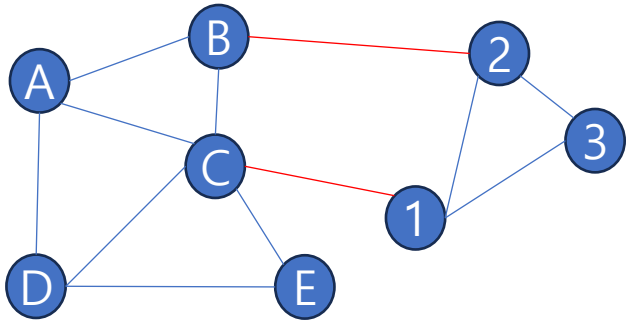
- Graph Connectivity: the minimum number of elements (nodes or edges) that need to be removed to separate the remaining nodes into two or more isolated subgraphs.



Unconnected graph



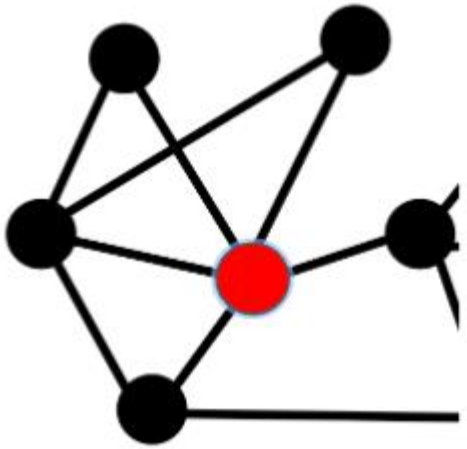
1- connected graph



2- connected graph

Local Features: Node Degree and Centrality Overview

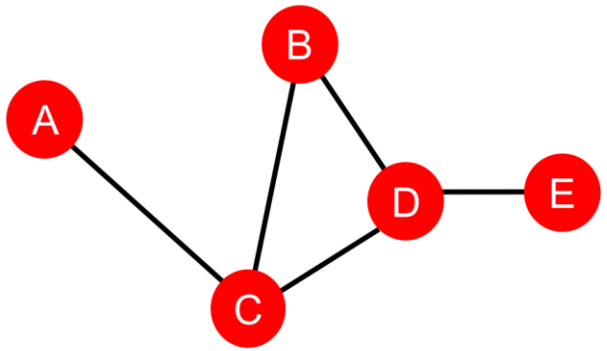
- Node degree counts the neighbouring nodes without capturing their importance.
- Node centrality takes the node importance in a graph into account.
- Different ways to evaluate importance:
  - Eigenvector centrality
  - Betweenness centrality
  - Closeness centrality
  - and many others….



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

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

  - A graph betweenness centrality is average of all the nodes' betweenness centrality.
  - For example:



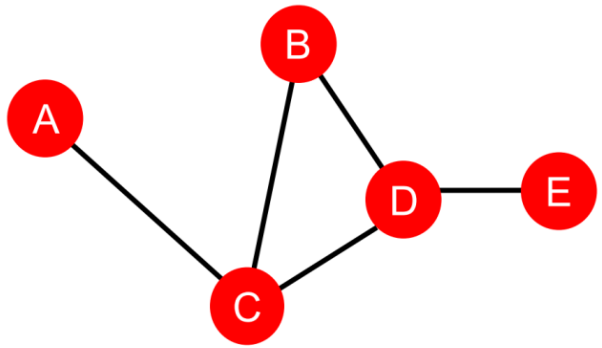
- $C_A = C_B = C_E = 0$
- $C_C = 3$ (A-C-B, A-C-D, A-C-D-E)
- $C_D = 3$ (A-C-D-E, B-D-E, C-D-E)
- $C_G = \frac{0+0+3+3+0}{5} = 1.2$

➢ Closeness Centrality

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

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

- ➢ A graph closeness centrality is average of all the nodes' closeness centrality.
- ➢ For 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)

- $C_G = (\frac{1}{8} + \frac{1}{5} + \frac{1}{6} + \frac{1}{5} + \frac{1}{8})/5 \approx 0.1633$

➢ 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 recursively:

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

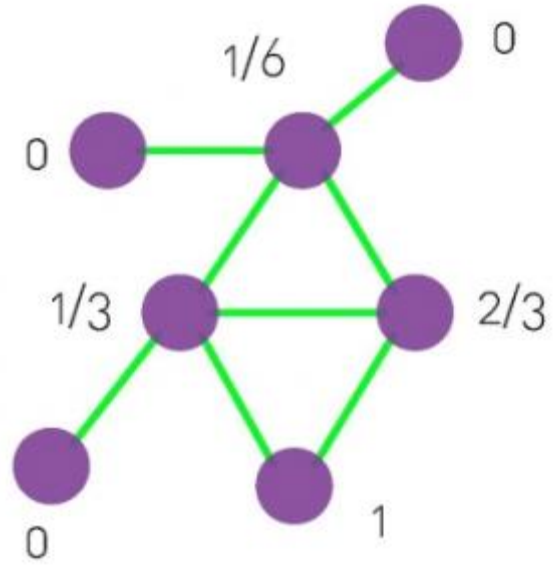
- $\boldsymbol{A}$: Adjacency matrix
  $\boldsymbol{A}_{uv} = 1$ if $u \in N(v)$
- $\boldsymbol{c}$: Centrality vector
- λ: Eigenvalue

- ➢ We can obtain the graph-level feature by averaging of all the nodes' eigenvector centrality.

Local Features: Average Clustering Coefficient

- The degree of clustering of a whole network is captured by the average clustering coefficient, namely $\langle C \rangle$, representing the average of all the local clustering coefficient C_i over all nodes $i = 1, \ldots, N$.

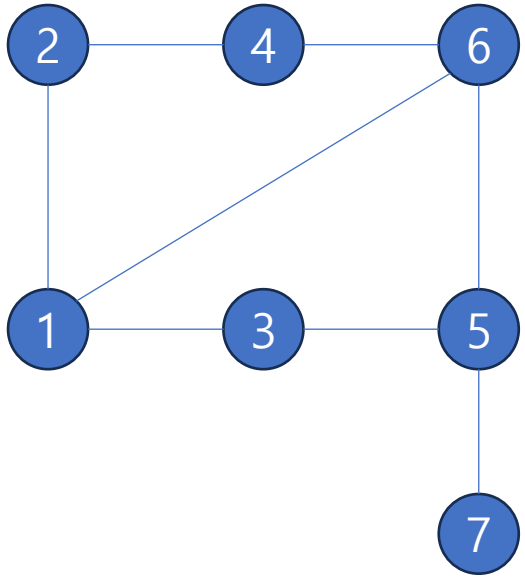
$$\langle C \rangle = \frac{1}{N} \sum_{i=0}^{N} C_i$$



$$\langle C \rangle = \frac{1}{7} * \left(0 + \frac{1}{6} + \frac{1}{3} + \frac{2}{3} + 1 + 0 + 0 \right) = 0.333$$

Local Features: Diameter

- The diameter of a graph is the length of the shortest path between the most distanced nodes.
- d measures the extent of a graph and the topological length between two nodes.



Diameter of this graph is 4

Local Features: Average Shortest Path Length

- The average number of steps along the shortest paths for all possible pairs of network nodes.
- A measure of the efficiency of information in a graph.
  - i.e. the average number of clicks which will lead you from one website to another,
  - or the number of people you will have to communicate through, on an average, to contact a complete stranger.

$$a = \sum_{\substack{s,t \in V \\ s \neq t}} \frac{d(s,t)}{n(n-1)}$$

Where V is the set of nodes in G, $d(s,t)$ is the shortest path from s to t, and n is the number of nodes in G

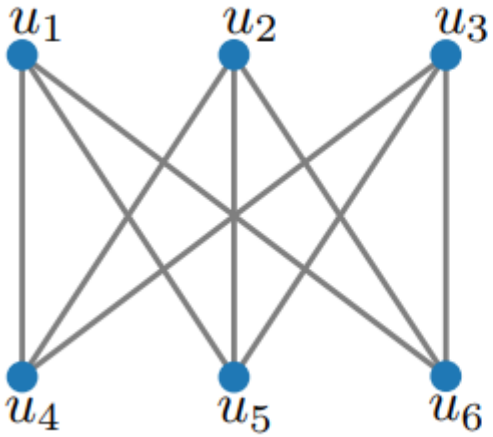
Background: Isomorphism

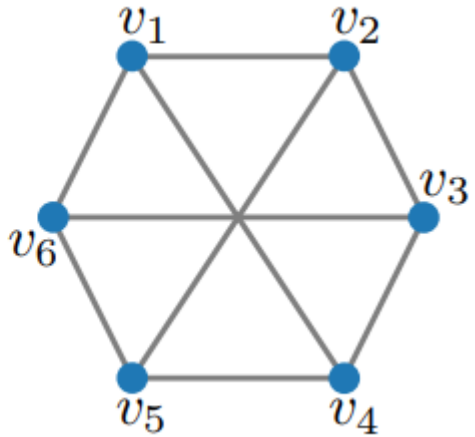
- For graphs $G = (V^G, E^G)$ and $G' = (V^{G'}, E^{G'})$, if we can define a bijection $\psi: V^G \rightarrow V^{G'}$, such that:

$$\forall v_i^G, v_j^G \in V^G, \left(v_i^G, v_j^G\right) \in E^G \text{ iff } \left(\psi\left(v_i^G\right), \psi\left(v_j^G\right)\right) \in E^{G'}$$

- The graphs G and G' are said to be isomorphic and denoted as

$$G \simeq G'$$





$$\psi: \begin{array}{ll} V^G & V^{G'} \\ v_1 & \rightarrow u_1 \\ v_2 & \rightarrow u_4 \\ v_3 & \rightarrow u_2 \\ v_4 & \rightarrow u_5 \\ v_5 & \rightarrow u_3 \\ v_6 & \rightarrow u_6 \end{array}$$

Global Features: Induced Subgraph

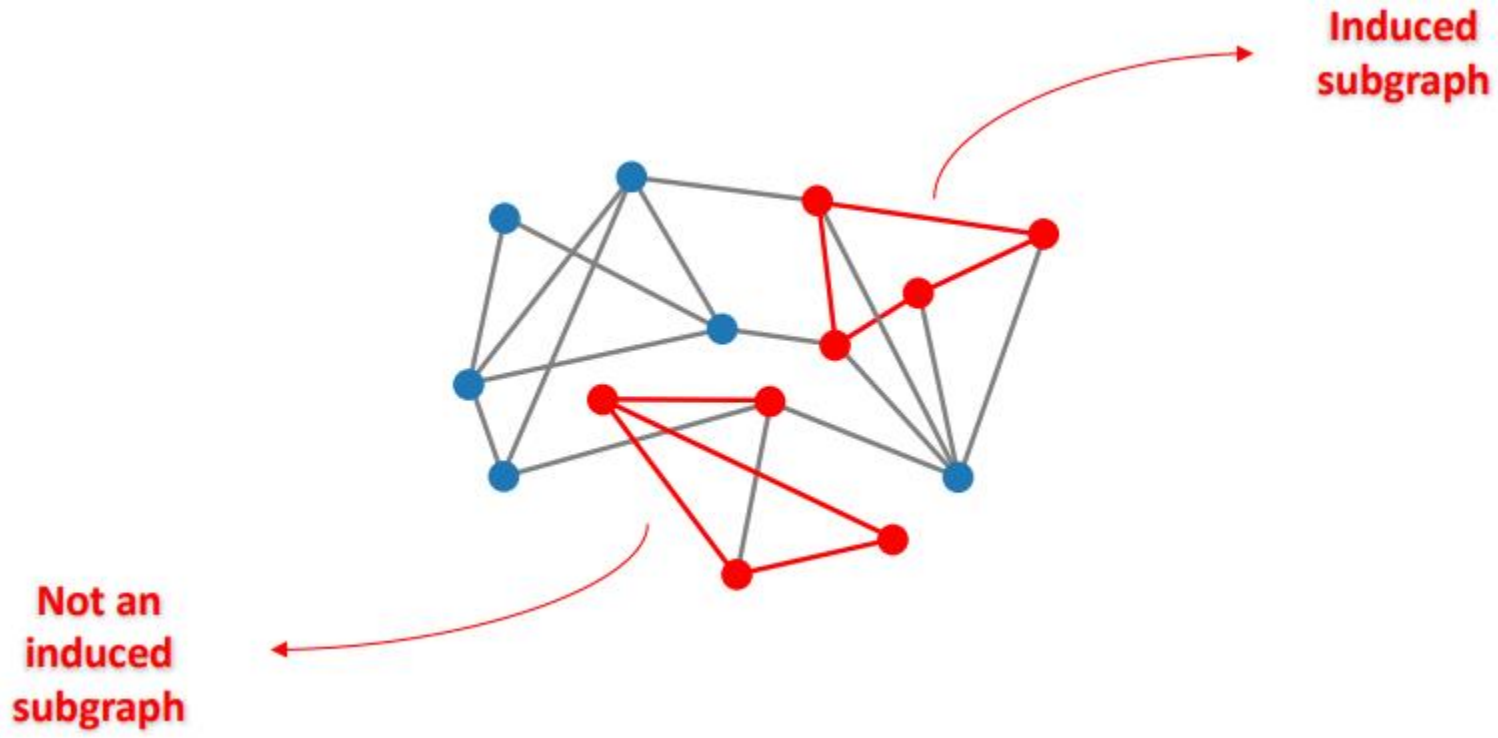
- An induced subgraph is a subgraph $G' = (V', E')$ consist of a subset of the nodes in the graph $G = (V, E)$ and all edges that connect them

$$E' = \{(v_i, v_j) \mid v_i, v_j \in V', (v_i, v_j) \in E\}$$

Global Features: Induced Subgraph

- An induced subgraph is a subgraph $G' = (V', E')$ consist of a subset of the nodes in the graph $G = (V, E)$ and all edges that connect them

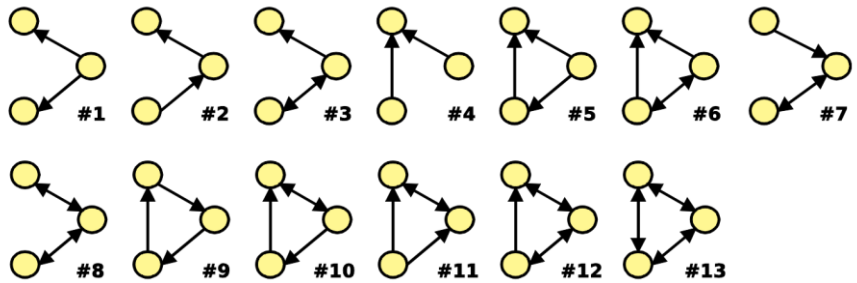
$$E' = \{(v_i, v_j) \mid v_i, v_j \in V', (v_i, v_j) \in E\}$$



- A measure of similarity for finding graph similarity.

Global Features: Motifs

- Given a network, most of the time, some subgraphs are “overrepresented”.
- A connected graph that has many occurrences in a network is called a motif of the network.
- Assume set of occurrences G' in G is $occ_G(H)$.
  - cardinality of $occ_G(H)$ in G is frequent.
  - How to know if G' is frequent in G?



⇒ Compute the probability that $occ_N(G') \geq occ_G(G')$ for a random network N.

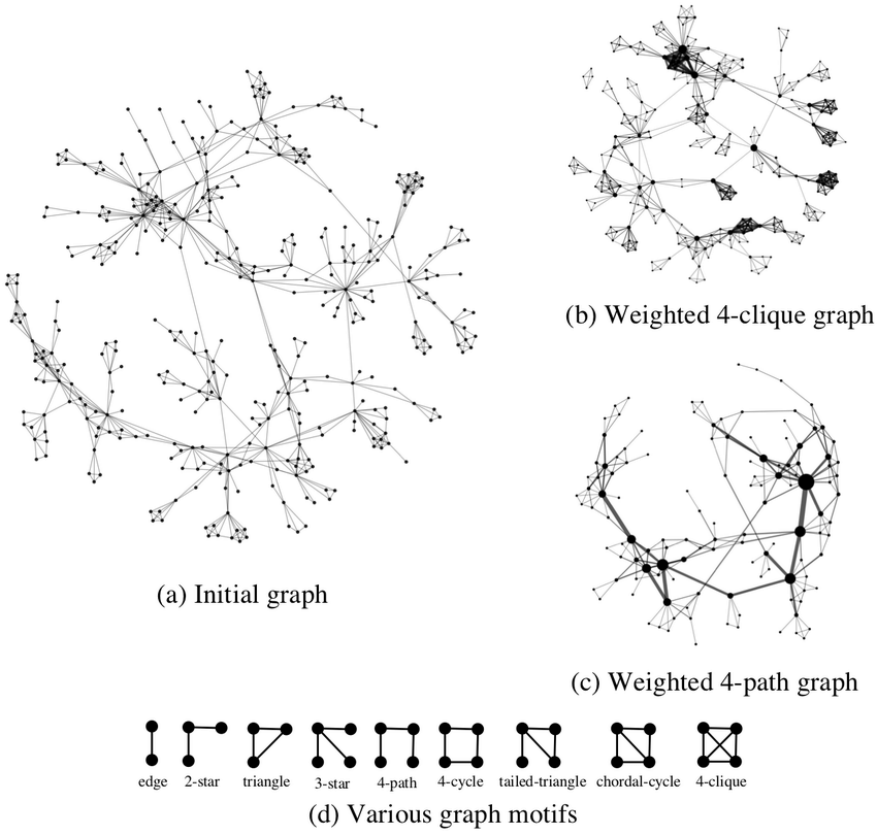
G' is said to be frequent in G if this probability is small enough.

To compute this probability, we need to have a distribution over networks.

Global Features: Motifs – Related problem

- Subgraph Isomorphism:
  - Input: Two graphs G' and G
  - Question: Does G' has at least one occurrence in G?
  - Determining if a graph contains a clique of size k is already NP-complete.

- Occurrences counting:
  - Input: Two graphs G' and G
  - Question: Determine occurrence $occ_G(H)$.
  - This problem is #P-complete.



(a) Initial graph

(b) Weighted 4-clique graph

(c) Weighted 4-path graph

(d) Various graph motifs

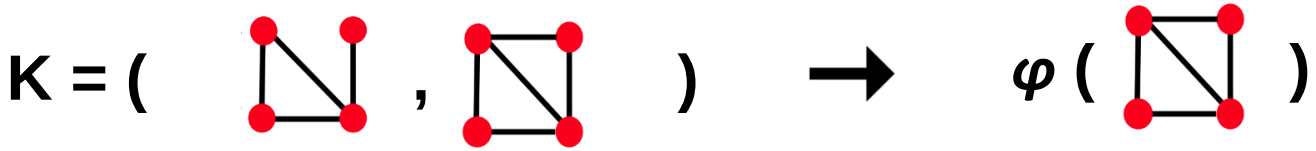
https://www.researchgate.net/figure/Graphs-defined-by-different-motif-adjacencies-can-differ-significantly-Size-weight-of_fig1_327790436

Background: Kernel Methods

- A quick introduction to Kernels:
  - Kernel $K(G, G') \in \mathbb{R}$ measures similarity between two graphs (data)
  - There exists a feature representation $\phi(\cdot)$ such that:

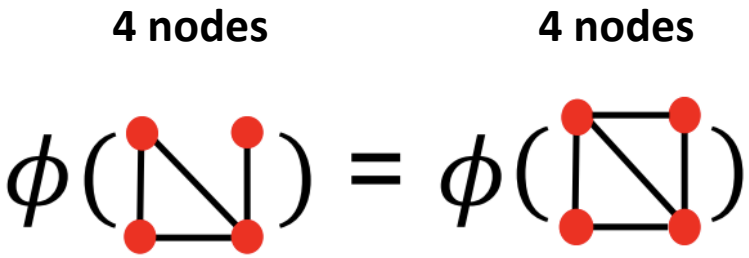
$$K(G, G') = \phi(\mathrm{G})^{\mathrm{T}} \phi(G')$$

  - Kernel enables vectors to be operated in higher dimension
  - Once the kernel is defined, off-the-shelf ML model, such as kernel SVM, can be used to make predictions.



Global Features: Graph Kernel - Key Idea

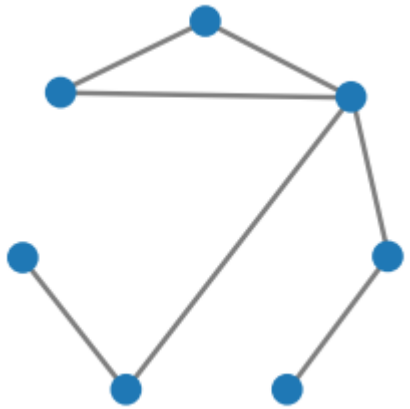
- **Goal**: Design graph kernel $\phi(G)$
- Key Idea: Bag-of-Words (BoW) for a graph
  - In NLP, BoW counts the word's frequency in a document as feature
  - Simplest way on graph: Regard nodes as words**.**
  - For example: in both graph have 4 nodes, we found the features of 2 graphs are same.



Global Features: Graph Kernel - Key Idea

- Problem: Bag of node counts doesn't work well…
- What if we use **Bag of Node Degrees**?
  - Characterizes a graph G based on frequency of different degree values in that graph.
  - For bag of degrees, the set of nodes σ_n is defined as

$$\sigma_n(G) = \{v_i | v_i \in V^G, d_i = n\}$$



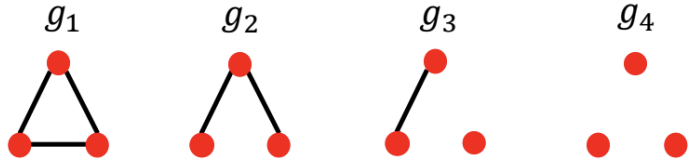
$d = 1$	$d = 2$	$d = 3$	$d = 4$
2	4	0	1

$$\phi_{BN}(G) = (2, 4, 0, 1)$$

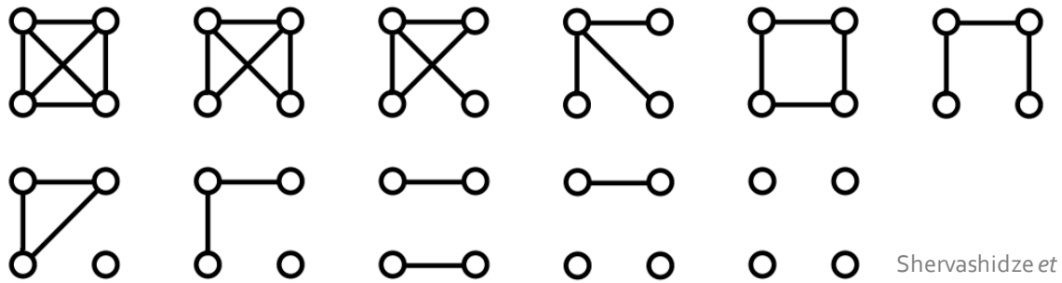
- Does not reflect the global structure of the graph.

Global Features: Graphlet-based Features

- **Key Idea**: Count the number of different graphlets in a graph.
- Graphlet Differences:
  - Nodes do not need to be connected.
  - Graphlets are not rooted.
- Let $G_k = (g_1, g_2, g_3, g_4)$ be a list of graphlet size k.
  - For $k = 3$, there are 4 graphlets.



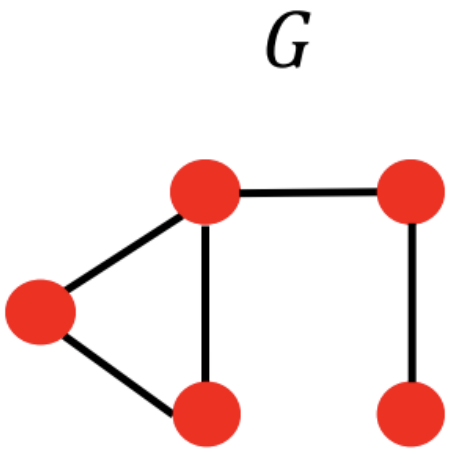
  - For $k = 4$, there are 11 graphlets.

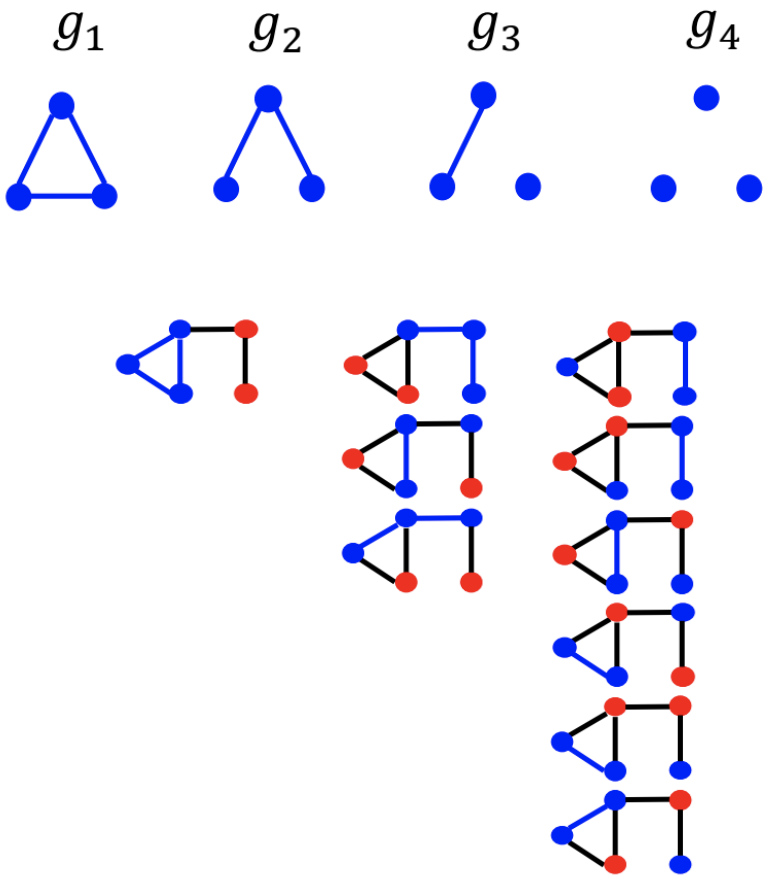


Shervashidze *et al.*, AISTATS 2011

Global Features: Graphlet-based Features

- Example for k = 3:

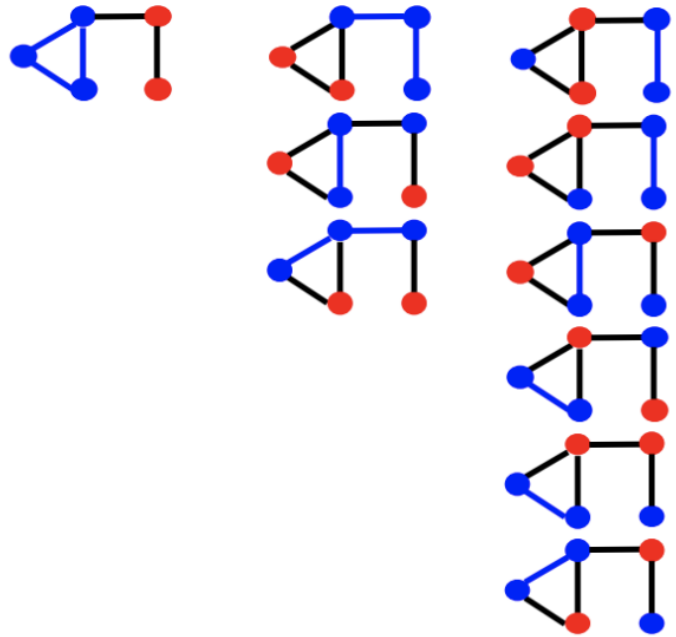




$$f_G = (1, \quad 3, \quad 6, \quad 0)^{\mathrm{T}}$$

Limitations of Graphlet Kernel

- Counting graphlets is expensive!
- Counting size k graphlets for graph with n nodes by enumeration takes n^k time.
- If our graph changes with time, we must recalculate the features again.
- Worst-case scenario: unavoidable 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?**

Global Features: Weisfeiler-Lehman Kernel

- **Goal**: Design an efficient graph feature descriptor $\phi(G)$.
- **Key Idea**:
  - Iteratively use neighborhood structure to describe node's neighboring topology.
  - Generalized version of **Bag of node degrees** (node degree only contains one-hop neighborhood information).

→ **Color Refinement Algorithm**

Global Features: Color Refinement

- For a graph G with nodes V:
- Assign initial color $c^{(0)}(v)$ to each node v
- Iteratively refine node colors by:

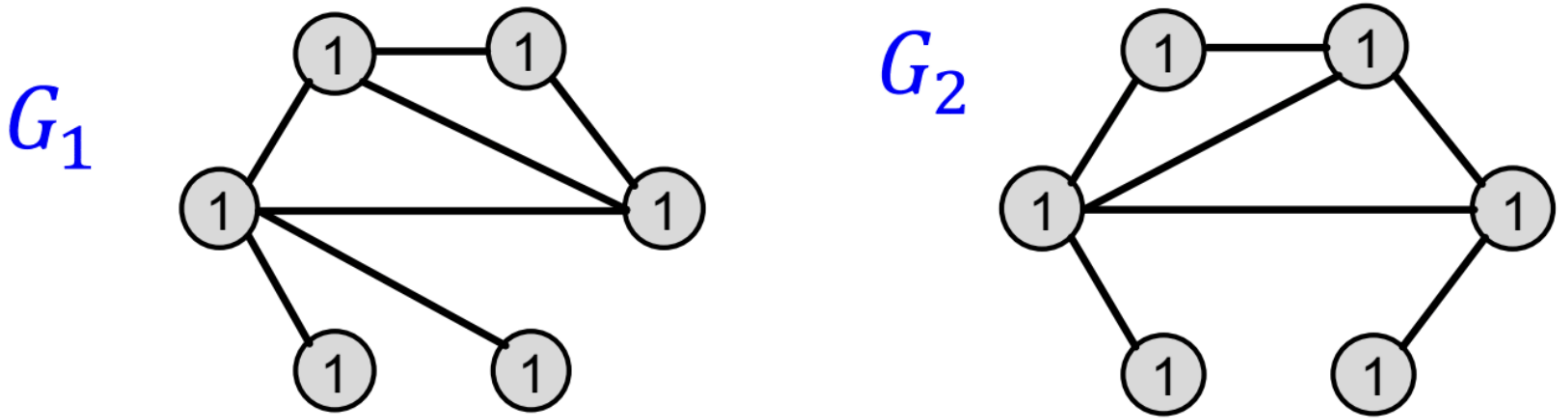
$$c^{(k+1)}(v) = \text{HASH}\left(\left\{c^{(k)}(v), \{c^{(k)}(u)\}_{u \in N(v)}\right\}\right)$$

where HASH maps different inputs to different colors.

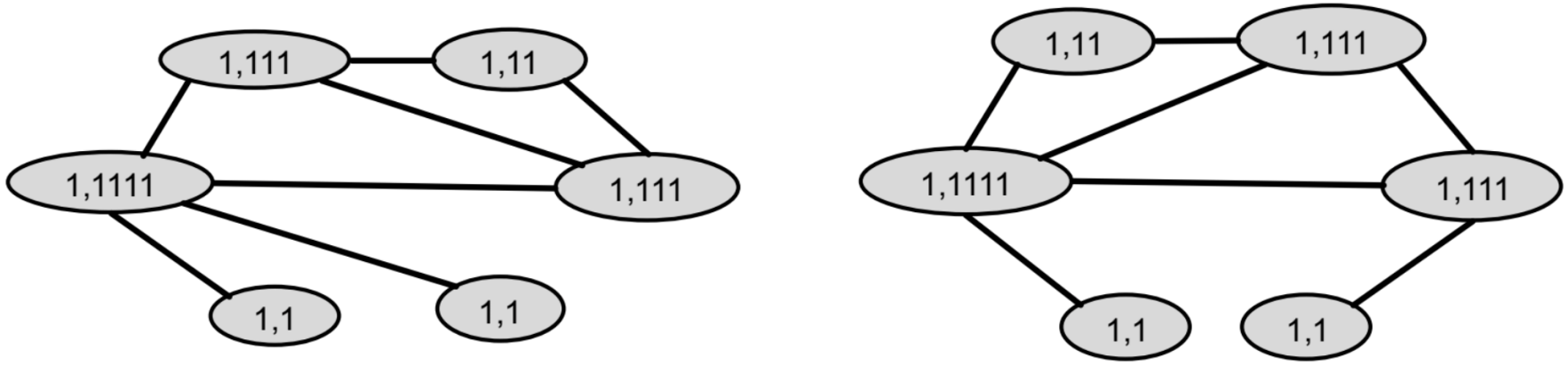
- After K steps of iteration, $c^{(K)}(v)$ represents the structure of the K-hop neighborhood.

Global Features: Color Refinement (1)

- Example with two graphs:
  - Assign initial color:

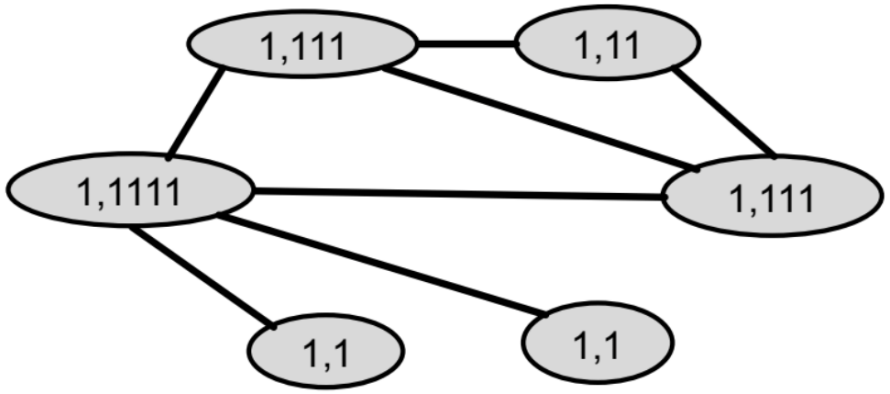


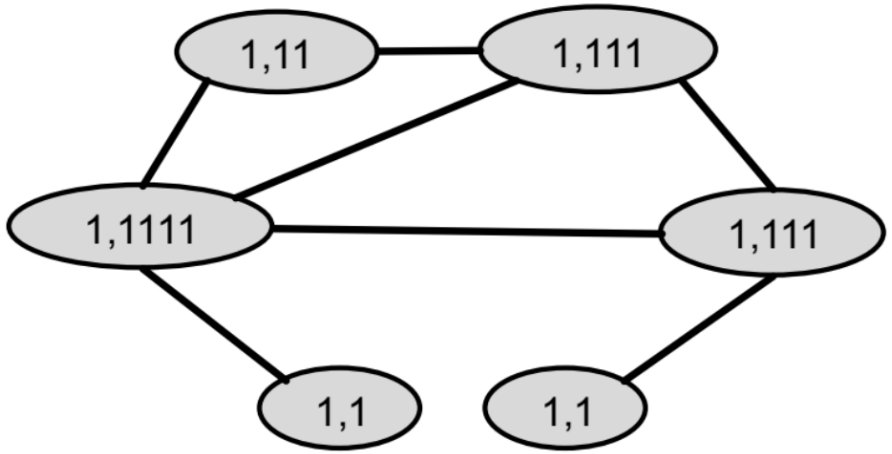
  - Aggregate neighboring colors:



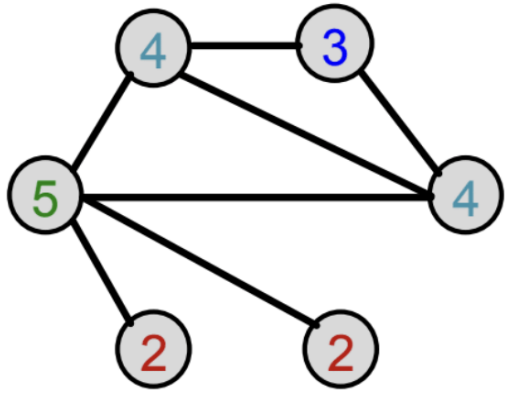
Global Features: Color Refinement (2)

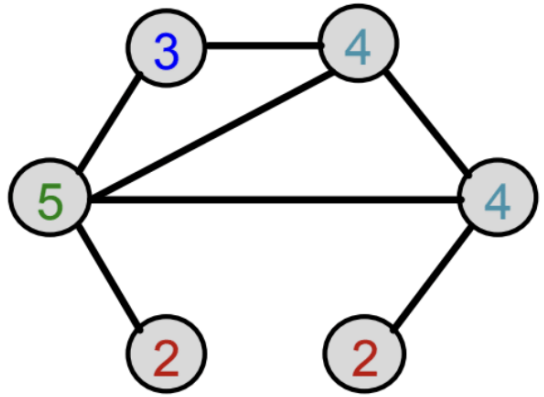
- Example with two graphs:
  - Aggregated colors:





  - Hash aggregated colors:



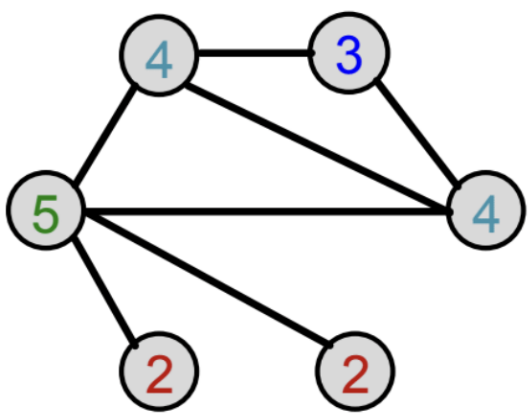


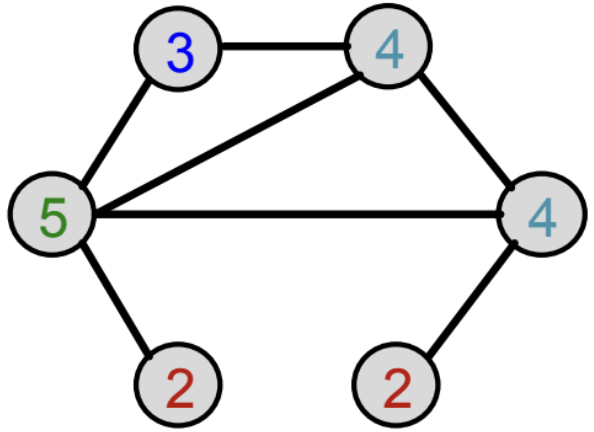
Hash table

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

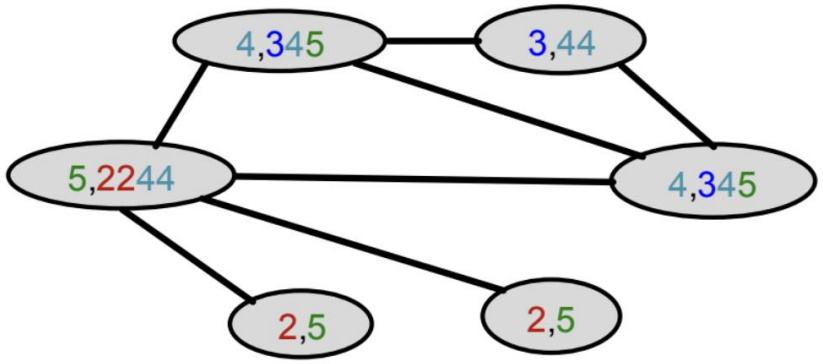
Global Features: Color Refinement (3)

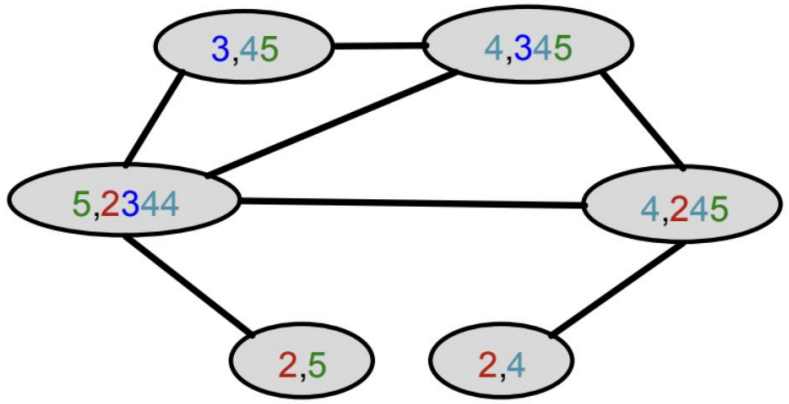
- Example with two graphs:
  - Aggregated colors:





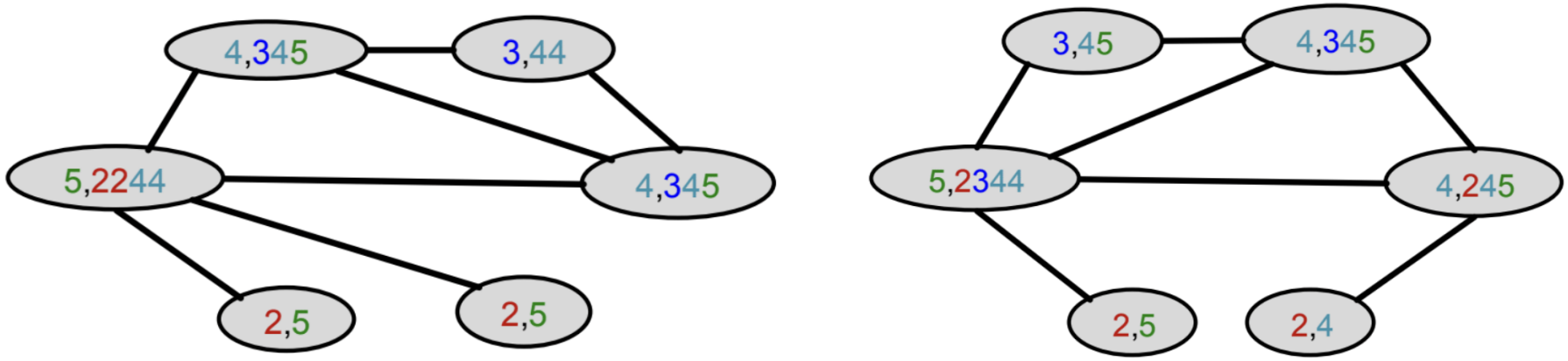
  - Hash aggregated colors:



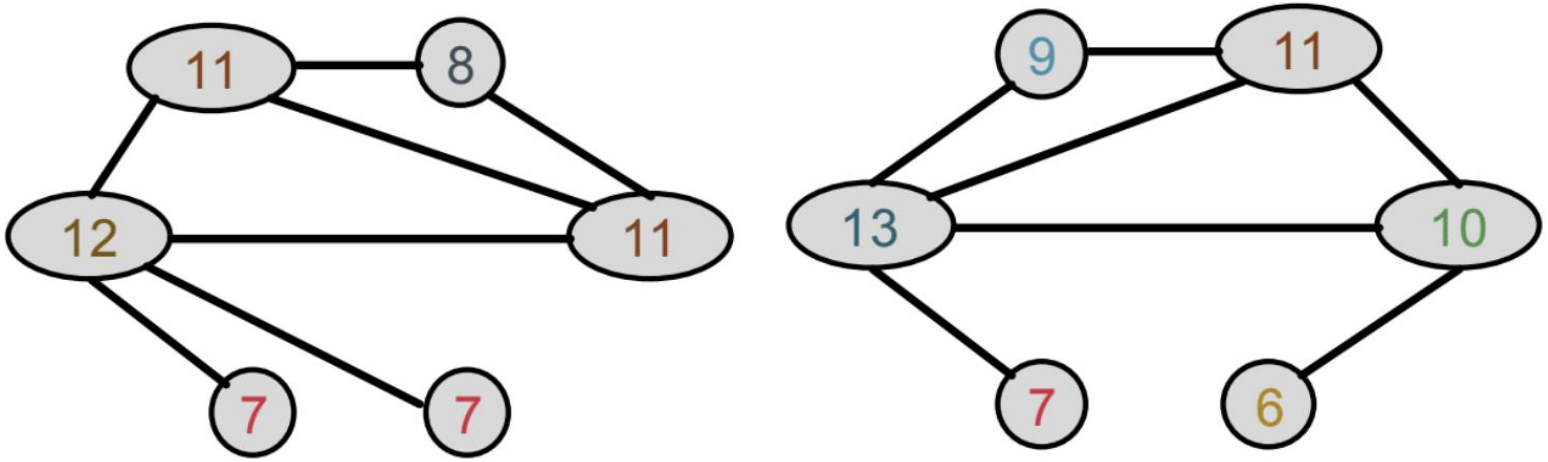


Global Features: Color Refinement (4)

- Example with two graphs:
  - Aggregated colors:



  - Hash aggregated colors:

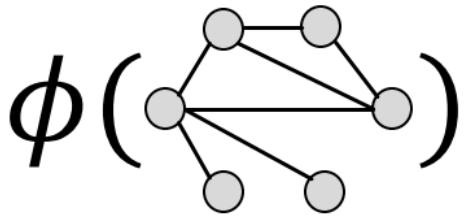


Hash table

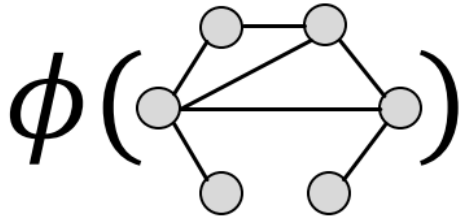
2,4	-->	6
2,5	-->	7
3,44	-->	8
3,45	-->	9
4,245	-->	10
4,345	-->	11
5,2244	-->	12
5,2344	-->	13

Global Features: Weisfeiler-Lehman Kernel

- After color refinement, WL Kernel counts # of nodes within given colors:

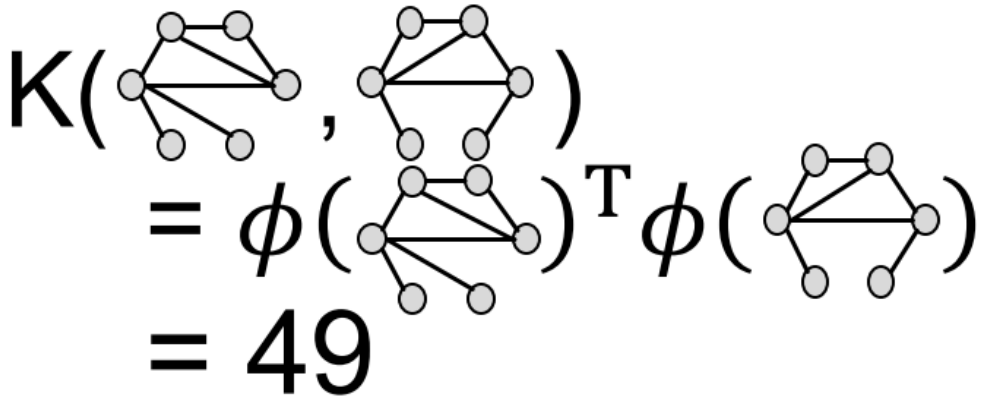


Colors
1,2,3,4,5,6,7,8,9,10,11,12,13
= [6,2,1,2,1,0,2,1,0, 0, 0, 2, 1]
Counts



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]

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

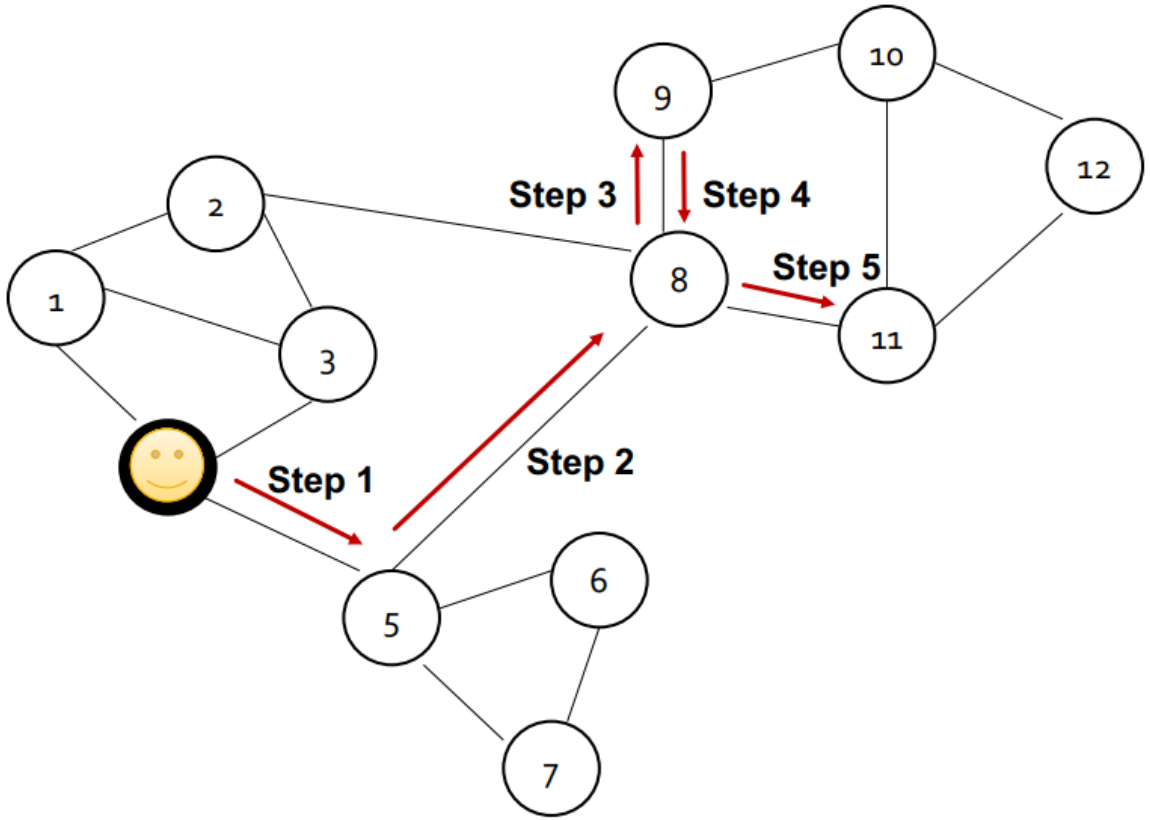


Global Features: Weisfeiler-Lehman Kernel

- WL kernel benefits:
  - Computationally efficient (color refinement need #(edges) steps).
  - #(colors) depends on total number of nodes - only colors appeared in the two graphs need to be tracked.
  - Time complexity is linear in #(edges).
  - Can be used to check graph isomorphism.

Global Features: Random Walk-based Kernel

- For a graph and a starting point, select a neighbor of it at random, and move to this neighbor.
- Select a neighbor of this point at random, and move to it, etc.
- The (random) sequence of points visited this way is a random walk on the graph.



Global Features: Shortest Path-based Kernel

- Compute all-pairs-shortest-paths for G and G' via Floyd-Warshall.
- Define a kernel by comparing all pairs of shortest path lengths from G and G':

$$k(G, G') = \sum_{v_i, v_j \in G} \sum_{v'_k, v'_l \in G'} k_{length}(d(v_i, v_j), d(v'_k, v'_l))$$

where $d(v_i, v_j)$ is the length of the shortest path between node v_i and v_j.

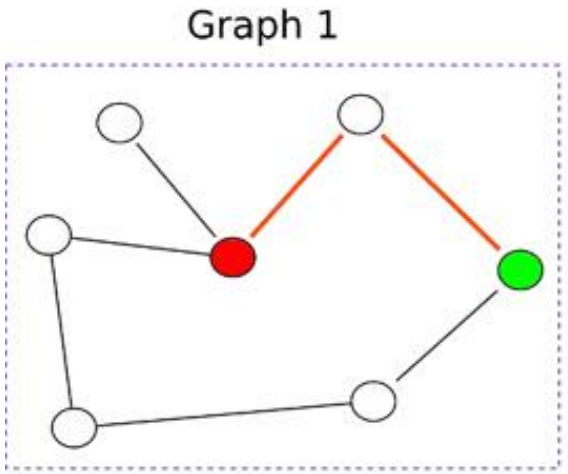
- k_{length} is a kernel that compares the lengths of two shortest paths:

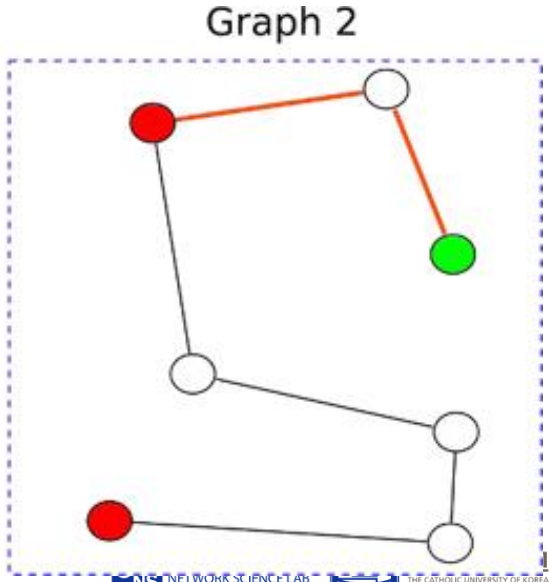
  - a linear kernel

    $$k(d(v_i, v_j), d(v'_k, v'_l)) = d(v_i, v_j) * d(v'_k, v'_l)$$

  - a delta kernel

    $$k\left(d(v_i, v_j), d(v'_k, v'_l)\right) = \begin{cases} 1, if\, d(v_i, v_j), = d(v'_k, v'_l) \\ 0, otherwise \end{cases}$$



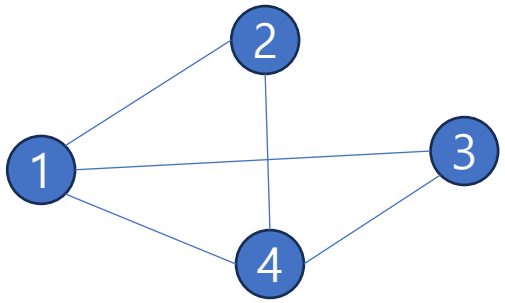


Karsten M. Borgwardt and Hans-Peter Kriegel. Shortest-path kernels on graphs

Global Features: Other Graph Kernels

- RWR [Kashima+ ’03, Gaertner+ ’03, Vishwanathan ’10]
- Shortest path kernels [Borgwardt & Kriegel ’05]
- Cyclic path kernels [Horvath+ ’04]
- Depth-first search kernels [Swamidass+ ’05]
- Subtree kernels [Shervashidze+ ’09 NIPS, JMLR’11 , Ralaivola+’05]
- Graphlet / Subgraph kernels [Shervashidze+ ’09, Thoma+ ’10]
- All-paths kernels [Airola+ ’08]
- …

- Graph and Associated Matrices



$$G = (V, E)$$
$$|V| = 4$$
$$|E| = 5$$

- Laplacian matrix

$$L_G = D_G - A_G$$
$$= B_G B_G^T$$

- Adjacency matrix

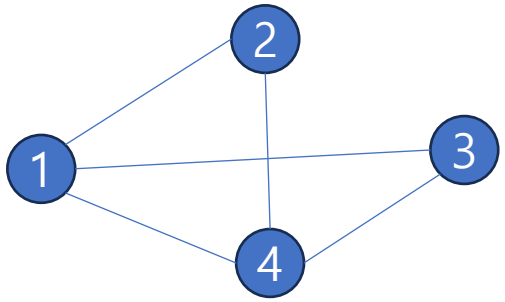
$$A_G = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

- Degree matrix

$$D_G = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix}$$

- Incidence matrix

$$B_G = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & -1 & -1 & -1 \end{bmatrix}$$



$$L_G = \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix}$$

Eigenvalue $\lambda = \{0,2,4,4\}$

Eigenvector $\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} 0 \\ -1 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} -1 \\ -1 \\ -1 \\ 3 \end{bmatrix} \begin{bmatrix} -2 \\ 1 \\ 1 \\ 0 \end{bmatrix}$

- Symmetric → real eigenvalues; eigenvectors are mutually orthogonal.
- Orthogonally diagonalizable → an eigenvalue with multiplicity k has k-dimensional eigenvectors.

Graph Spectral: Laplacian Matrix's Properties

- For entries $x = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$

$$x^T L_G x = x^T B_G B_G^T x = (x^T B_G)(B_G^T x) = \sum_{(i,j)\in E} (x_i - x_j)^2 \geq 0$$

- Meaning that: positive semidefinite → eigenvalues in Laplacian is non-negative.
- Row sum = 0 → singular
  - At least one eigenvalue = 0, unity eigenvector (since row sum = 1).
- Orthogonal eigenvector u = eigenvector of non-zero eigenvalue.

$$\sum_{i=1}^{n} u_i = 0$$

$$\lambda = \{0,2,4,4\}$$

$$\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad \begin{bmatrix} 0 \\ -1 \\ 1 \\ 0 \end{bmatrix} \quad \begin{bmatrix} -1 \\ -1 \\ -1 \\ 3 \end{bmatrix} \quad \begin{bmatrix} -2 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$

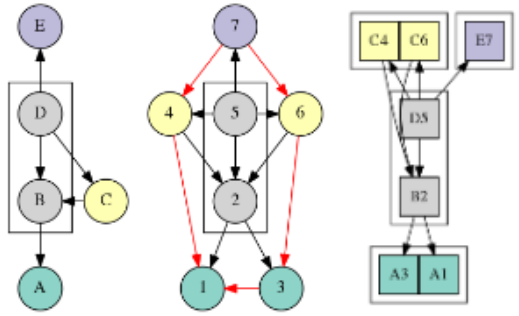
Graph Spectral: Spectrum of Some Graphs

- Which graphs are determined by their spectrum?
  - Complete Graphs.
  - Graphs with one edge.
  - Graphs missing 1 edge.
  - Regular graphs with degree 2.
  - Regular graphs of degree n – 3.

	Eigenvalues
Complete	$\{0, n^{n-1}\}$
Line	$2 - 2\cos\left(\frac{\pi k}{n}\right), k = 1, \dots, n$
Ring	$2 - 2\cos\left(\frac{2\pi k}{n}\right), k = 1, \dots, \frac{n}{2}$
Star	$\{0, 1^{n-2}, 2\}$

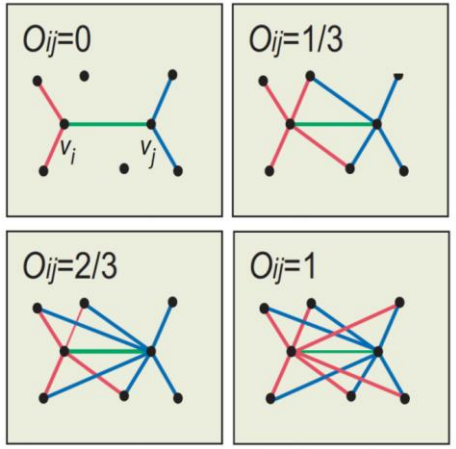
Global Features: Community Structure

- Reminder: Communities in networks is defined with respect to the whole graph.
  - identifying sets of nodes that are densely connected with each other.
- A graph has a community structure if it is different from a random graph.
- Common methods:
  - Structural equivalence: share the same neighbors and are not adjacent



  - Edge Overlap between the number of neighbor $N(i)$ and $N(j)$ of node i and j

$$O_{ij} = \frac{|(N(i) \cap N(j)) \backslash \{i, j\}|}{|(N(i) \cup N(j)) \backslash \{i, j\}|}$$



Summary: Graph-level Features

- Local:
  - Fundamental: Graph size, density, connectivity, Node degree.
  - Graph Centrality: Betweenness, Closeness, Eigenvector.
  - Average Clustering Coefficient.
  - Diameter: the length of the shortest path between the most distanced nodes.
  - Average Shortest Path Length: average number of steps along the shortest paths for all possible pairs of nodes.
- Global:
  - Subgraph/Motif counts.
  - Kernel-based: Graphlet, Weisfeiler-Lehman, Random Walk, Shortest Path, etc.
  - Spectral: Laplacian matrix.
  - Community Structure.

Graph-level Tasks

- There are many graph-level tasks:
  - Graph regression.
  - Graph classification.
  - Graph generation.
  - Graph clustering.
  - Graph similarity.
  - Graph embeddings.

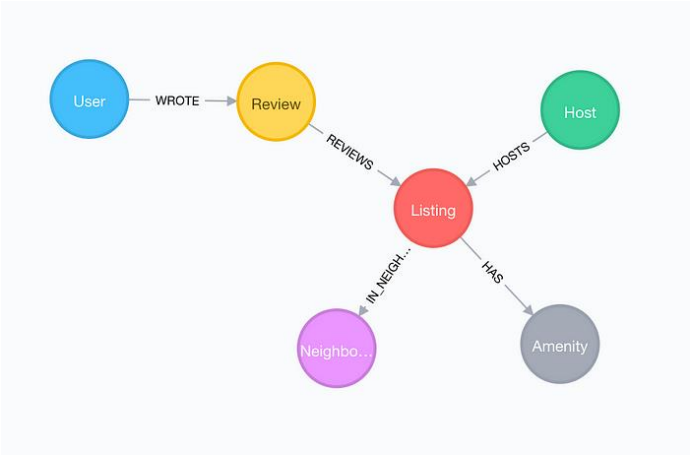
Graph-level Tasks: Graph Regression

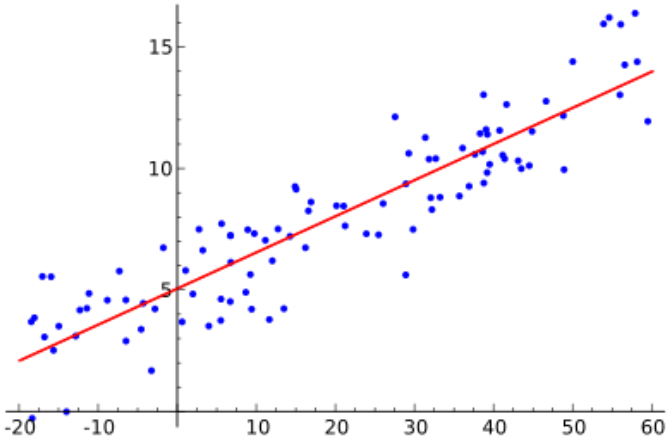
- Graph regression:
  - Given a set of graphs $G = \{G_1, G_2, \ldots, G_n\}$ and their associated target value $y = \{y_1, y_2, \ldots, y_n\}$.
  - The goal is to learn a function f that map each graph G_i to a continuous target value $\hat{y}_i = f(G_i)$ such that the predicted values $\hat{y}_i$ are close to the true values.

$$\hat{y}_i = f(G_i) + \epsilon_i$$

Where ϵ_i represents the error or residual between the predicted and true values

  - Conventional methods.
    - Kernel method: Subgraph matching, Weisfeiler-Lehman Subtree Kernel, Shortest path, Random walk, etc.

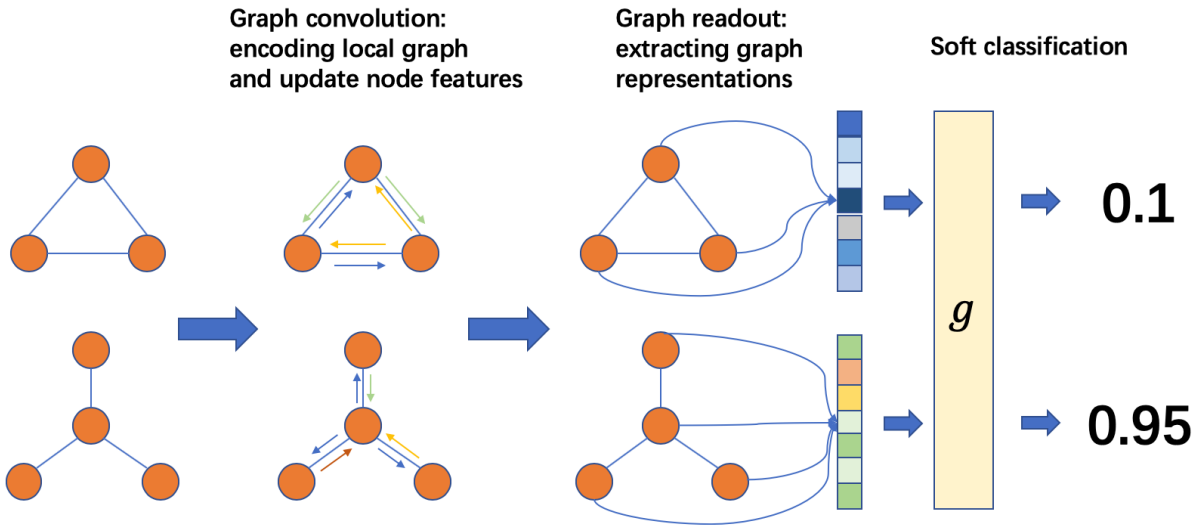




Source: https://towardsdatascience.com/graphs-and-linear-regression-734d1446e9cd

Graph-level Tasks: Graph Classification

- Graph classification:
  - Given a set of attributed graphs $D = \{(G_1, l_1), (G_2, l_2), \ldots, (G_n, l_n)\}$, the goal is to learn a function $f : G \rightarrow L$, where G is the input space of graphs and L is the set of graph labels.
  - Each graph $G_i = (A_{G_i}, D_{G_i})$ is comprised of an adjacency matrix A_{G_i}, an attribute matrix D_{G_i} and corresponding label l_i.
  - Conventional methods.
    - Kernel method: Subgraph matching, Weisfeiler-Lehman Subtree Kernel, Shortest path, Random walk, etc.



Source: https://docs.dgl.ai/en/0.8.x/guide/training-graph.html

Graph Classification: Subgraph Matching Kernel

- Counts the number of matchings between subgraphs of bounded size in two graphs.
- Given two graphs $G = (V, E)$ and $G' = (V', E')$:
  - $B(G, G')$ denote the set of all bijections between sets $S \subseteq V$ and $S' \subseteq V'$
  - $\lambda: B(G, G') \rightarrow \mathbb{R}^+$ be a weight function.
  - The subgraph matching kernel is defined as

$$k(G, G') = \sum_{\phi \in \mathcal{B}(G,G')} \lambda(\phi) \prod_{v \in S} \kappa_V(v, \phi(v)) \prod_{e \in S \times S} \kappa_E(e, \psi(e))$$

Where $S = \mathrm{dom}(\phi)$ and κ_V, κ_E are kernel functions defined on vertices and edges.

Nils Kriege and Petra Mutzel: Subgraph Matching Kernels for Attributed Graphs

Graph Classification: Subgraph Matching Kernel

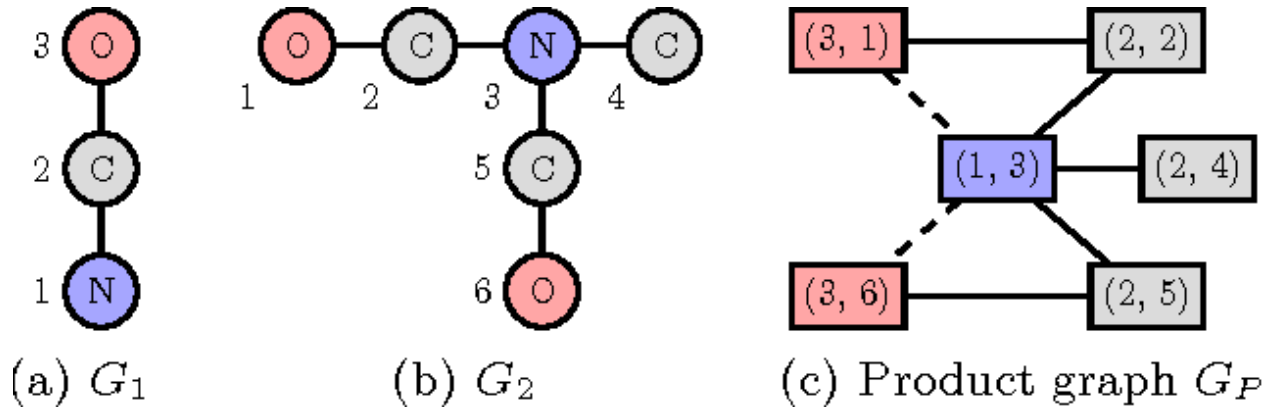
- The instance of the subgraph matching kernel that is obtained if we set the κ_V, κ_E functions as follows.

$$\kappa_V(v, v') = \begin{cases} 1, & \text{if } \ell(v) \equiv \ell(v'), \\ 0, & \text{otherwise and} \end{cases}$$

$$\kappa_E(e, e') = \begin{cases} 1, & \text{if } e \in E \wedge e' \in E' \wedge \ell(e) \equiv \ell(e') \text{ or } e \notin E \wedge e' \notin E', \\ 0, & \text{otherwise.} \end{cases}$$

is known as the common subgraph isomorphism kernel.

- This kernel counts the number of isomorphic subgraphs contained in two graphs.



(a) G_1 (b) G_2 (c) Product graph G_P

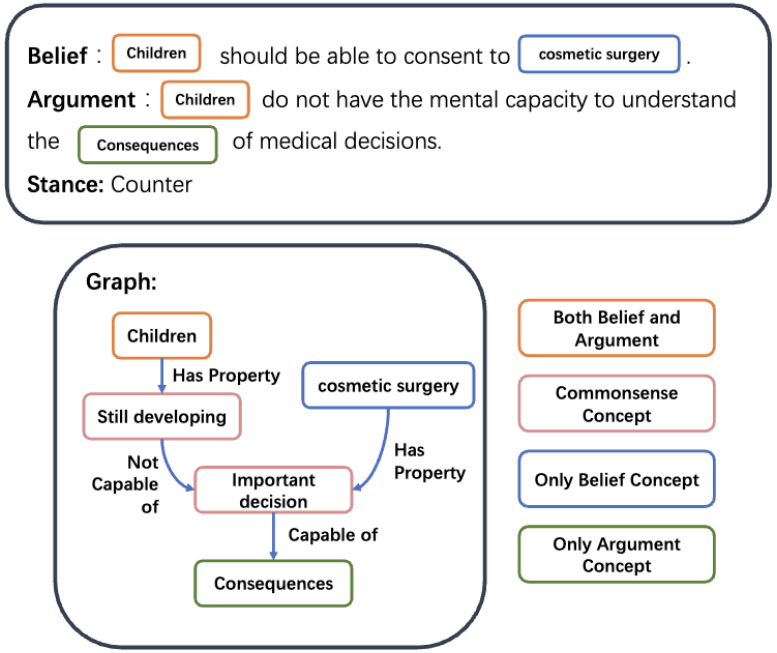
Nils Kriege and Petra Mutzel: Subgraph Matching Kernels for Attributed Graphs

Graph-level Tasks: Graph Generation

- Graph generation:
  - A quadruplet graph $G = (V, E, X, \boldsymbol{E})$, where V is the vertex set, $E \subseteq V \times V$ is the edge set, $X \in \mathbb{R}^{N \times D}$ is the node feature matrix, $\mathbf{E} \in \mathbb{R}^{N \times N \times F}$ is the edge attributes, and D, F are the feature dimensionality.
  - Given a set of M observed graphs $\mathcal{g} = \{G_i\}_{i=1}^{M}$, graph generation learns the distribution of these graphs $p(G)$, from which new graphs can be sampled $G_{new} \sim p(\mathcal{g})$.
  - Conventional methods
    - Preferential Attachment

$$PA = |N(x)|.|N(y)| = d_x.d_y$$

Where $N(x), N(y)$ are number of neighbors of node x and y.



Han Cui et al: Explanation Graph Generation via Generative Pre-training over Synthetic Graphs

Graph-level Tasks: Graph Clustering

- Graph clustering:
  - Given a set of graphs, partitioning a set of graphs into different groups that share some form of similarity.
  - Conventional methods:
    - Hierarchical clustering, K-means clustering, spectral clustering.
    - Modularity: To qualify the graph partitions.
    - Louvian Algorithm: to find partition of a given network with high modularity score

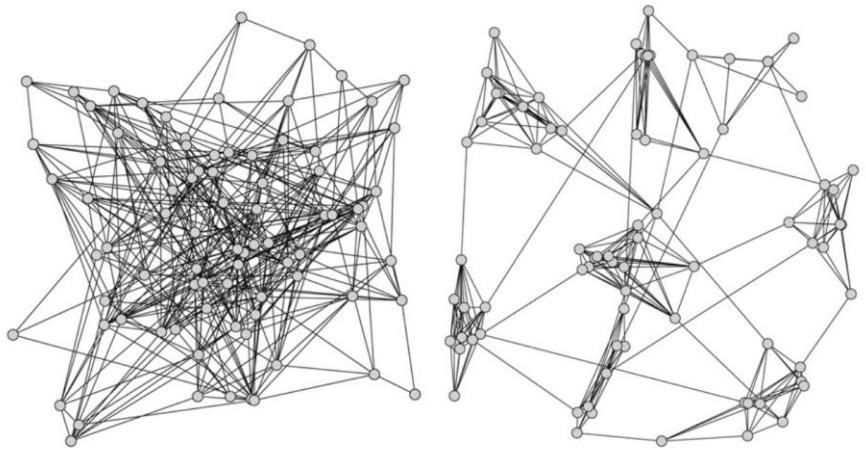
normalization

adjacency matrix

probability a random edge would go between i and j

$$Q = \frac{1}{4m} \sum_{i,j} \left(A_{ij} - \frac{k_i k_j}{2m} \right)$$

m = # edges in graph
k_i = degree(i)



Satu Elisa Schaeffer: Graph clustering

Graph Clustering: Modularity

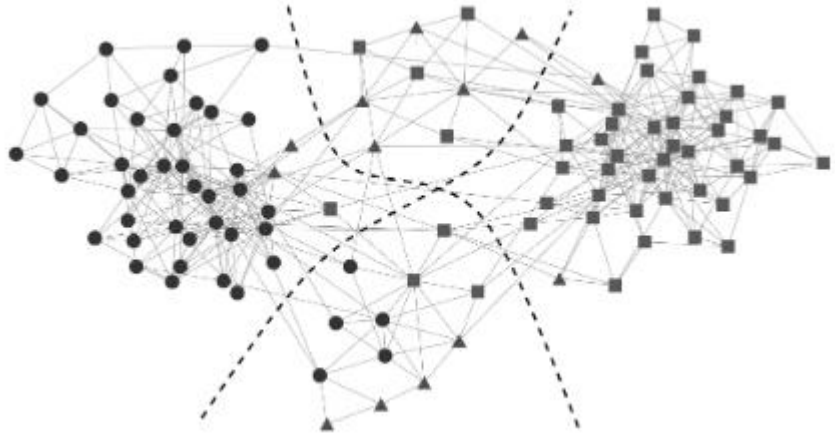
- Normally, modularity only consider to qualify into two graph partition.
- To divide network into more than two communities:

$$\Delta Q = \frac{1}{2m}\left[\frac{1}{2}\sum_{i,j\in g} B_{ij}(s_i s_j + 1) - \sum_{i,j\in g} B_{ij}\right]$$

$$= \frac{1}{4m}\left[\sum_{i,j\in g} B_{ij} s_i s_j - \sum_{i,j\in g} B_{ij}\right]$$

$$= \frac{1}{4m}\sum_{i,j\in g}\left[B_{ij} - \delta_{ij}\sum_{k\in g} B_{ik}\right] s_i s_j$$

$$= \frac{1}{4m}\mathbf{s}^T\mathbf{B}^{(g)}\mathbf{s},$$



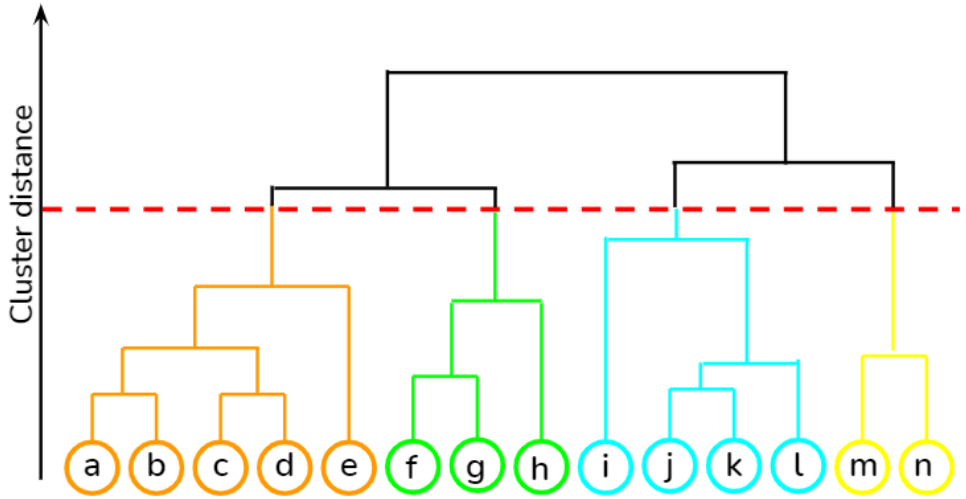
Where δ_{ij} is the Kronecker δ-symbol, $s_i^2 = 1$ and B^g is the $n_g \times n_g$ matrix with elements indexed by the labels i, j of nodes within group g and having values

$$B_{ij}^{(g)} = B_{ij} - \delta_{ij}\sum_{k\in g} B_{ik}.$$

M. E. J. Newman: Modularity and community structure in networks

Graph Clustering: Hierarchical clustering

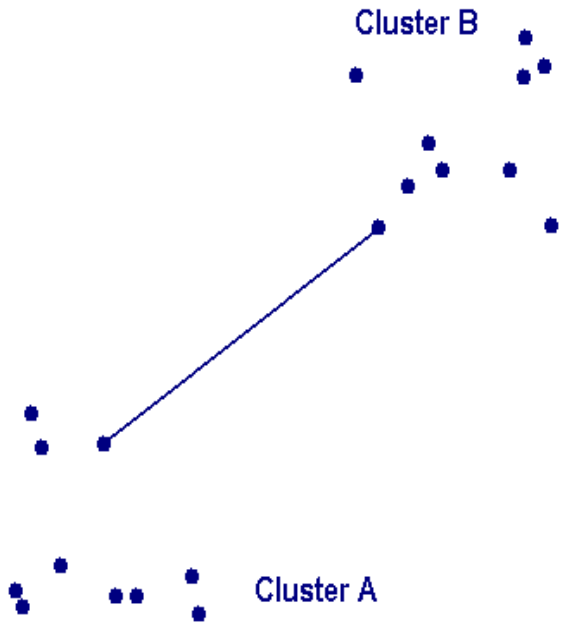
- Hierarchical clustering is a method of cluster analysis which seeks to build a hierarchy of clusters. Two approaches:
  - **Agglomerative** ("bottom up“): each point starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy – popular one.
  - **Divisive** ("top down“): all points start in one cluster, and splits are performed recursively as one moves down the hierarchy:
- Agglomerative clustering algorithm:
  - Maintain a set of clusters.
  - Initially, each instance in its own cluster.
  - Repeat:
    - Pick the two closest clusters.
    - Merge them into a new cluster.
    - Stop when there’s only one cluster left.



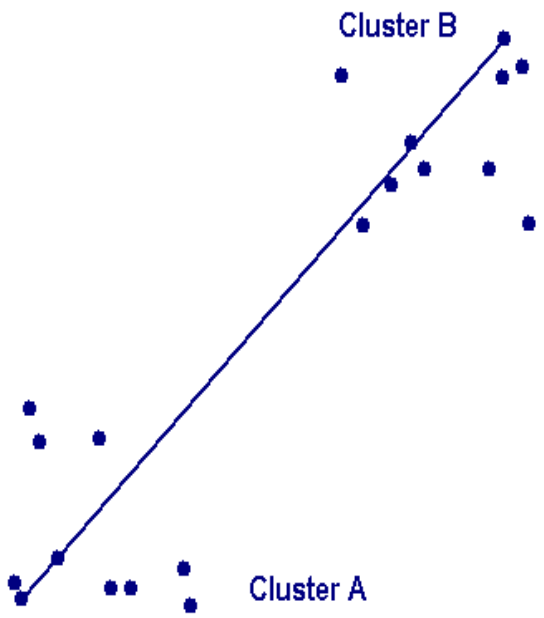
Source: https://towardsdatascience.com/hierarchical-clustering-explained-e59b13846da8

Graph Clustering: Hierarchical clustering

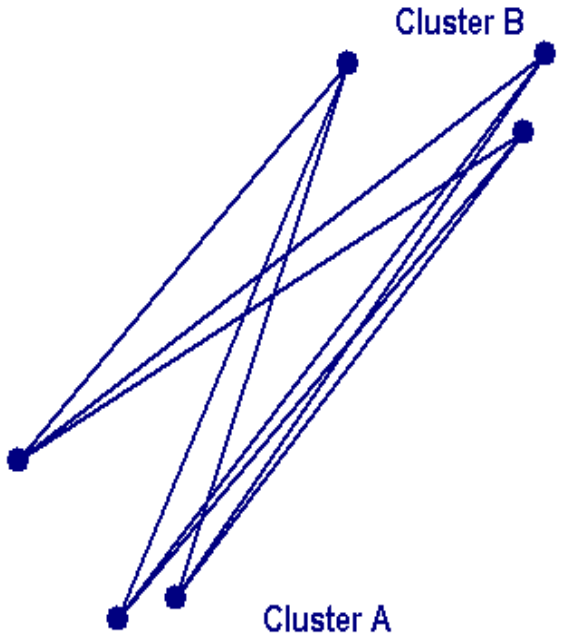
- Three Different Distance Measures to define closest cluster:
  - Minimum distance / Closest distance (single linkage).
  - Maximum distance / Farthest distance(complete linkage).
  - Group Average (average linkage).



Single linkage



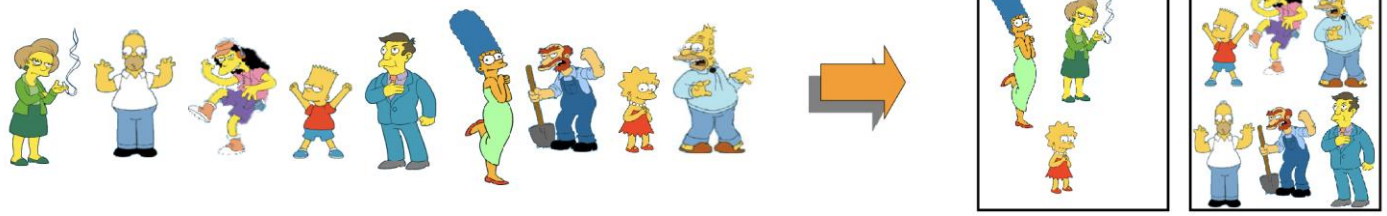
Complete linkage



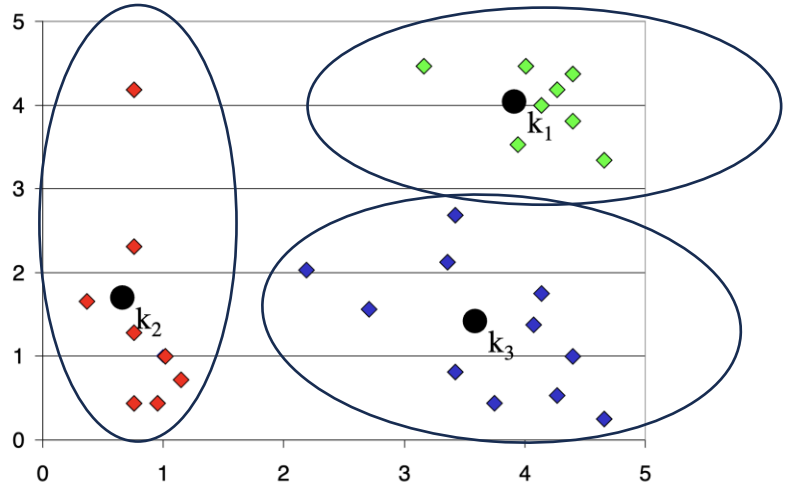
Average linkage

Graph Clustering: K-mean Clustering

- Partition clustering:
  - Nonhierarchical, each instance is placed in exactly one of K non-overlapping clusters.
  - Since the output is only one set of clusters the user has to specify the desired number of clusters K.



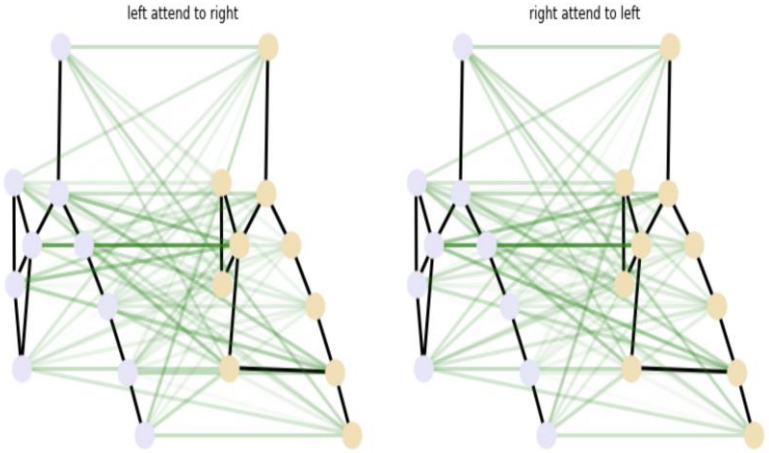
- K-mean clustering algorithm:
  - Re-assign and move centers, until ...no objects changed membership.



Source: School of Computer Science – Carnegie Mellon University

Graph-level Tasks: Graph Similarity

- Graph similarity:
  - Given two graphs G_1 and G_2, a graph similarity model can be written as a function $f(G_1, G_2)$ that computes a scalar similarity value.
  - Output: find the similarity score between graphs(from 0 to 1).
  - Conventional methods:.
    - Graph matching, isomorphism testing, etc.



    - Graph edit distances.

$$GED(g_1, g_2) = \min_{(e_1,\ldots,e_k)\in\mathcal{P}(g_1,g_2)} \sum_{i=1}^{k} c(e_i)$$

Where $P(g_1, g_2)$ denotes the set of edit paths transforming $g_1$into g_2 and $c(e) \geq 0$ is the cost of each graph edit operation e.

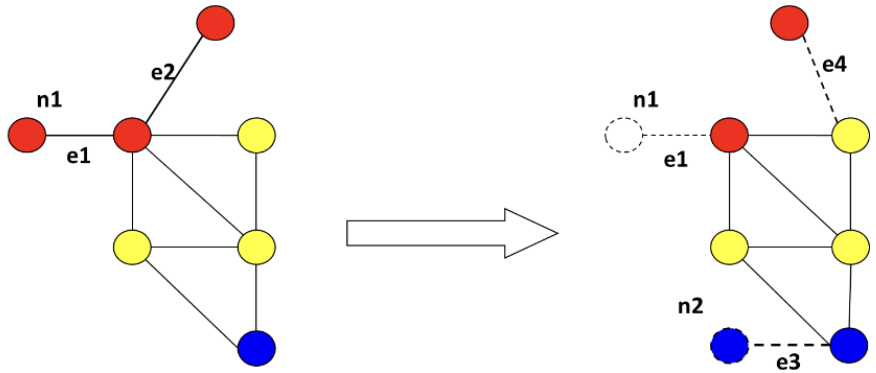
Source: https://notebook.community/deepmind/deepmind-research/graph_matching_networks/graph_matching_networks

Graph Similarity: Graph Edit Distance

- Compute the minimum cost to transform g_1 into g_2.
- assign cost for operations, e.g.,
  - vertex or edge insertion
  - vertex or edge deletion
  - vertex or edge substitution.

$$GED(g_1, g_2) = \min_{(e_1,\ldots,e_k)\in\mathcal{P}(g_1,g_2)} \sum_{i=1}^{k} c(e_i)$$

Where $P(g_1, g_2)$ denotes the set of edit paths transforming $g_1$into g_2 and $c(e) \geq 0$ is the cost of each graph edit operation e.

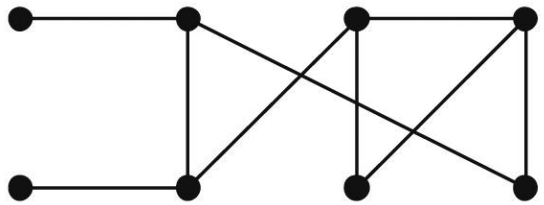


Graph Similarity: Graph Spectral Distance

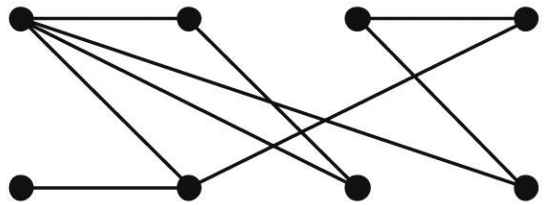
- Given graph G and G' of size n with adjacency spectra λ^A and $\lambda^{A'}$.
- Adjacency spectral distance between the two graphs is defined:

$$d_A(G, G') \stackrel{\text{def}}{=} \sqrt{\sum_{i=1}^{n} (\lambda_i^A - \lambda_i^{A'})^2},$$

- Smaller distance means that two graph are similarity.
- Spectral distances do not require node correspondence.



G



G'

Richard C. Wilson et al: A study of graph spectra for comparing graphs and trees

Graph Similarity: Graphlet Kernel

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

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

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

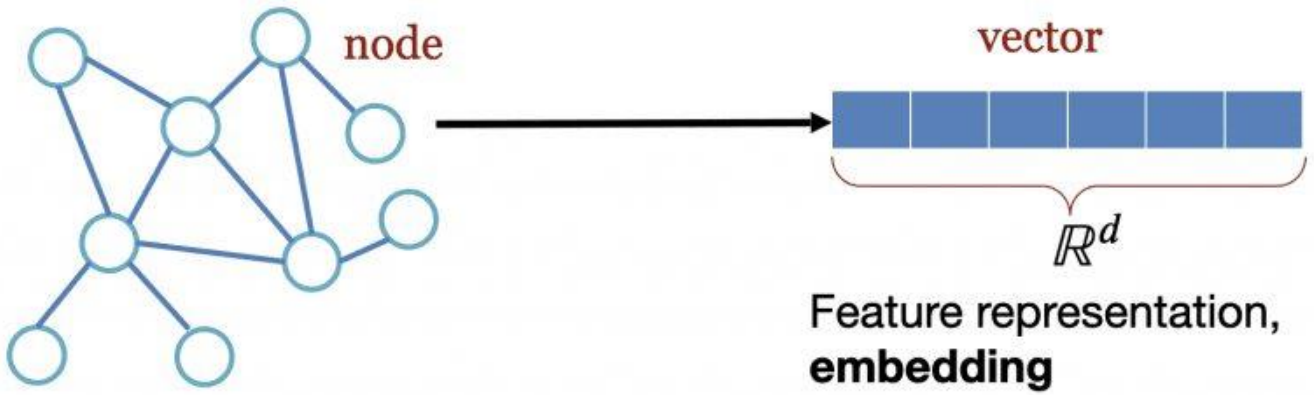
$$\boldsymbol{h}_G = \frac{\boldsymbol{f}_G}{\text{Sum}(\boldsymbol{f}_G)} \qquad K(G, G') = \boldsymbol{h}_G{}^{\text{T}} \boldsymbol{h}_{G'}$$

Graph-level Tasks: Graph Embeddings

- Graph Embedding:
  - Given a graph $G = (N, E)$, where V is the vertex set, $E \subseteq V \times V$ is the edge set. Graph embedding aims to learn a low-dimensional vector representation x_i for each node v_i from embedding function Φ maps: $x_i = \Phi(v_i) \in \mathbb{R}^d$.

  where d is the dimensionality of the embedding space.

  - Goal: to learn embeddings that preserve important structural properties of the graph, such as node proximity or graph topology, in the low-dimensional space.



https://www.graphable.ai/blog/knowledge-graph-embeddings/

- Graph Embedding:
  - Conventional methods
    - Euclidean distance and Cosine similarity.

$$cos(A,B) = \frac{A \cdot B}{||A|| \cdot ||B||} = \frac{\sum_i A_i B_i}{\sqrt{\sum_i A_i^2}\sqrt{\sum_i B_i^2}}$$

Where A, B denotes two vectors of two graphs.

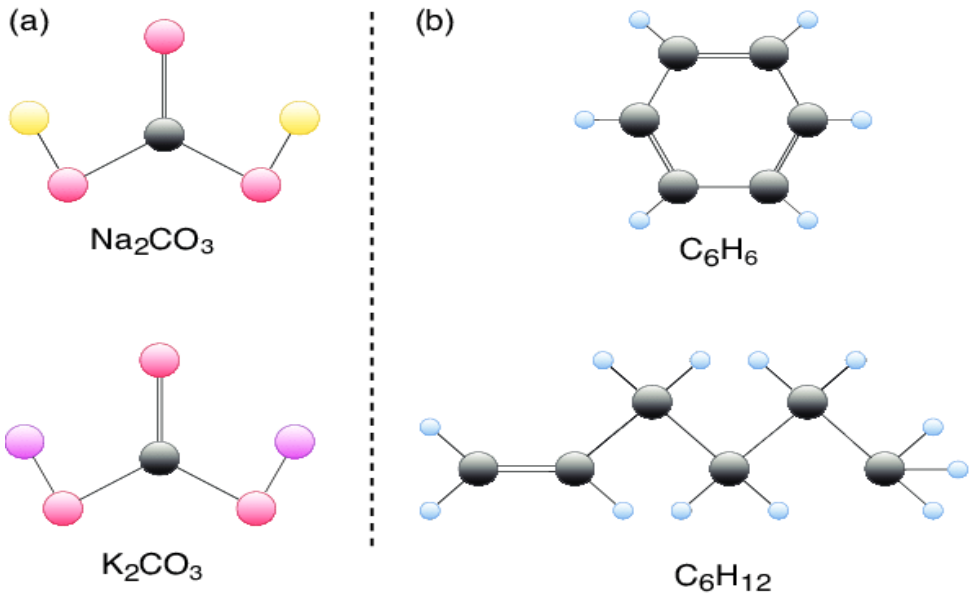
- Laplacian matrix factorization: singular value decomposition, nonnegative matrix factorization.
  - Singular value decomposition:

$$A = UDV^T$$

Where A denotes adjacency matrix. U, V are orthonormal and the matrix D is diagonal with positive real entries.

Graph-Level Applications

- Drug Discovery:
  - Classifying a graph itself into different categories.
  - Inputs: A collection of graphs.
  - For example, determining if a chemical compound is toxic or non-toxic by looking at its graph structure.



https://www.researchgate.net/figure/An-illustration-of-molecule-graph_fig1_349880436

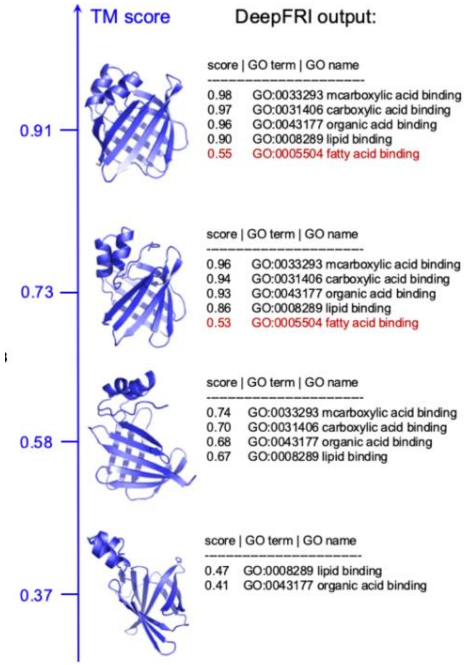
Graph-Level Applications

- Programming code recommendation: graph classification tasks
  - Program-derived graphs
    - Contains bugs or not.

```
function clearEmployeeListOnLinkClick(){
  document.querySelector("a").addEventListener("click",
    function(event){
      document.querySelector("ul").InnerHTML = "";
    }
  );
}
```

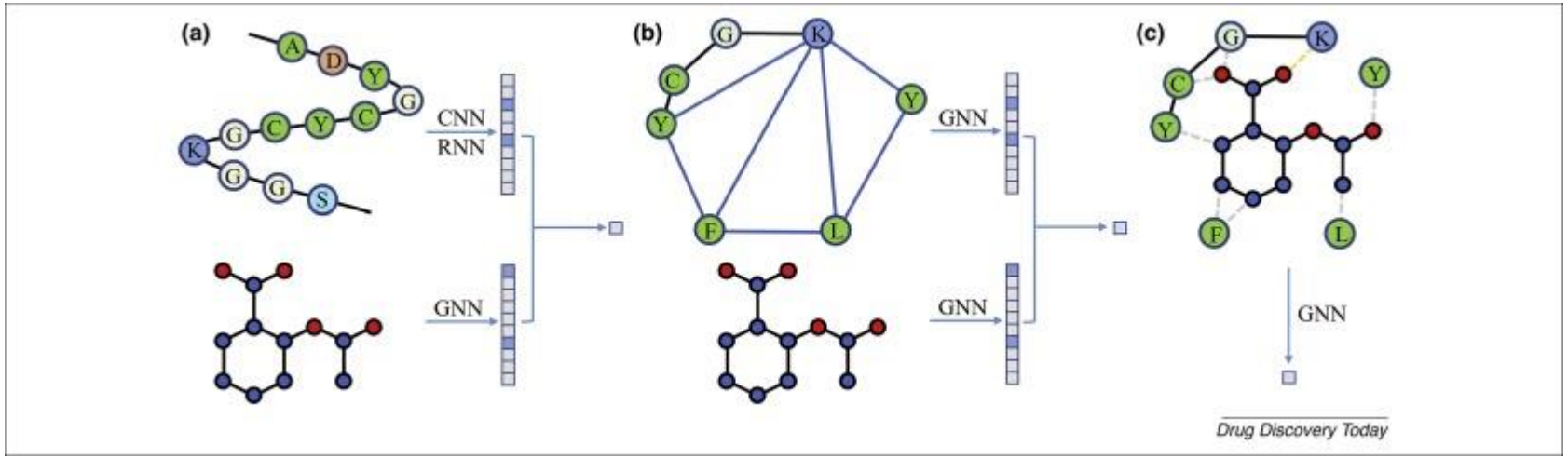
```
if (matches) {
  return {
    episode: Number(matches.groups.episode),
    hosts: matches.groups.hosts.split(/([,&]+|\sand\s)/).
              map(el => S(el).trim().s)
  };
}
```

- Drug Discovery: graph regression tasks
  - Proteins.
    - Predict protein function from molecular.



Vladimir Gligorijević et al: Structure-based protein function prediction using graph convolutional networks

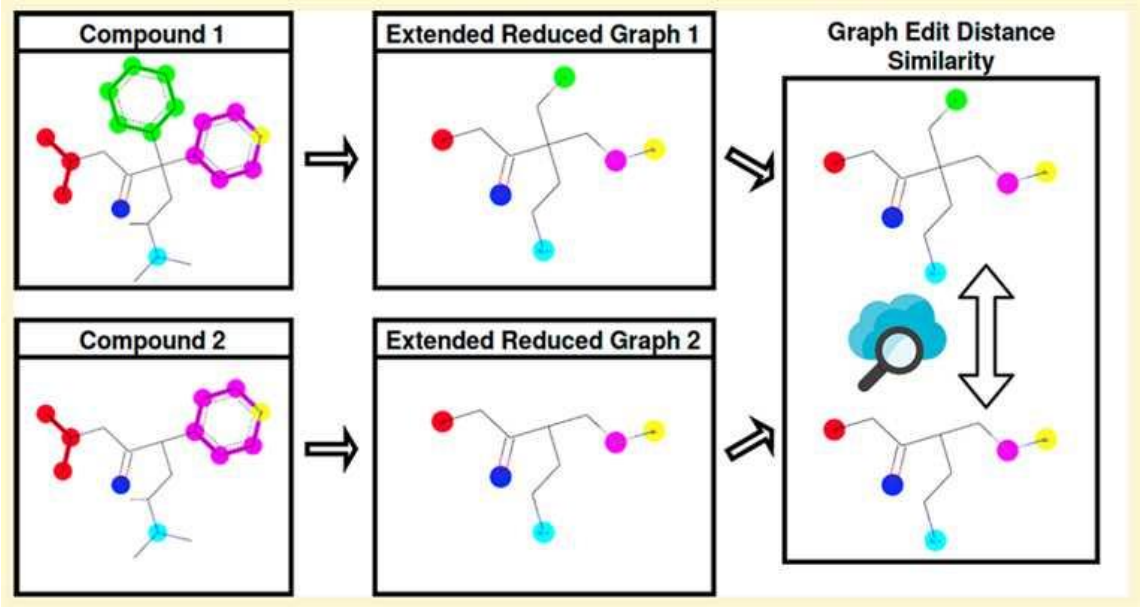
- Drug-Discovery:
  - Molecular-design for drug-discovery using **graph generation**:
    - Generate syntactically valid molecules.
    - Generated molecule should possess certain properties.



Jiacheng Xiong et al: Graph neural networks for automated de novo drug design

Graph-Level Applications

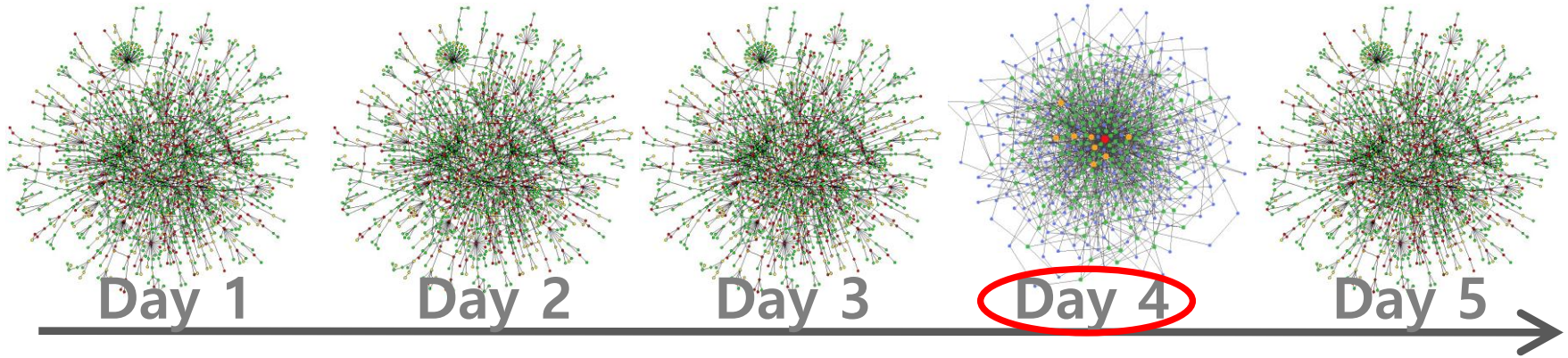
- Drug database:
  - Drug similarity search using **graph similarity**:



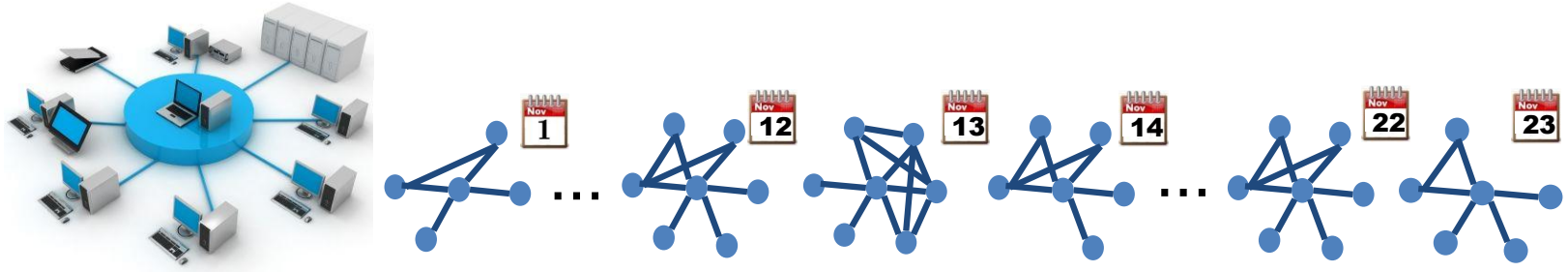
  - Program database:
    - Code recommendation using graph similarity.

Source: https://www.creative-biolabs.com/drug-discovery/therapeutics/graph-based-similarity-assessment.htm

- Network Analysis - Graph similarity:
  - Discontinuity Detection.

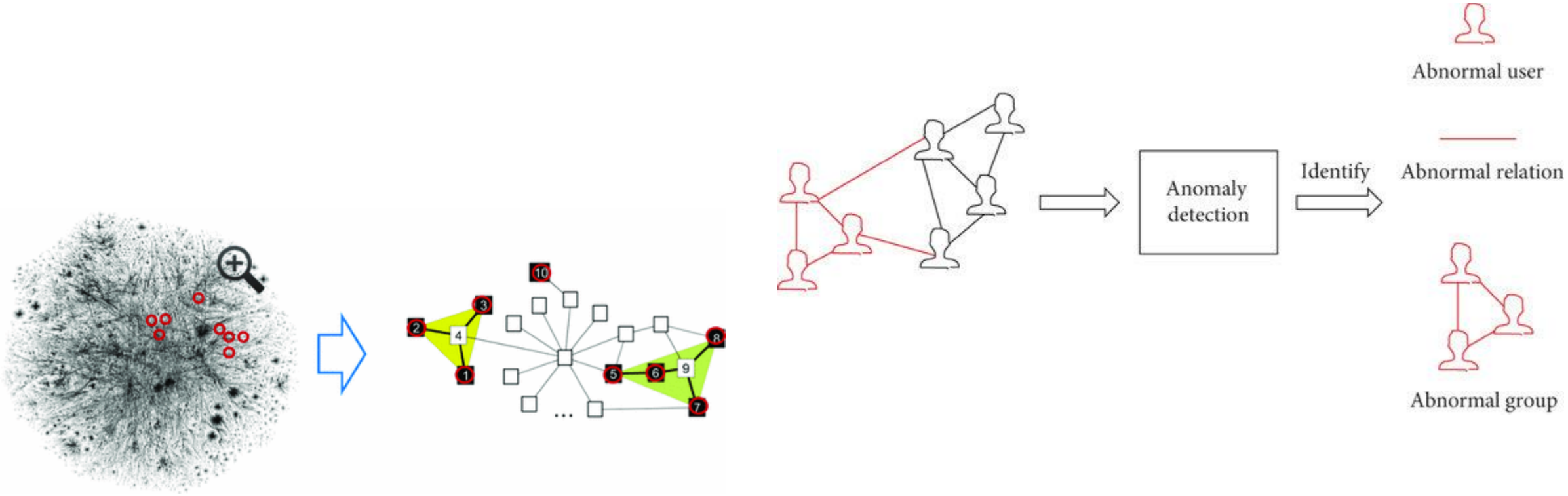


  - Intrusion detection:
    - Network intrusion.



Source: School of Computer Science – Carnegie Mellon University

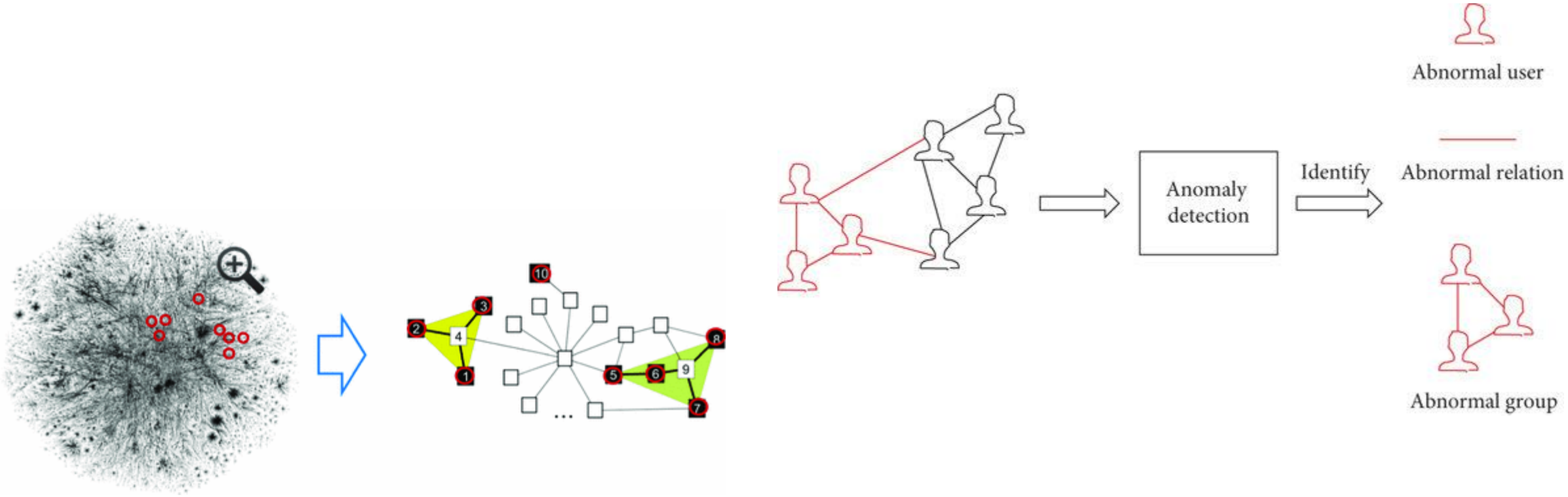
- Anomaly detection:
  - Abnormal group vs normal group in social network using graph similarity:



Source: School of Computer Science – Carnegie Mellon University

Graph-Level Applications

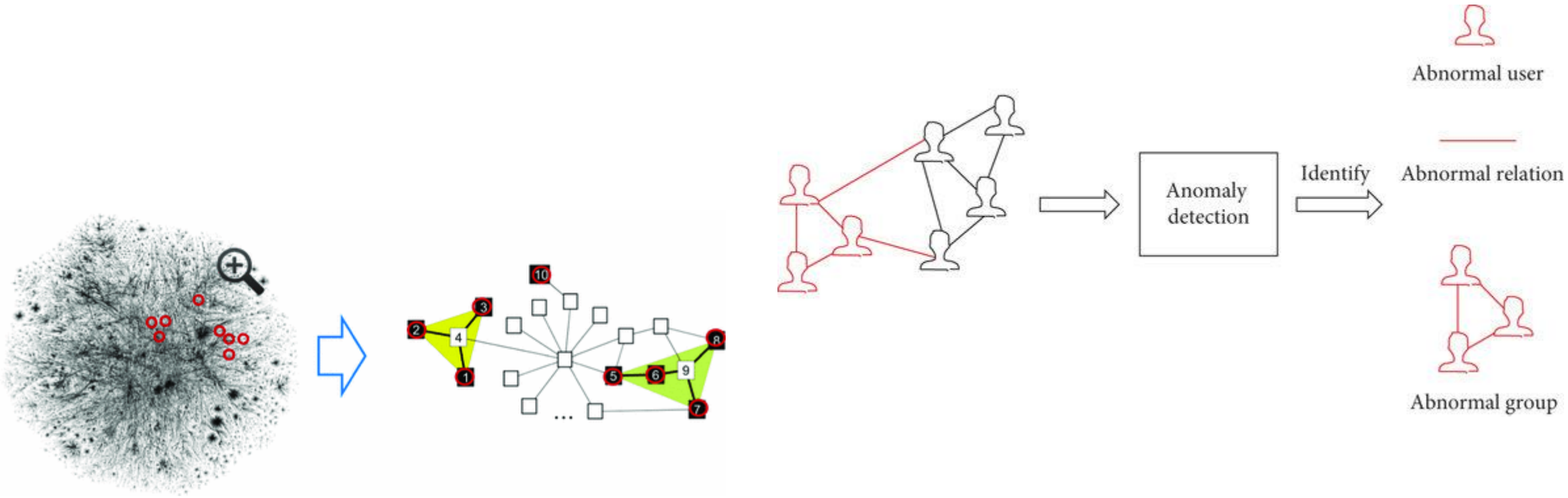
- Anomaly detection:
  - Abnormal group vs normal group in social network using graph similarity:



Source: School of Computer Science – Carnegie Mellon University

Graph-Level Applications

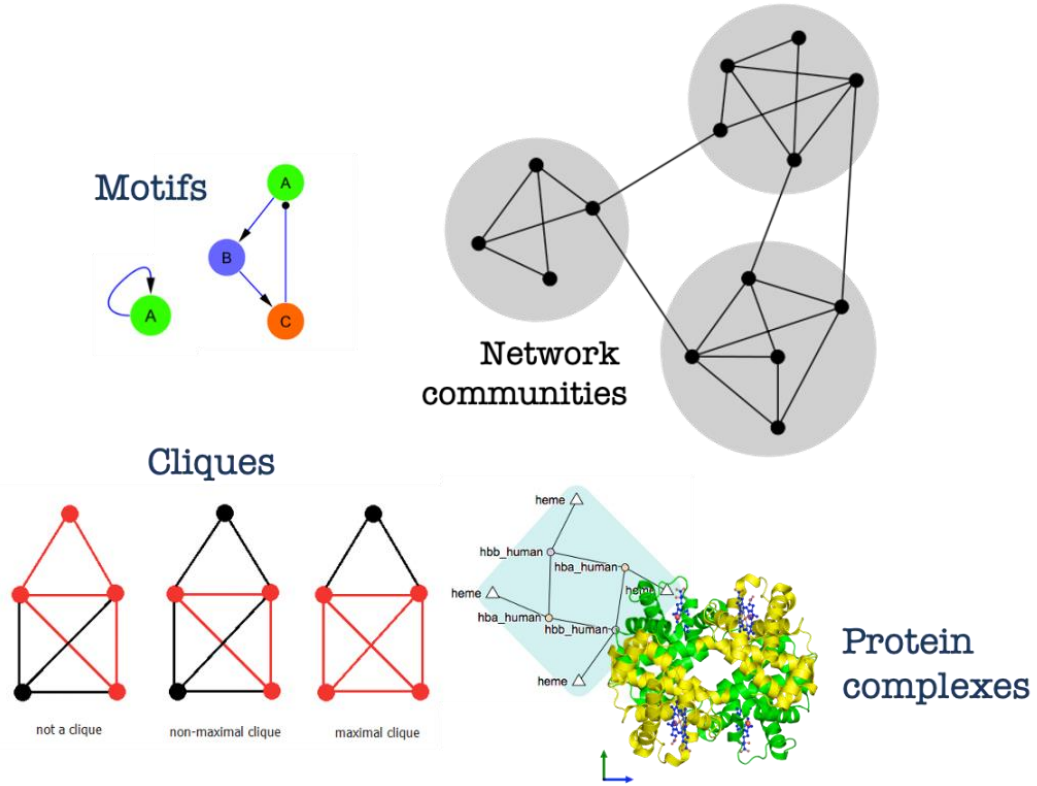
- Anomaly detection:
  - Abnormal group vs normal group in social network using graph similarity:



Source: School of Computer Science – Carnegie Mellon University

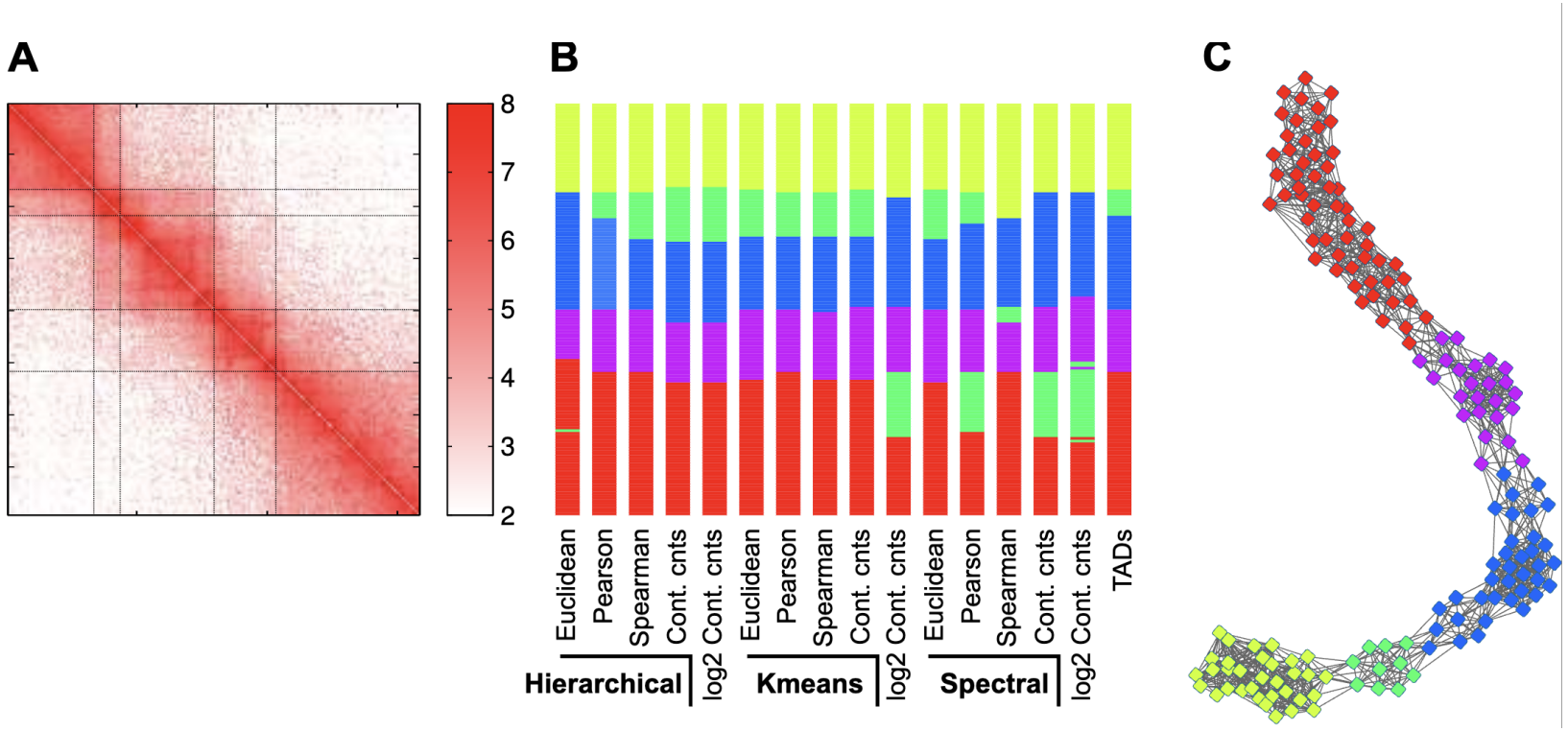
Graph-Level Applications

- Biological network analysis:
  - Identifying functional modules in Protein-protein interaction networks using graph clustering.



https://www.ebi.ac.uk/training/online/courses/network-analysis-of-protein-interaction-data-an-introduction/building-and-analysing-ppins/topological-ppin-analysis/clustering-analysis/

- Genome analysis in Bioinformatics:
  - Finding higher-order Topologically Associated Domain using graph clustering.



네트워크 과학 연구실
NETWORK SCIENCE LAB

가톨릭대학교
THE CATHOLIC UNIVERSITY OF KOREA