Graph Mining and Graph Representation Learning

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Contents

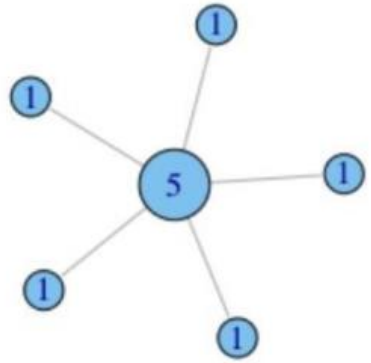
- Graph Representation.
- Centrality Measurements:
  - Betweenness Centrality, Closeness Centrality, PageRank Centrality.
- Graph Measurements:
  - Clustering Coefficients, Conductance, Modularity.
- Additional Metrics:
  - Jaccard's Coefficient, Katz Index.
- Graph Kernels:
  - Shortest Path Kernel, Weisfeiler-Lehman Kernel.
- Graph Representation Learning (GRL):
  - From traditional machine learning for graph to GRL.
  - WalkLet, Node2Vec, LINE, HOPE, Struc2Vec, Role2Vec, metapath2vec.
  - Dynnode2vec, Continuous-Time Dynamic Network Embeddings.

Graph Representations

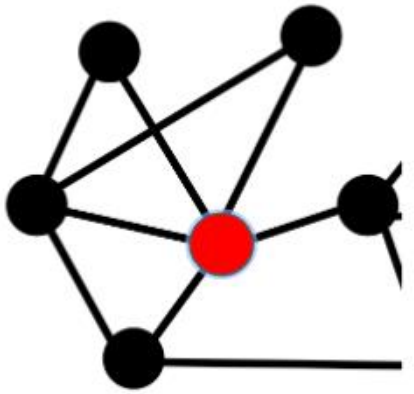
- Graphs efficiently model relationships, perfect for addressing questions like "What's the lowest-cost path from A to B?"
- We need a data structure that represents graphs
- Determining the "Best" Data Structure can depend on:
  - Properties of the graph (dense vs. sparse)
  - Common queries
    - For example: "is (u ,v) an edge?" vs "what are the neighbors of node u?"
- There are two standard graph representations:
  - Adjacency Matrix.
  - Adjacency List.

Introduction of Centrality Measures

- **Node degree**: the degree k_v of node v is the number of edges (neighboring nodes) the node has.
  - In-degree: Number of incoming edges to the node.
  - Out-degree: Number of outgoing edges from the node.
  - Total degree: Sum of in-degree and out-degree



- Knowing the network structure, we can calculate various useful quantities or measures that capture important features of network topology
- Centrality measures represent the most important nodes in graphs:
  - The most influential person in a social network.
  - The most critical nodes in an infrastructure.
  - The highest spreaders of disease.



➢ Betweenness Centrality:

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

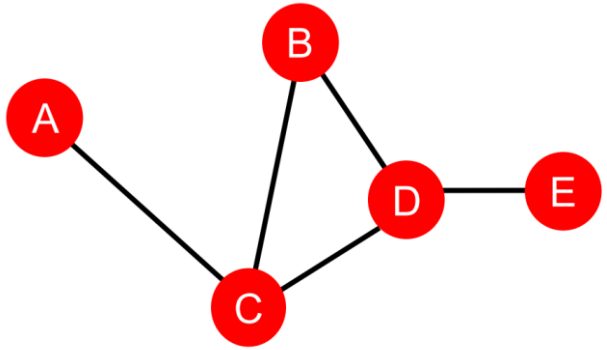
$$c_v = \sum_{s \neq v \neq t} \frac{\#(\text{shortest paths betwen } s \text{ and } t \text{ that contain } v)}{\#(\text{shortest paths between } s \text{ and } t)}$$

- ➢ Usually normalized by:

No. of nodes in the graph

$$\bar{B}(v_i) = B(v_i) / [(n-1)(n-2)/2]$$

- ➢ 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)

Centrality Measurement: Betweenness Centrality

- Vertices with high betweenness centrality have influence in the network by virtue of their control over information passing between others.
  - They get to see the messages as they pass through
  - They could get paid for passing the message along
- Thus, they get a lot of power: their removal would disrupt communication

➢ Closeness Centrality:

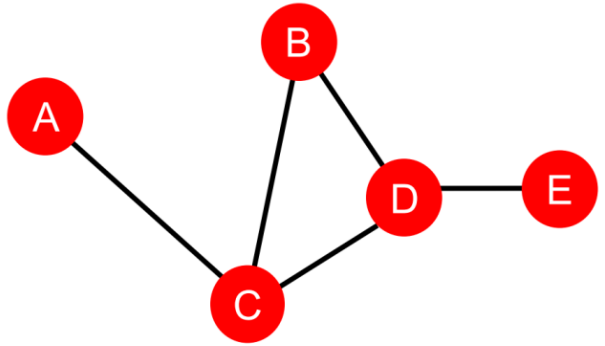
- A node is important if it has **small shortest path lengths** to all other nodes.

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

- Usually normalized by:

$$\bar{C}(v_i) = \frac{\mathrm{n} - 1}{\sum_{j=1}^{n} \left| \mathrm{d}(v_i, v_j) \right|}$$

- For example:



- $C_A = 1/(2 + 1 + 2 + 3) = 1/8$

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

- $C_D = 1/(2 + 1 + 1 + 1) = 1/5$

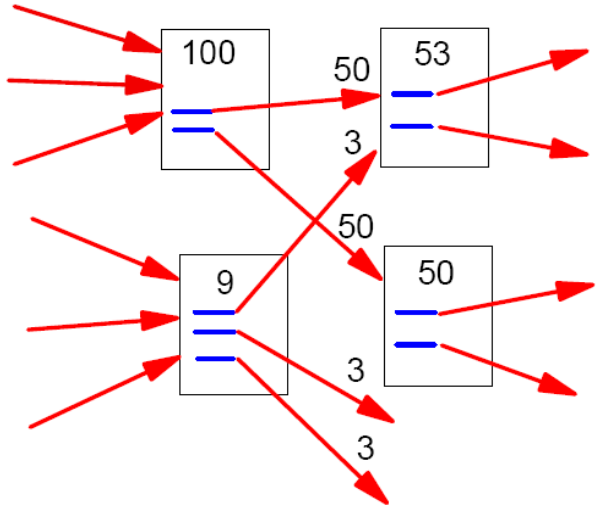
(D-C-A, D-B, D-C, D-E)

Centrality Measurement (3): PageRank

- PageRank is a numeric value that represents how important a page is on the web.
- Webpage importance
  - One page links to another page = A vote for the other page A link from page A to page B is a vote on A to B.
  - If page A is more important itself, then the vote of A to B should carry more weight.
  - More votes = More important the page must be.

Simplified PageRank: A simplified version from Google

- Importance Computation
  - The importance of a page is distributed to pages that it points to.
  - The importance of a page is the aggregation of the importance shares of the pages that points to it.
    - If a page has 5 outlinks, the importance of the page is divided into 5 and each link receives one fifth share of the importance.

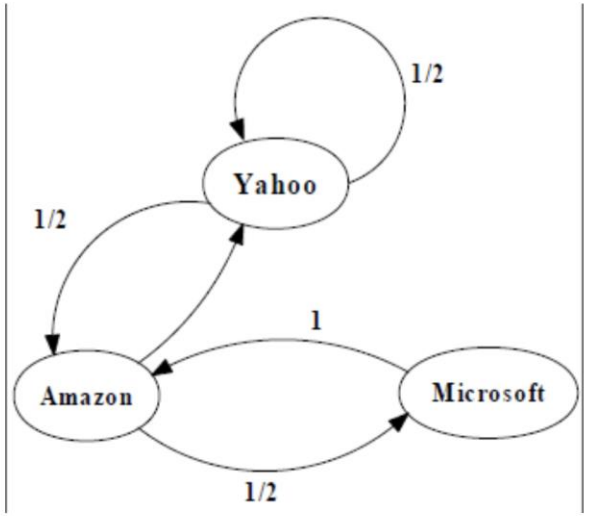


A Simple Version of PageRank

$$R(u) = c \sum_{v \in B_u} \frac{R(v)}{N_v}$$

- u: a web page.
- B_u: the set of u's backlinks.
- N_v: the number of forward links of page v.
- c: the normalization factor to make $\|R\|_{L1} = 1 (\|R\|_{L1} = |R_1 + \cdots + R_n|)$.

➢ For example:



$$M = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix}$$

$$\begin{bmatrix} \text{yahoo} \\ \text{Amazon} \\ \text{Microsoft} \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

$$\begin{bmatrix} 1/3 \\ 1/2 \\ 1/6 \end{bmatrix} = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix} \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

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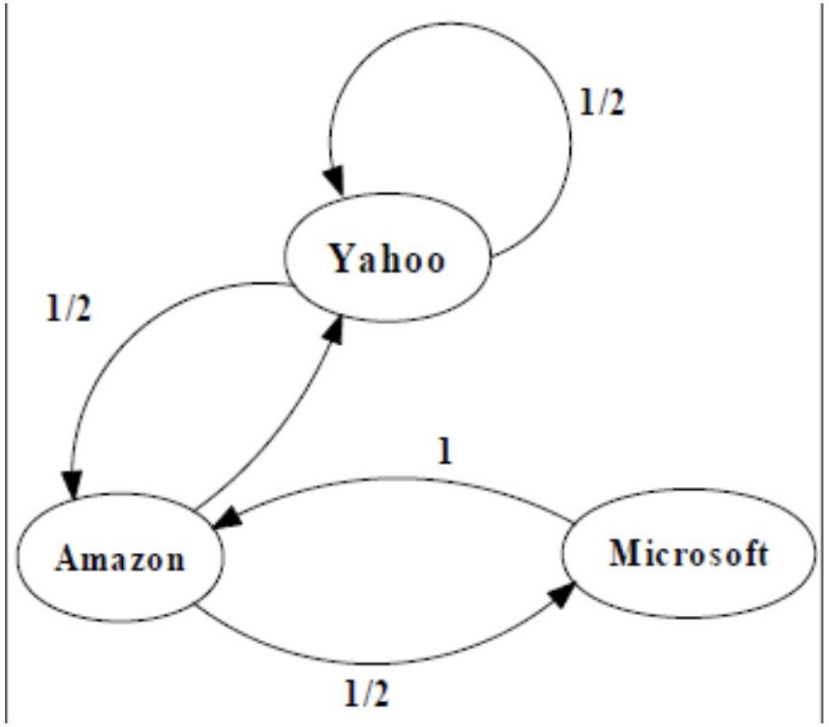
A Simple Version of PageRank



$$M = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix}$$

$$\begin{bmatrix} \text{yahoo} \\ \text{Amazon} \\ \text{Microsoft} \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

$$\begin{bmatrix} 5/12 \\ 1/3 \\ 1/4 \end{bmatrix} = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix} \begin{bmatrix} 1/3 \\ 1/2 \\ 1/6 \end{bmatrix}$$

PageRank Calculation: second iteration

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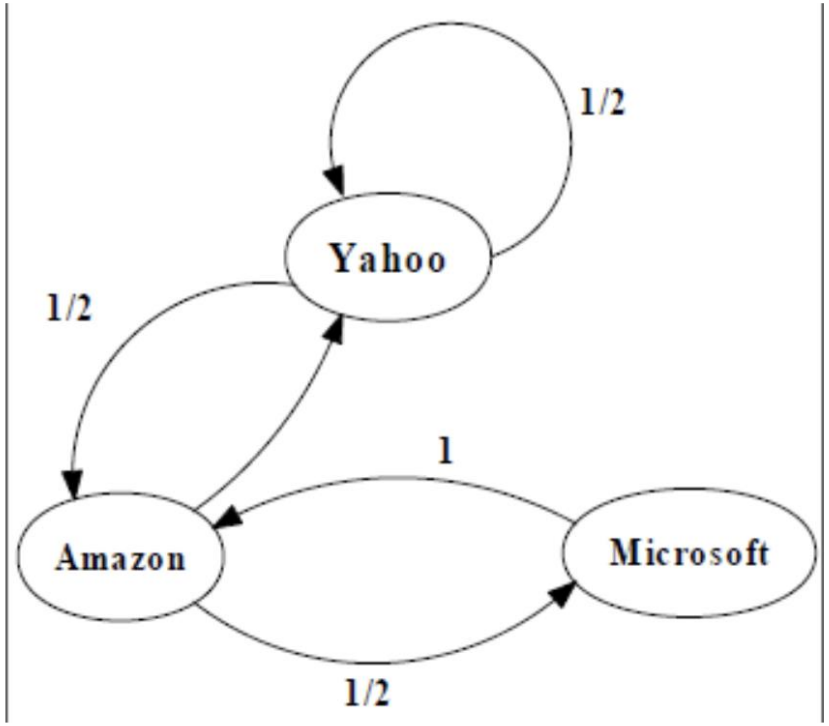
A Simple Version of PageRank



$$M = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 0 & 1 \\ 0 & 1/2 & 0 \end{bmatrix}$$

$$\begin{bmatrix} \text{yahoo} \\ \text{Amazon} \\ \text{Microsoft} \end{bmatrix} = \begin{bmatrix} 1/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

$$\begin{bmatrix} 3/8 \\ 11/24 \\ 1/6 \end{bmatrix} \begin{bmatrix} 5/12 \\ 17/48 \\ 11/48 \end{bmatrix} \ldots \begin{bmatrix} 2/5 \\ 2/5 \\ 1/5 \end{bmatrix}$$

Convergence after some iterations

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Clustering Coefficient

- The clustering coefficient measures how connected a node's neighbors are to one another.
- The range is from 0 to 1 (from non-neighbor are connected to each other to all neighbors are fully connected).
- There are three types of clustering coefficient:
  - Local clustering coefficient.
  - Average clustering coefficient.
  - Global clustering coefficient.

Local Clustering Coefficient

- How close its neighbours are to being a clique (complete graph).
- For a node i with degree d_i and L_i represents the number of edges between neighbors of node i.

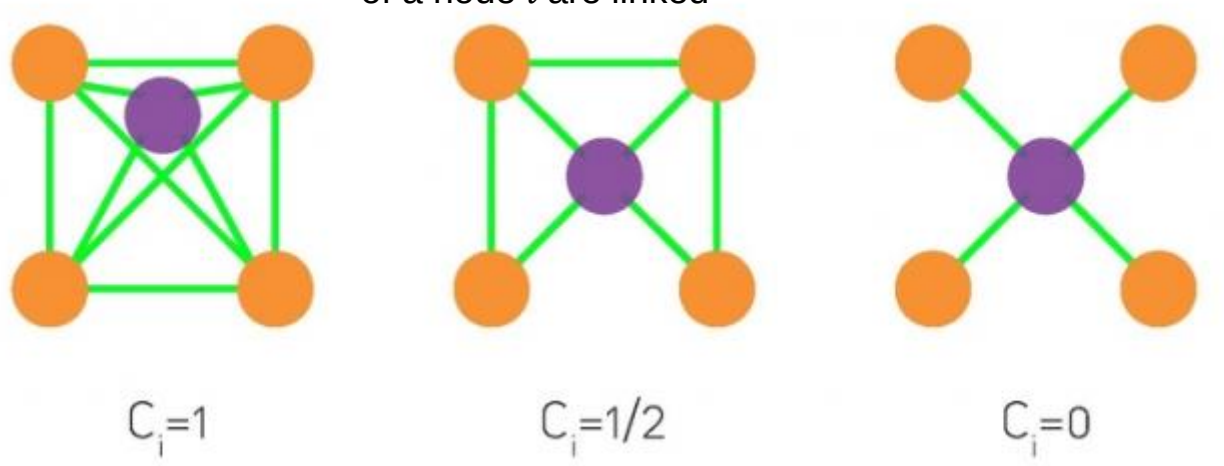
  The local clustering coefficient C_i for a node i is defined as:

$$C_i = \frac{2L_i}{d_i(d_i - 1)}$$

neighbors of node i form a complete graph

50% chance that two neighbors of a node i are linked

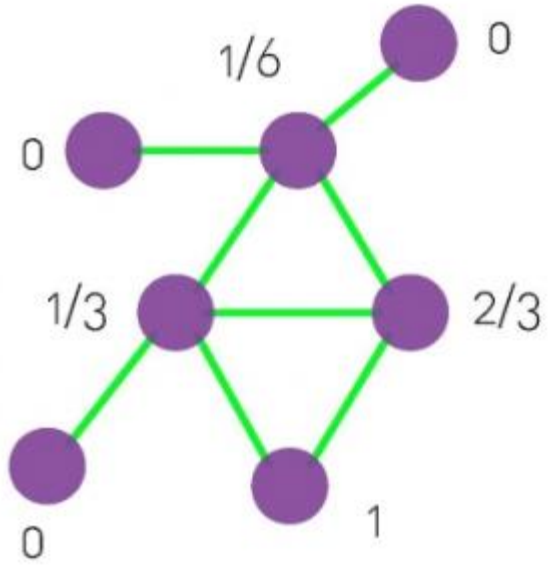
None of neighbors of node i link to each other



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 $i = 1, \ldots, N$.

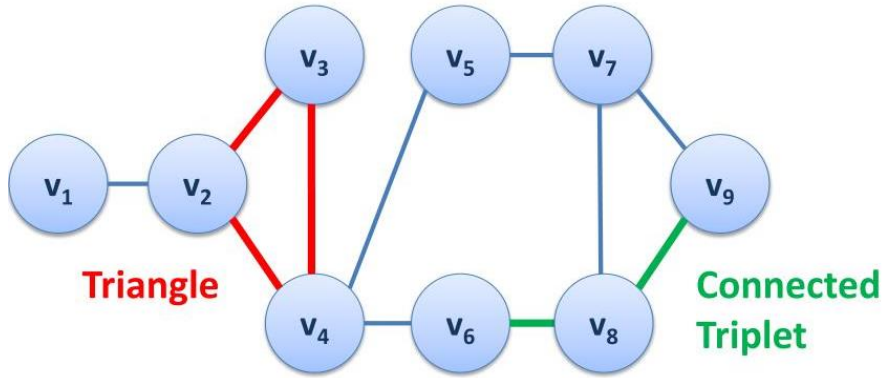
$$\langle C \rangle = \frac{1}{N} \sum_{i=0}^{N} C_i$$



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

Global Clustering Coefficient

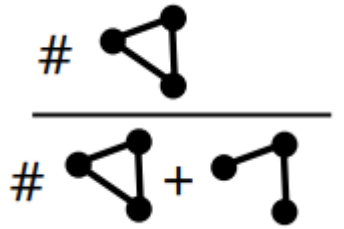
- The global clustering coefficient is based on triplets of nodes.
- A triplet consists of three connected nodes. A triangle therefore includes three closed triplets, one centered on each of the nodes.



- The global clustering coefficient is the number of closed triplets over the total number of triplets (both open and closed)

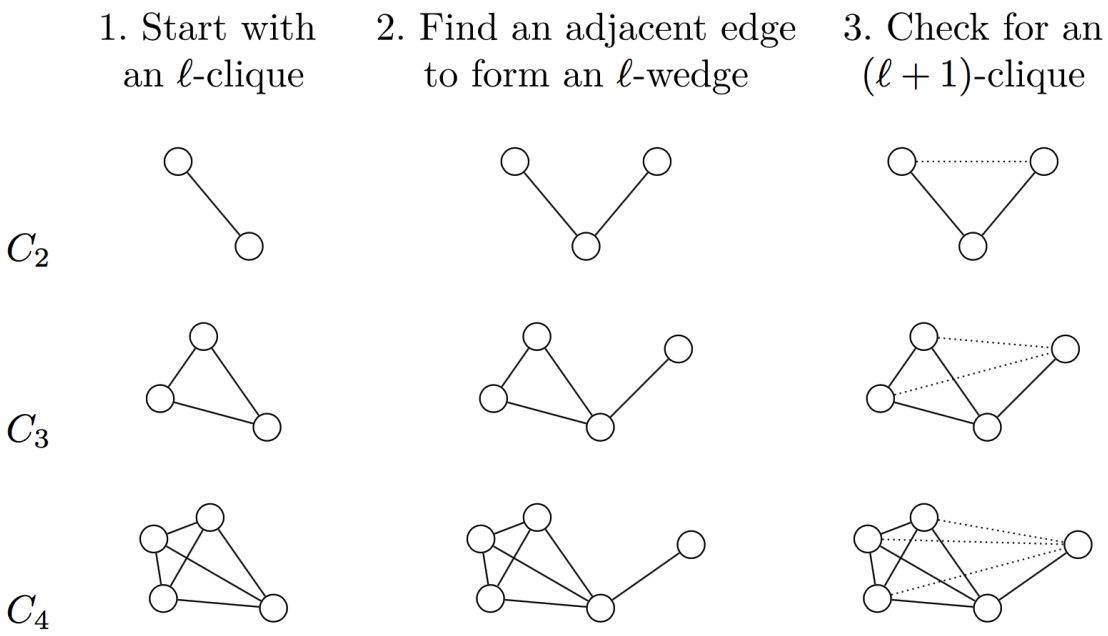
Closed triplets: (v_2, v_3, v_4), (v_7, v_8, v_9)
Connected triplets: $(v_6, v_8, v_9), \cdots$

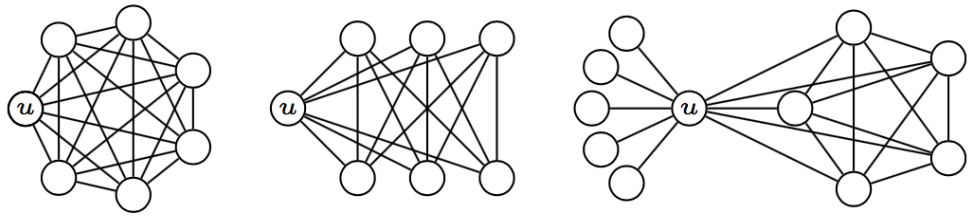
$$C(G) = \frac{\#of\ closed\ triplets}{\#\ of\ connected\ triplets}$$



Higher-order Clustering Coefficient

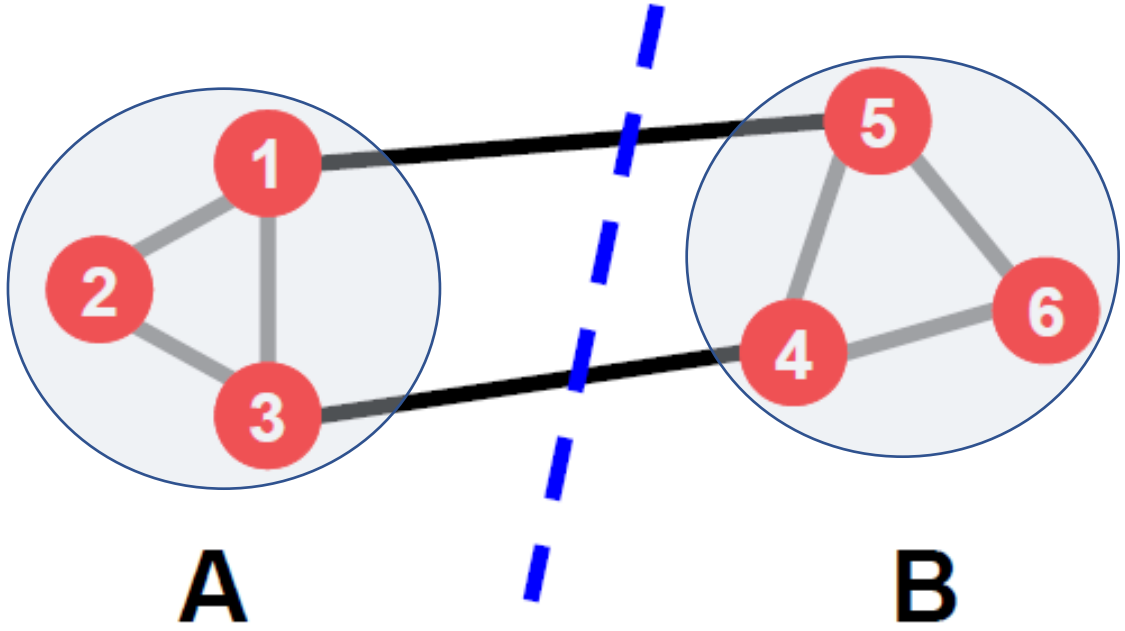
- The clustering coefficient can be extended to higher order structures with k-cliques.





$C_2(u)$	1	$\frac{d}{2(d-1)} \approx \frac{1}{2}$	$\frac{d-2}{4d-4} \approx \frac{1}{4}$
$C_3(u)$	1	0	$\frac{d-4}{2d-4} \approx \frac{1}{2}$
$C_4(u)$	1	0	$\frac{d-6}{2d-6} \approx \frac{1}{2}$

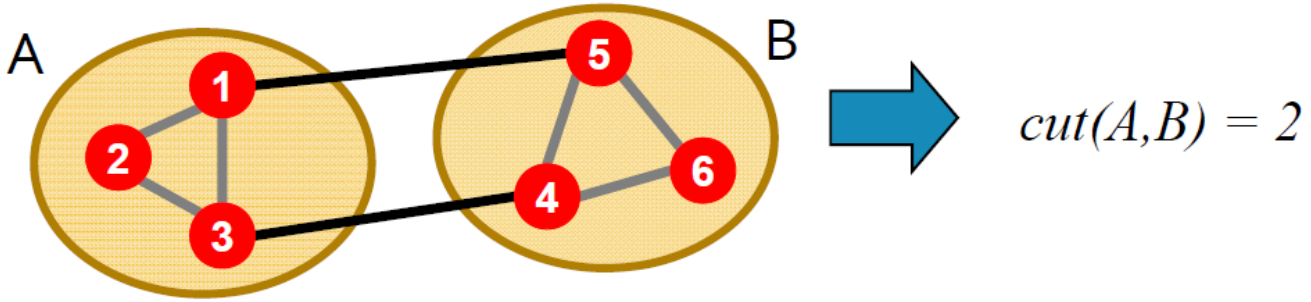
- Basic principle for graph partitioning:
  - Minimize the number of between-group connections.
  - Maximize the number of within-group connections.



Graph partitioning : A & B

Mathematical expression: Cut (A,B)

- For considering between-group:



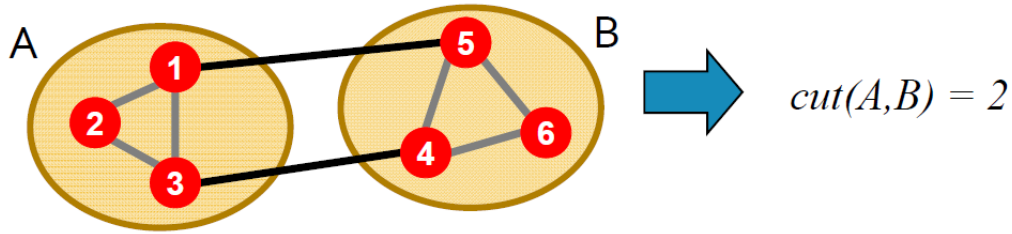
$$cut(A,B) = 2$$

Cut: Set of edges with only one vertex in a group: $cut(A,B) = \sum_{i \in A, j \in B} w_{ij}$

Mathematical expression: Normalized-cut (N-cut), Conductance

- For considering within-group.
- Assoc(A,V): the total connection from nodes in A to all nodes in the graph.

$$assoc(A,V) = \sum_{u \in A, t \in V} w(u,t)$$



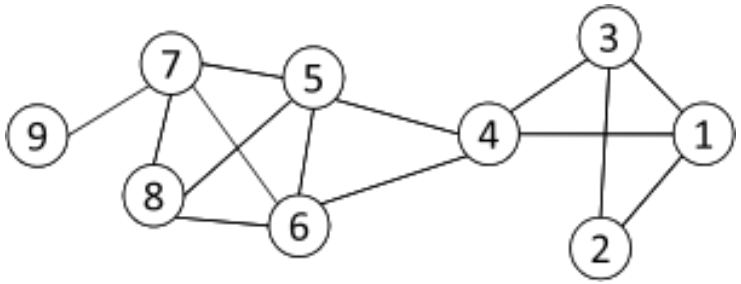
$$Ncut(A,B) = \frac{cut(A,B)}{assoc(A,V)} + \frac{cut(A,B)}{assoc(B,V)}$$

$$Conductance(A,B) = \frac{cut(A,B)}{\min(assoc(A,V), assoc(B,V))}$$

Modularity Maximization

- Modularity measures the strength of a community partition by considering the degree distribution
- Given a graph with m edges, the expected number of edges between two nodes with degree d_i and d_j is

$$d_i d_j / 2m$$



The expected number of edges between nodes 1 and 2 is 3*2/ (2*14) = 3/14

- Modularity:

$$Q = \frac{1}{2m}\sum_{ij}(A_{ij} - \gamma\frac{d_i d_j}{2m})\delta(C_i, C_j)$$

probability a random edge would go between i and j

Adjacency matrix of graph

$\delta(C_i, C_j)$: 1 if i and j are in the same community else 0

Modularity Matrix

- We have modularity matrix:

$$B = A - \mathbf{d}\mathbf{d}^T/2m \qquad (B_{ij} = A_{ij} - d_i d_j/2m)$$

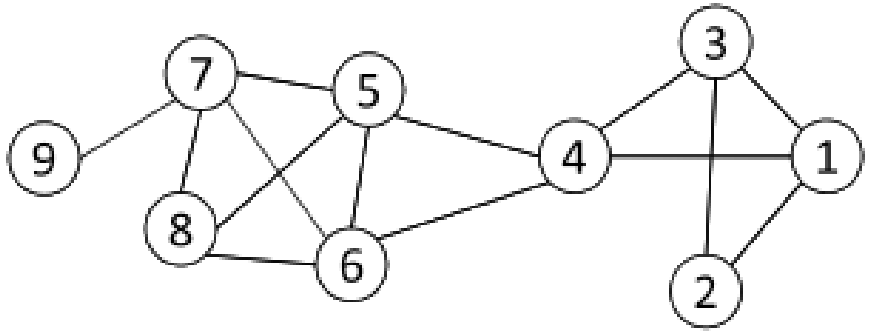
Where: d is node degree.

- Similar to spectral clustering, modularity maximization can be reformulated as

$$\max Q = \frac{1}{2m} Tr(S^T B S) \quad s.t.\ S^T S = I_k$$

- Optimal solution: top eigenvectors of the modularity matrix.
- Apply k-means to S as a post-processing step to obtain community partition.

Modularity Maximization Example



Two Communities:
{1, 2, 3, 4} and {5, 6, 7, 8, 9}

k-means

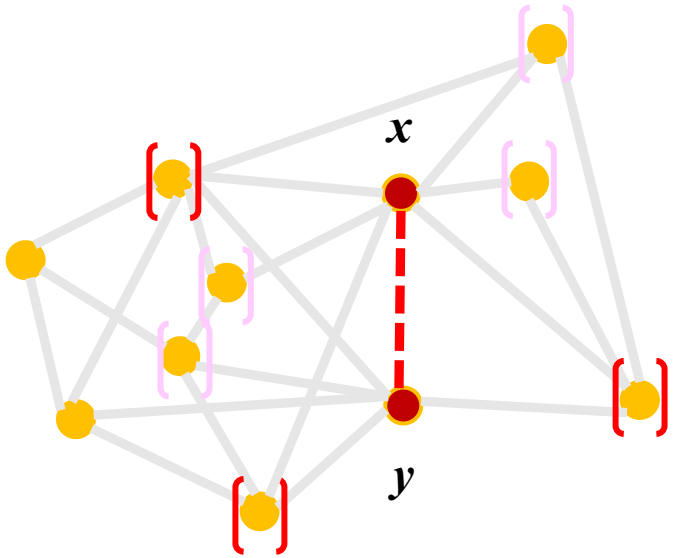
$$B = \begin{bmatrix} -0.32 & 0.79 & 0.68 & 0.57 & -0.43 & -0.43 & -0.43 & -0.32 & -0.11 \\ 0.79 & -0.14 & 0.79 & -0.29 & -0.29 & -0.29 & -0.29 & -0.21 & -0.07 \\ 0.68 & 0.79 & -0.32 & 0.57 & -0.43 & -0.43 & -0.43 & -0.32 & -0.11 \\ 0.57 & -0.29 & 0.57 & -0.57 & 0.43 & 0.43 & -0.57 & -0.43 & -0.14 \\ -0.43 & -0.29 & -0.43 & 0.43 & -0.57 & 0.43 & 0.43 & 0.57 & -0.14 \\ -0.43 & -0.29 & -0.43 & 0.43 & 0.43 & -0.57 & 0.43 & 0.57 & -0.14 \\ -0.43 & -0.29 & -0.43 & -0.57 & 0.43 & 0.43 & -0.57 & 0.57 & 0.86 \\ -0.32 & -0.21 & -0.32 & -0.43 & 0.57 & 0.57 & 0.57 & -0.32 & -0.11 \\ -0.11 & -0.07 & -0.11 & -0.14 & -0.14 & -0.14 & 0.86 & -0.11 & -0.04 \end{bmatrix}$$

Modularity Matrix

$$S = \begin{bmatrix} 0.44 & -0.00 \\ 0.38 & 0.23 \\ 0.44 & -0.00 \\ 0.17 & -0.48 \\ -0.29 & -0.32 \\ -0.29 & -0.32 \\ -0.38 & 0.34 \\ -0.34 & -0.08 \\ -0.14 & 0.63 \end{bmatrix}$$

Additional Metrics (1)

- Jaccard coefficient:
  - How likely a neighbour of x is also a neighbour of y.
  - Same as common neighbors, adjusted for degree.



$$JC = \frac{|N(x) \cap N(y)|}{|N(x) \cup N(y)|} = \frac{CN}{d_x + d_y - CN}$$

Additional Metrics (2)

- Katz index:

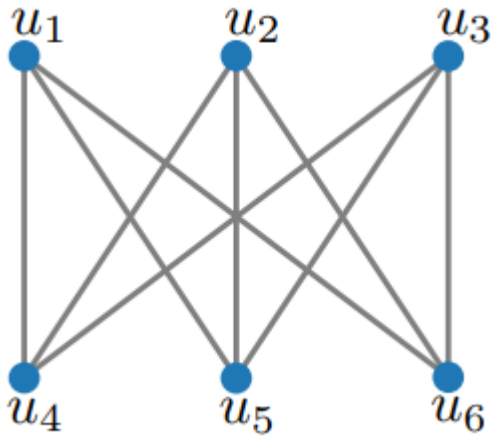
Element (x,y) in the adjacency matrix

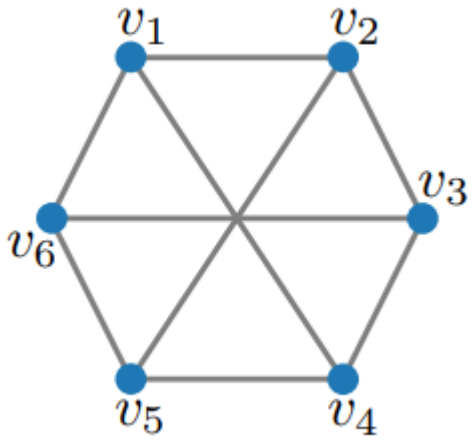
$$score(x,y) = \sum_{l=1}^{\infty} \beta^l \left| paths_{xy}^{(l)} \right| = \beta A_{xy} + \beta^2 A_{xy}^2 + \ldots$$

- Sum over ALL paths of length ℓ.
- $0 < \beta < 1$ is a parameter of the predictor, exponentially damped to count short paths more heavily.
- Small damped parameter = predictions much like common neighbours.

Graph Isomorphism

- Graph isomorphism:
  - Find a mapping f of the vertices of G_1 to the vertices of G_2 such that G_1 and G_2 are identical;
  - i.e. (u_i, u_j) is an edge of G_1 iff $(f(u_i), f(u_j))$ is an edge of G_2. Then f is an isomorphism, and G_1 and G_2 are called isomorphic.
  - No polynomial-time algorithm is known for graph isomorphism.
  - Neither is it known to be NP-complete.





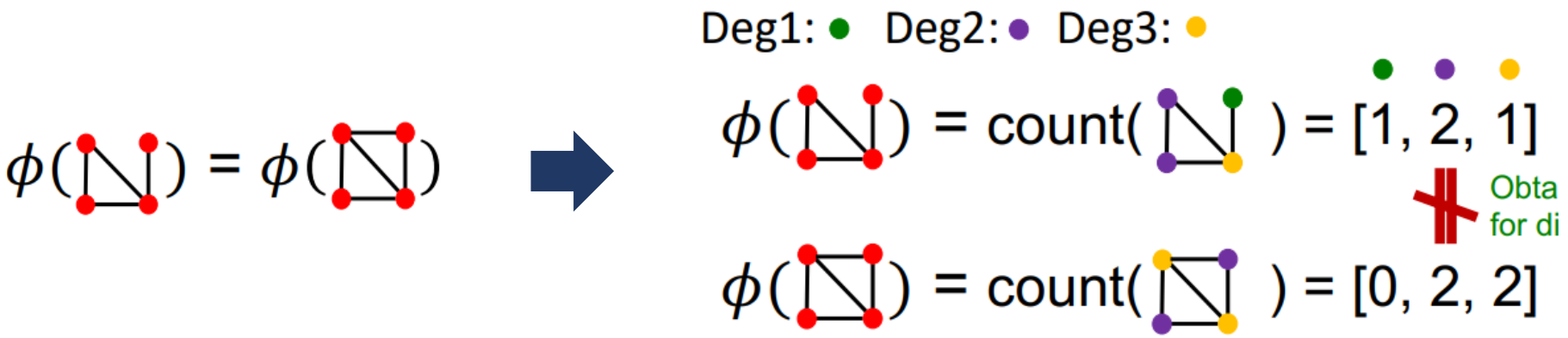
$$V^{G_1} \qquad V^{G_2}$$

$$\psi: \begin{array}{l} v_1 \to u_1 \\ v_2 \to u_4 \\ v_3 \to u_2 \\ v_4 \to u_5 \\ v_5 \to u_3 \\ v_6 \to u_6 \end{array}$$

What is a Kernel? (Schölkopf ,1997)

- Kernel is a type of measures of similarity.
- Mapping two objects x and x' via mapping ϕ into feature space *H.*
- Measure their similarity in *H* as $\langle \phi(x), \phi(x') \rangle$.
- **Kernel Trick**: Compute inner product in *H* as kernel in input space

$$k(x, x') = \langle \phi(x), \phi(x') \rangle.$$



What is a Graph Kernel?

- Instance of R-convolution kernels by Haussler (1999):
  - R-convolution kernels compare decompositions of two structured objects.

$$k_{convolution}(x, x') = \sum_{(x_d, x) \in \mathrm{R}} \sum_{(x'_d, x') \in \mathrm{R}} k_{parts}(x_d, x'_d)$$

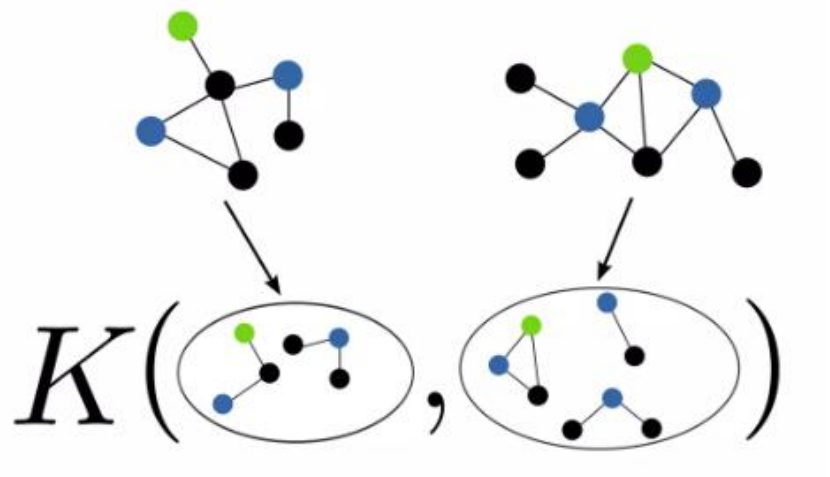
  - Decompose graphs into their substructures and add up the pairwise similarities between th ese substructures.

- Concept:
  - Kernel function to measure the similarity of pairs of graphs by computing an inner product o n graphs.
  - Compare substructures of graphs that are computable in polynomial time.

https://citeseerx.ist.psu.edu/document?repid=rep1&type=pdf&doi=5ee0d8aeb2cb01ef4d8a858d234e72a7400c03ac

Kenels based on bags of patterns

- Graph kernels based on bags of patterns:
  - Extraction of a set of patterns from graphs.
  - Comparison between patterns.
  - Comparison between bags of patterns.



Why Graph Kernels?

- Graph kernels are one of the most recent approaches to graph comparison.
- Interestingly, graph kernels employ concepts from all three traditional branches of graph comparison:
  - Measure similarity in terms of isomorphic substructures of graphs.
  - Allow for inexact matching of nodes, edges, and labels.
  - Treat graphs as vectors in a Hilbert space of graph features.

Shortest Path Kernel: More General Form

Floyd-transformation:

- Given an input graph G, outputs a shortest-path graph S.
  - S contains the same set of nodes as the input graph G.
  - There exists an edge between all nodes in S which are connected by a path in G.
  - Every edge in S between two nodes is labelled by the shortest distance between these two nodes.
  - This transformation can be done in $O(n^3)$ time.

Shortest Path Kernel: Definition

- 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.

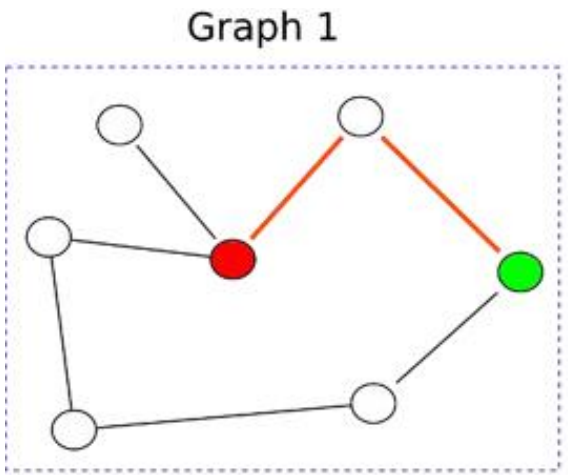
- k_{length} is a kernel that compares the lengths of two shortest paths:

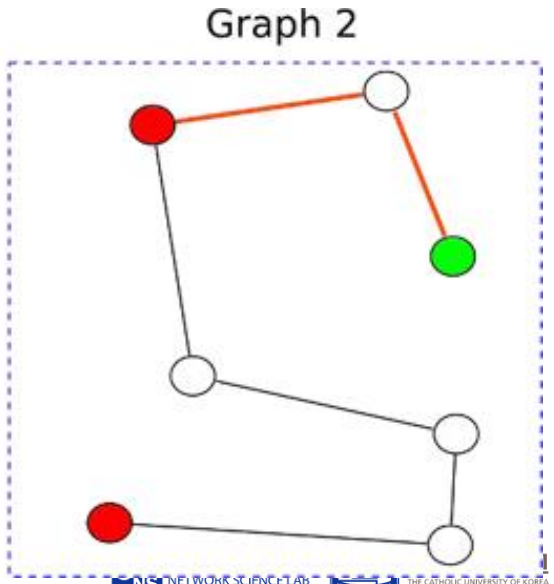
  - a linear kernel

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

  - a delta kernel

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

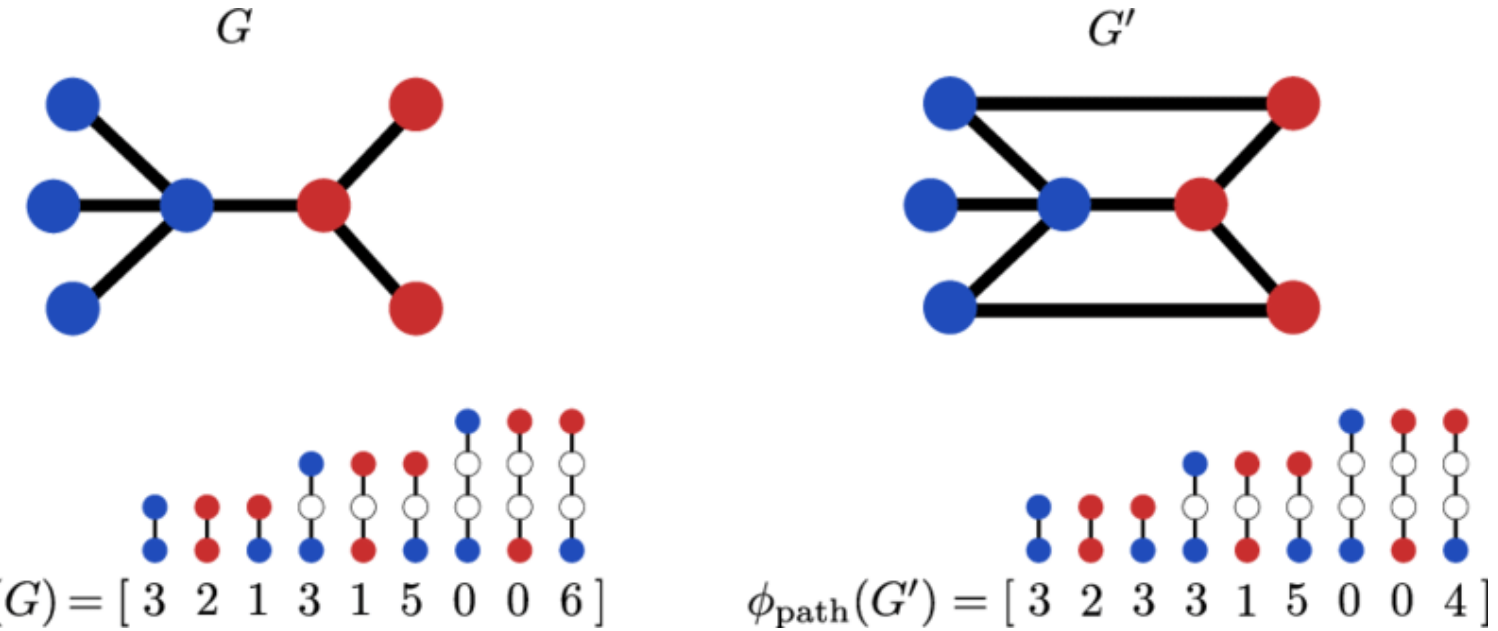




Karsten M. Borgwardt and Hans-Peter Kriegel. Shortest-path kernels on graphs

Shortest-path graph kernel:

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



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Isomorphism of Graphs

Definition:

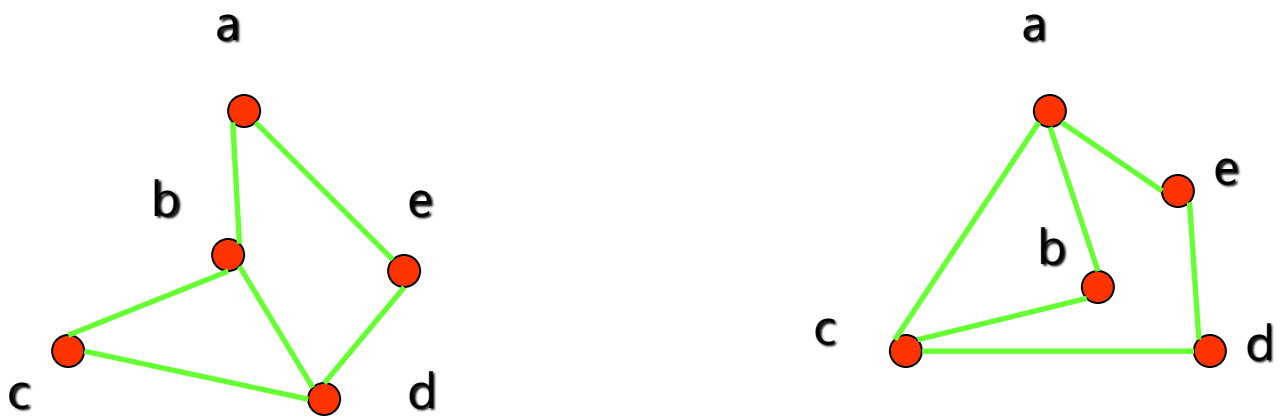
- The simple graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic if there is a bijection (a one-to-one and onto function) f from V_1 to V_2 with the property that a and b are adjacent in G_1 if and only if $f(a)$ and $f(b)$ are adjacent in G_2, for all a and b in V_1.
- Such a function f is called an isomorphism.
- In other words, G_1 and G_2 are isomorphic if their vertices can be ordered in such a way that the adjacency matrices $M(G_1)\ and\ M(G_2)$ are identical.

Isomorphism of Graphs

- For this purpose, we can check invariants, that is, properties that two isomorphic simple graphs must both have.
- For example, they must have
  - The same number of nodes,
  - the same number of edges,
  - And the same degrees of nodes.
- Note that two graphs that differ in any of these invariants are not isomorphic, but two graphs that match in all of them are not necessarily isomorphic.

Isomorphism of Graphs: Example 1

- Are the following two graphs isomorphic?

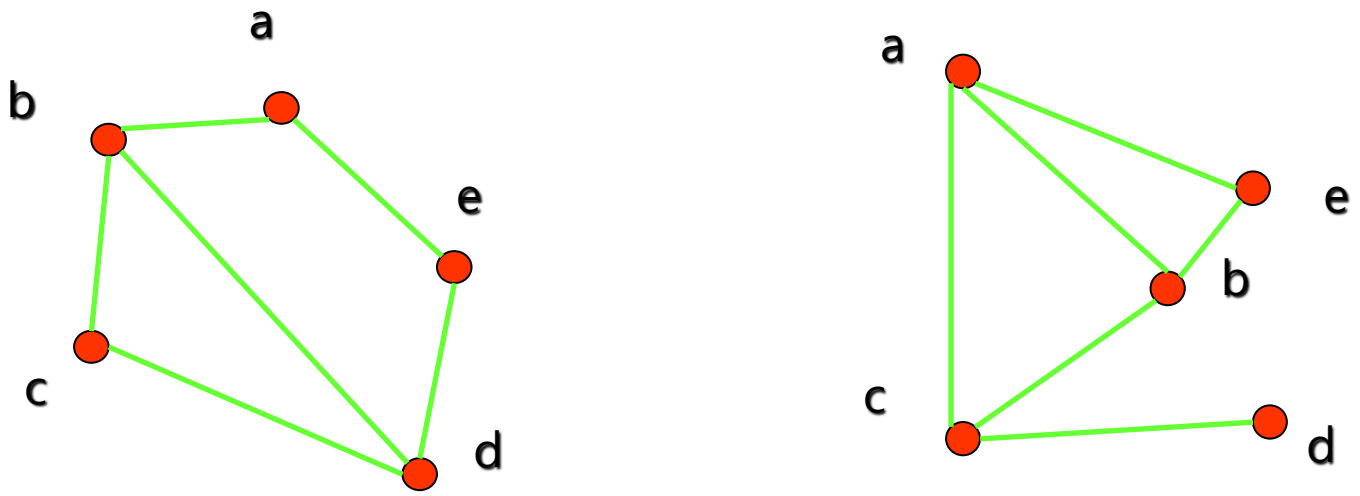


- **Solution**: Yes, they are isomorphic, because they can be arranged to look identical.
- You can see this if in the right graph you move vertex b to the left of the edge {a, c}. Then the isomorphism f from the left to the right graph is

$$f(a) = e,\ f(b) = a,\ f(c) = b,\ f(d) = c,\ f(e) = d.$$

Isomorphism of Graphs: Example 2

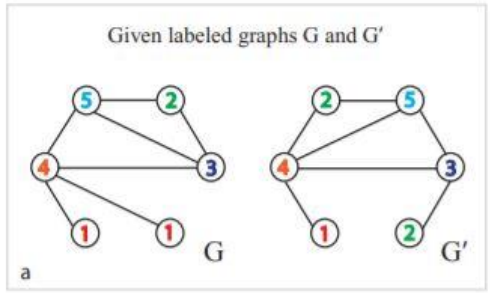
- Are the following two graphs isomorphic?

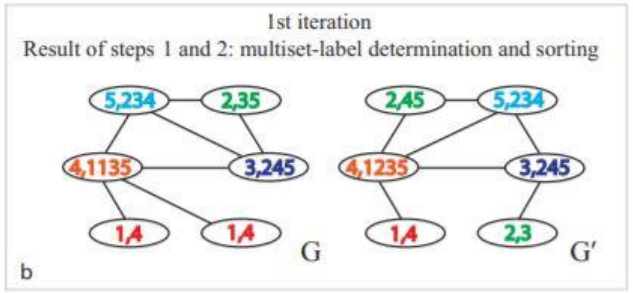


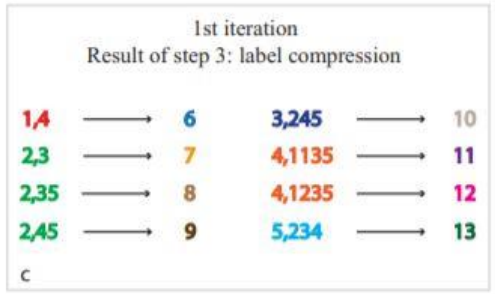
- **Solution**: No, they are not isomorphic, because they differ in the degrees of their vertices.
- Vertex d in right graph is of degree one, but there is no such vertex in the left graph.

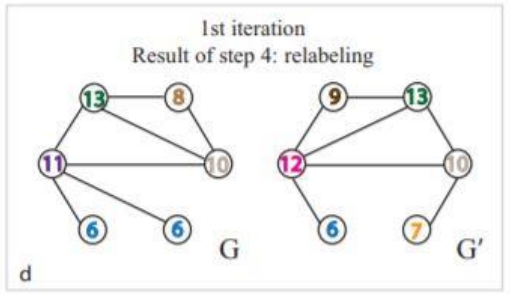
The Weisfeiler-Lehman Isomorphism Test

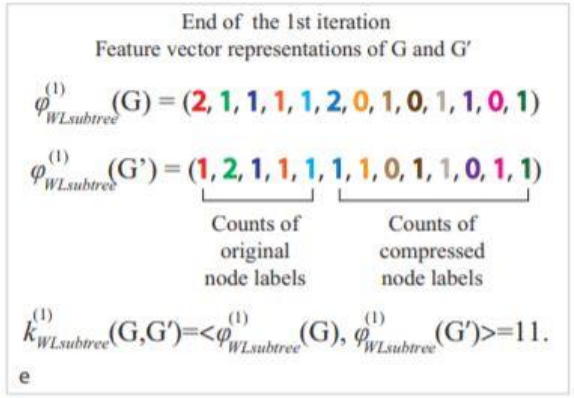
- Weisfeiler-Lehman Isomorphism Testing:









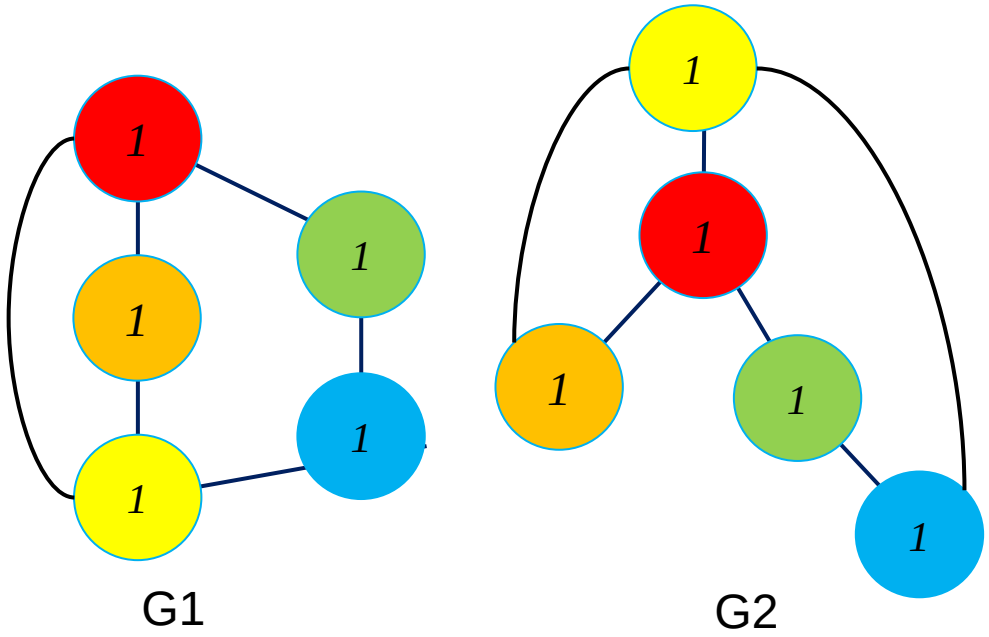


Algorithm 1: WL-1 algorithm (Weisfeiler & Lehmann, 1968)

Input: Initial node coloring $(h_1^{(0)}, h_2^{(0)}, ..., h_N^{(0)})$
Output: Final node coloring $(h_1^{(T)}, h_2^{(T)}, ..., h_N^{(T)})$
$t \leftarrow 0$;
repeat
  for $v_i \in \mathcal{V}$ **do**
    $h_i^{(t+1)} \leftarrow \text{hash}\left(\sum_{j \in \mathcal{N}_i} h_j^{(t)}\right)$;
  $t \leftarrow t + 1$;
until *stable node coloring is reached*;

The Weisfeiler-Lehman Isomorphism Test

- We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a m eans of illustrating the test.
- Step 1: Set node label =1 for all nodes



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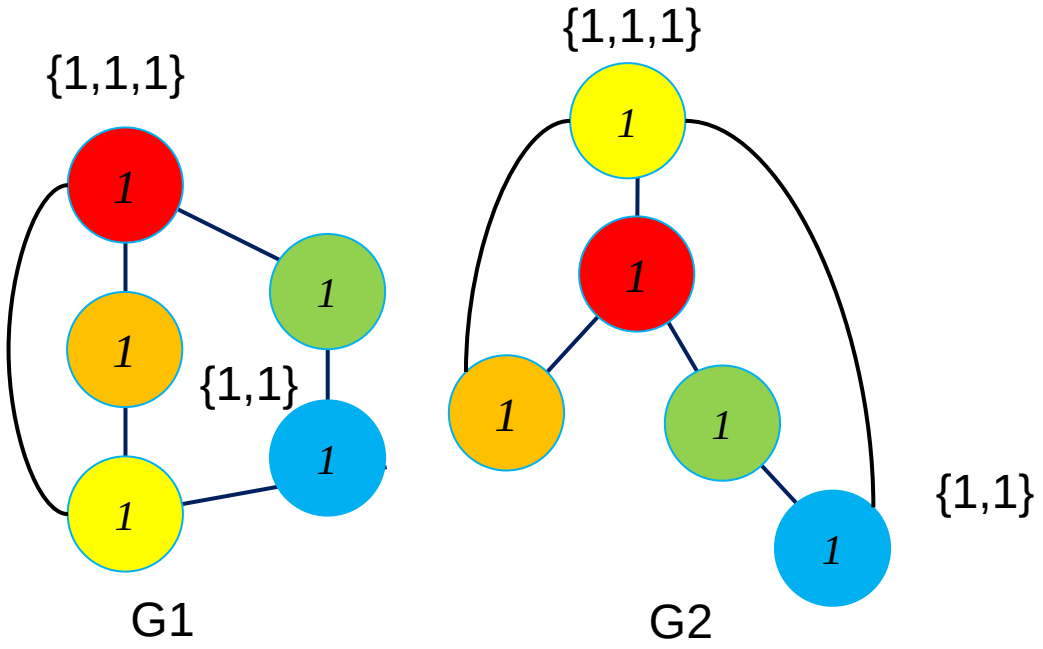
- Step 1: Set node label =1 for all nodes
- Step 2: Compute multiset of the neighboring nodes' compressed labels.



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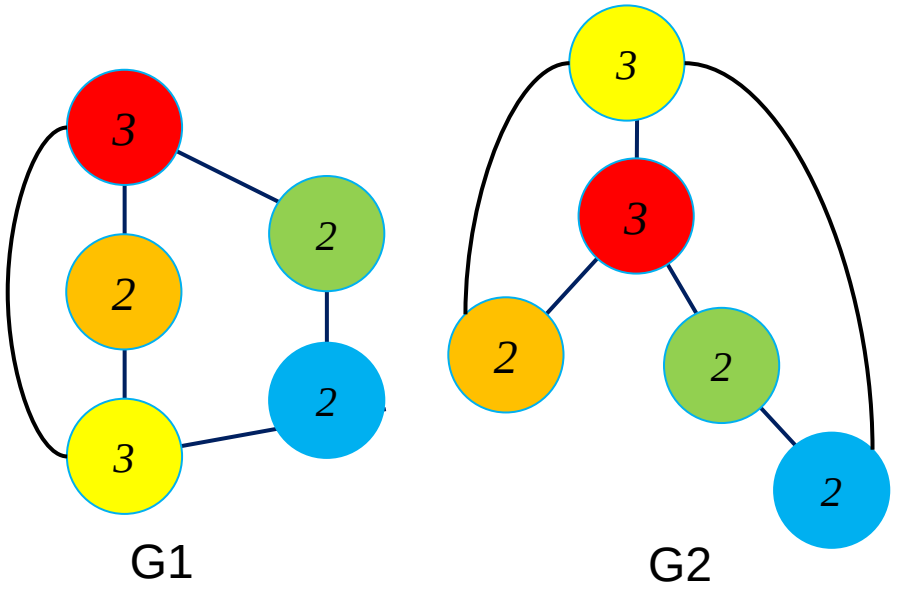

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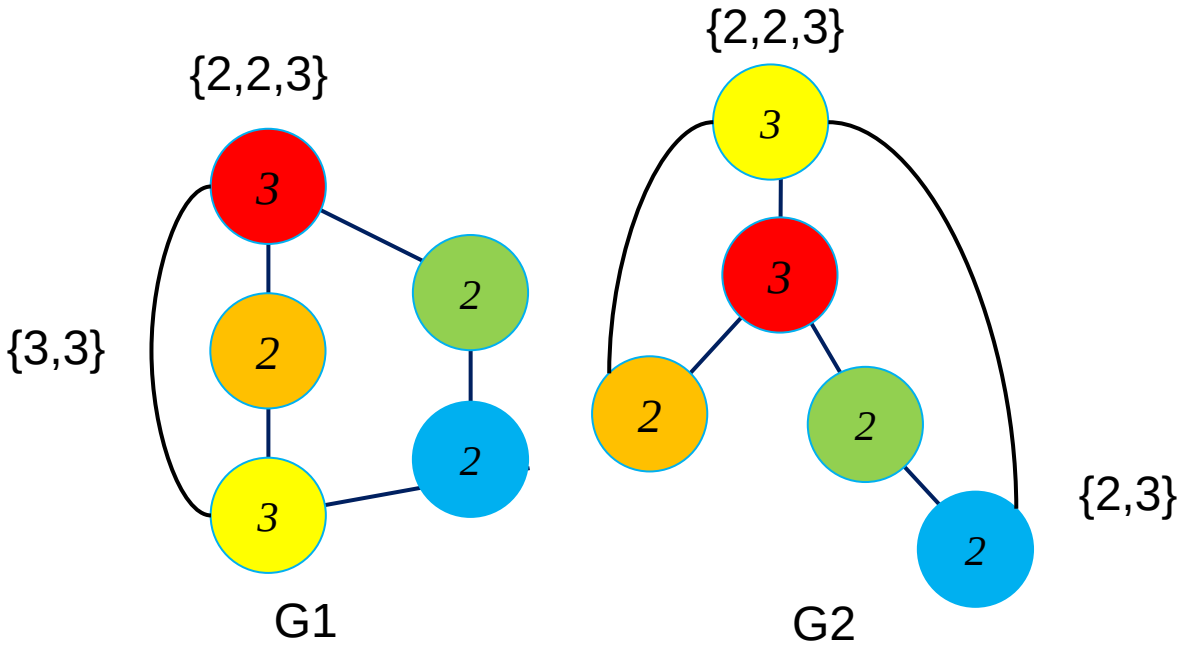
- Step 2: Compute multiset of the neighboring nodes' compressed labels.
- Step 3: Continuous.



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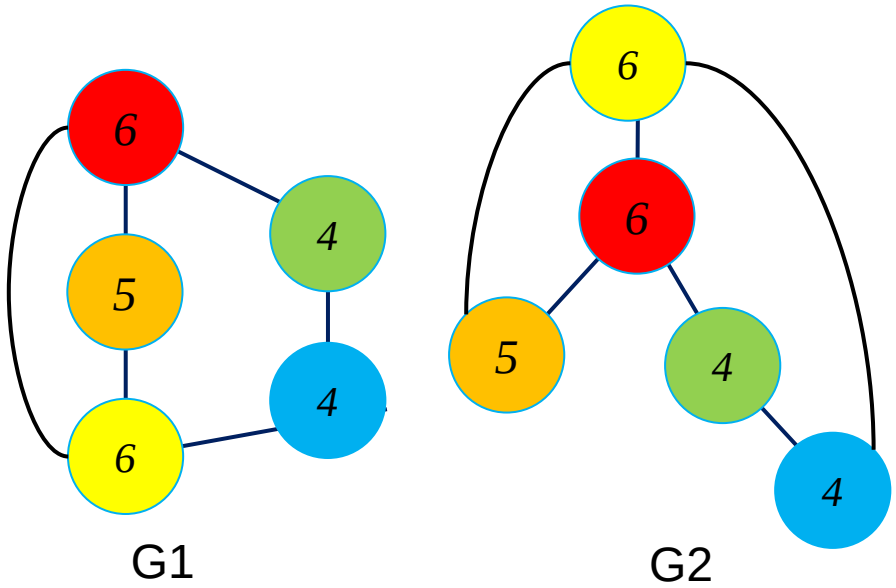

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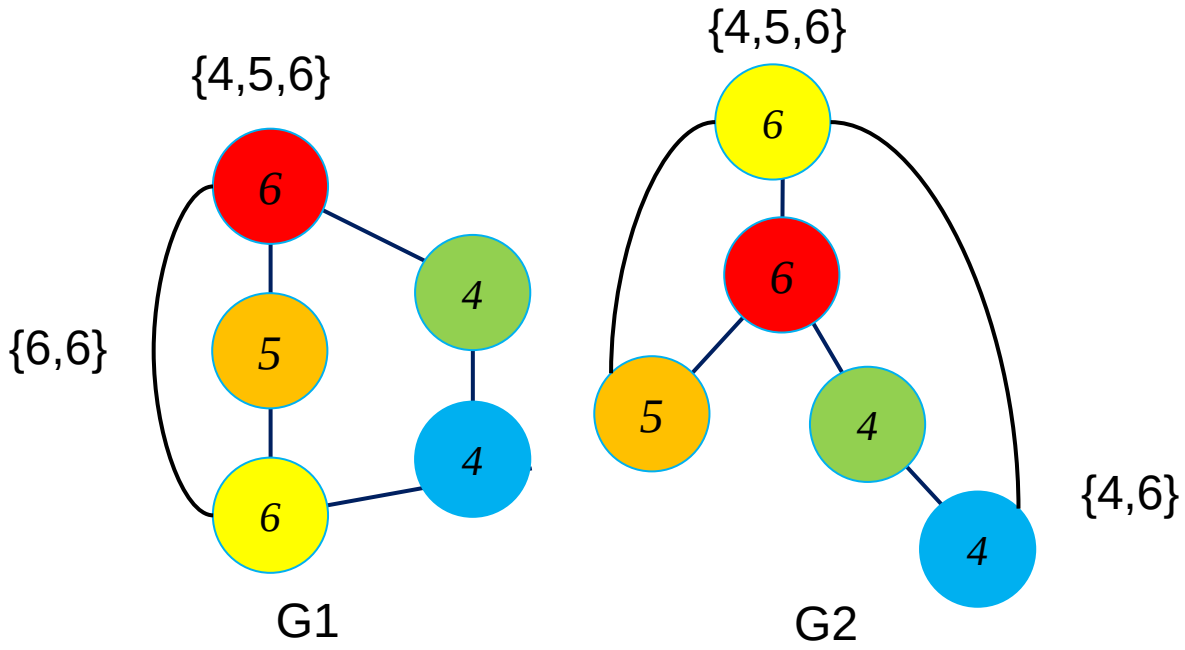

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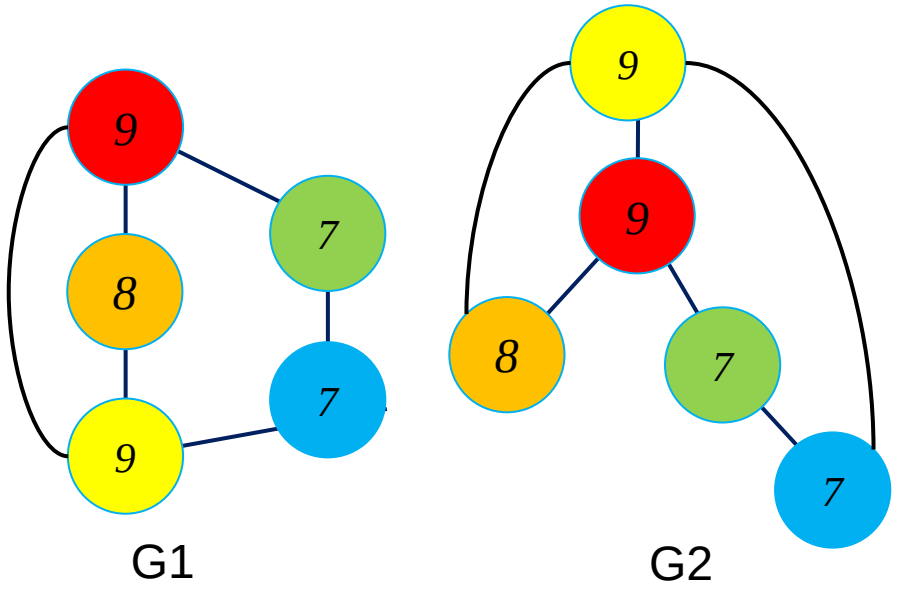
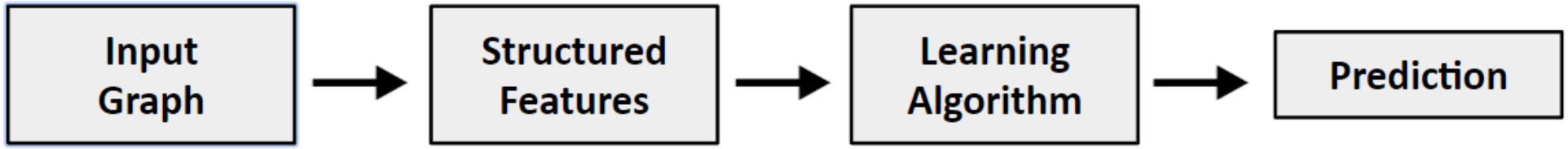
- Step 1: Set node label =1 for all nodes
- Step 2: Compute multiset of the neighboring nodes' compressed labels.
- Step 3: Continuous….
- Step 4: Since the partition of nodes by compressed label has not changed, we m ay terminate the algorithm here



- Given a graph, we can extract node, edge, graph-level features from the graph, then learn a model to map the features to the desired labels.



Feature Engineering

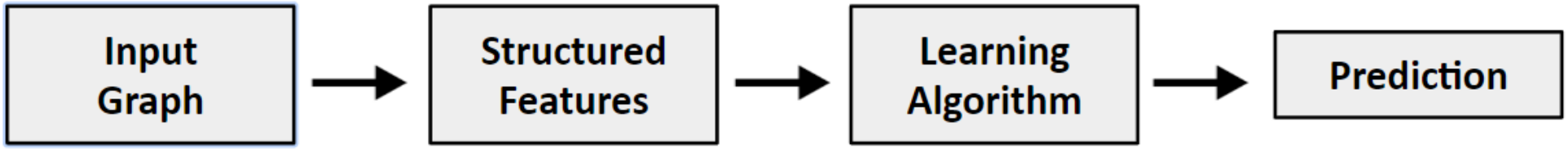
- Node feature
- Edge feature
- Graph feature

- SVM
- Random Forest
- XGBoost
- DNN

- Node-level
- Edge-level
- Graph-level

Graph Representation Learning

- Graph Representation Learning aims to generate graph representation vectors that describe graph's structure.
- We don't need to do feature engineering every single time.



Feature Engineering

Representation Learning

learn the features by itself

- SVM
- Random Forest
- XGBoost
- DNN

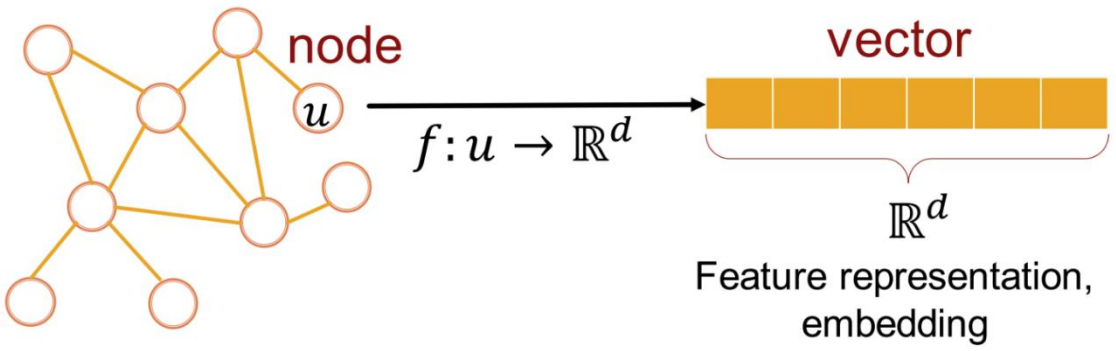
- Node-level
- Edge-level
- Graph-level

Why Embeddings?

- Graph Representation Learning's **goal**: Learn efficient task-independent feature for machine learning with graphs

  → Map nodes into an embedding space.

- Similarity of embeddings between nodes indicates their similarity in the network.
  - Example: both nodes are close to each other (connected by an edge).
- For simplicity, no node features or extra information is used.



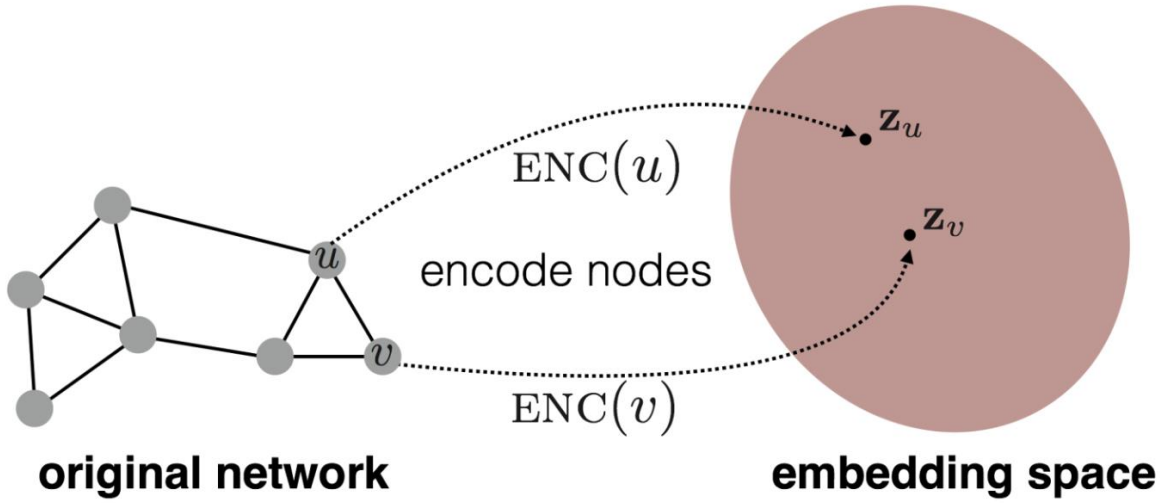
Tasks

- Node classification/regression
- Edge prediction
- Graph classification/regression.
- Graph clustering
- …

- Goal: Encode nodes → similarity in embedding space (dot product) ≈ similarity in the original graph

$$\underbrace{\text{similarity}(u, v)}_{\text{in the original network}} \approx \underbrace{\mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u}_{\text{Similarity of the embedding}}$$

We need to define:
ENC(u)
Similarity(u, v)



https://snap-stanford.github.io/cs224w-notes/machine-learning-with-networks/node-representation-learning

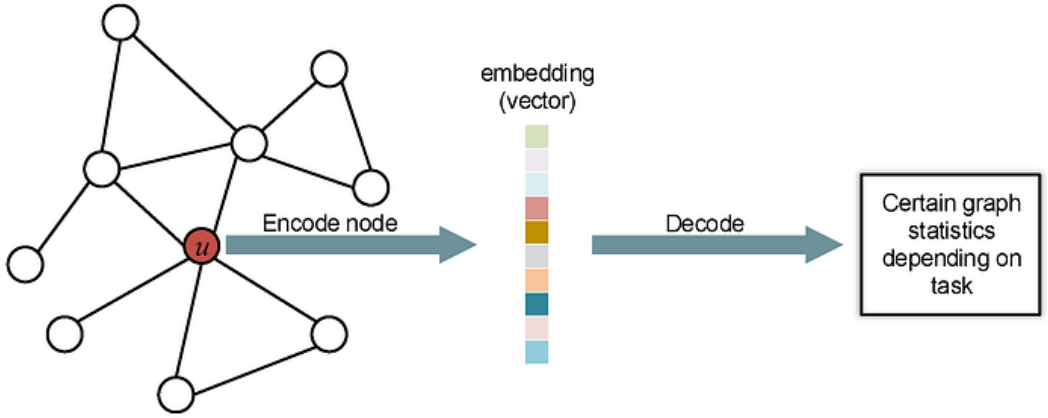
Learning Node Embeddings

- Encoder: node → embedding (d-dimensional vector, ENC(v) = Z_v)
- Decoder: map embedding → similarity score (dot product)
- Define a node similarity function:
  - whether 2 nodes are close in the graph, and how close are they?

Dot product between node embedding

- Optimize → $\underbrace{\text{similarity}(u, v)}_{\text{in the original network}} \approx \underbrace{\mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u}_{\text{Similarity of the embedding}}$

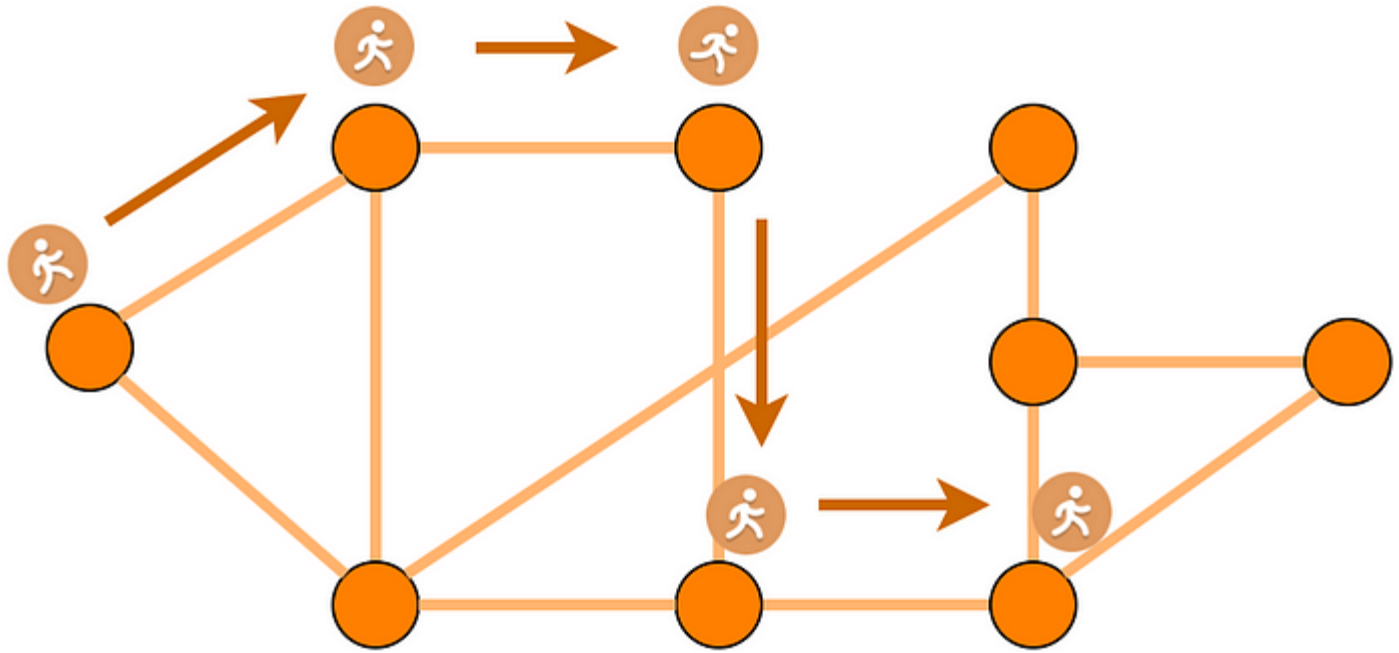
  - Maximize $\boldsymbol{z}_v^T \boldsymbol{z}_u$ for node pairs (u, v) that are similar.



https://medium.com/the-modern-scientist/graph-neural-networks-series-part-3-node-embedding-36613cc967d5

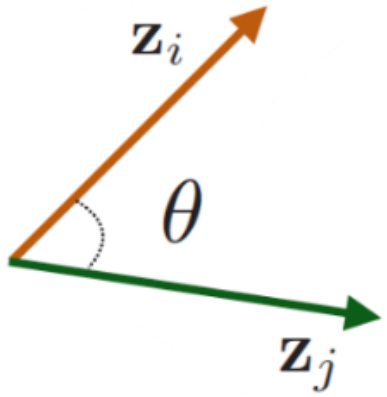
Random Walk

- Given a graph and a starting point, we select a neighbour of it at random, and move to this neighbour.
- Then, we select a neighbor of this point at random, and move to it,…
- The random sequence of nodes visited this way is **a random walk on the graph**

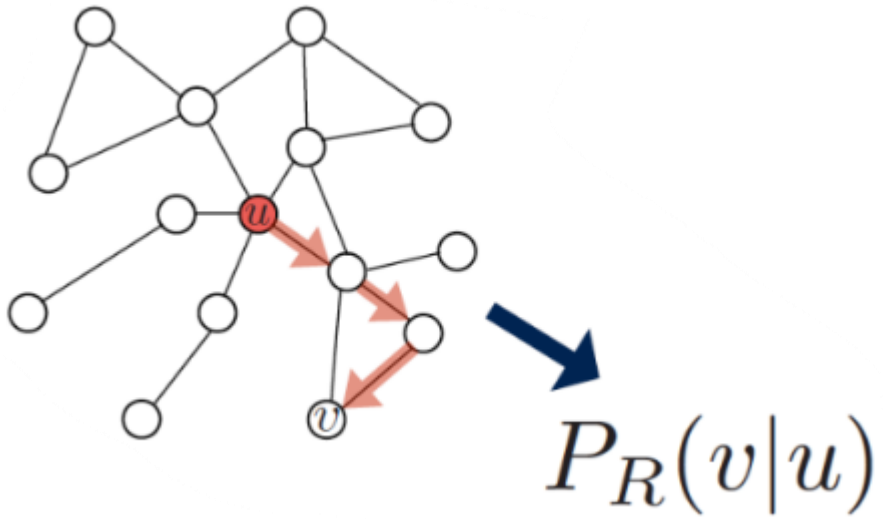


https://medium.com/analytics-vidhya/an-intuitive-explanation-of-deepwalk-84177f7f2b72

- Estimate probability of visiting node v on a random walk starting from node u using some random walk strategy R.
- Optimize embeddings to encode these random walk statistics.



$$\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v \approx$$



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Random Walk Optimization

- Run short random walks starting from each node on the graph using some strategy R.
- For each node u collect N(u), the multiset* of nodes visited on random walks starting from u.
- Optimize embeddings to according to:

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u))$$

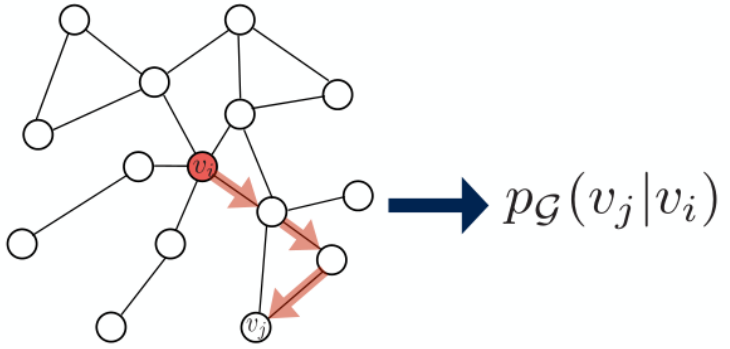
- * N(u) can have repeat elements since nodes can be visited multiple times on random walks.

Simple Random Walk on Network

- Employ short random walks on the graph to discover the structure

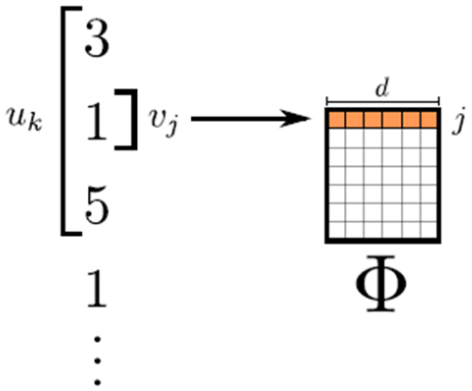
$$v_4 \rightarrow v_3 \rightarrow v_1 \rightarrow v_5 \rightarrow v_1 \rightarrow v_{46}$$

Random walks in Network
=
Sentences in NLP



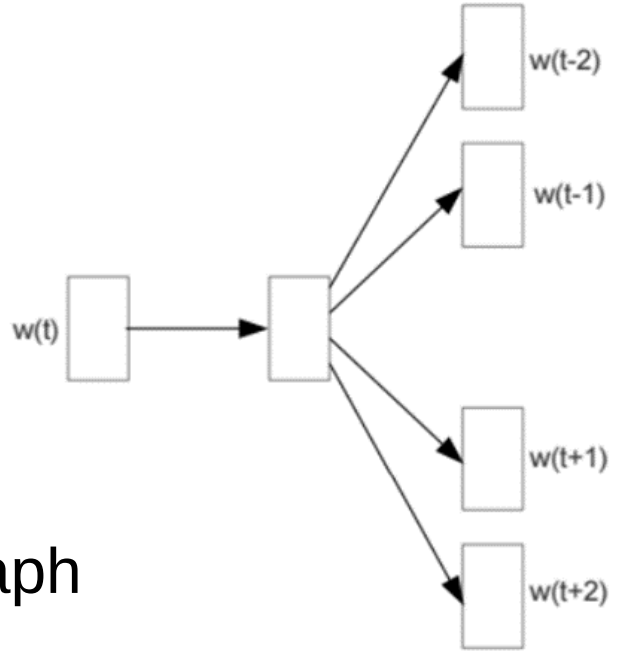
1. Run random walks to obtain co-occurrence statistics.

The quick brown fox jumps over the lazy dog.



Node sequence as the input of word2vec models

$$\Phi : v \in V \mapsto \mathbb{R}^{|V| \times d}$$

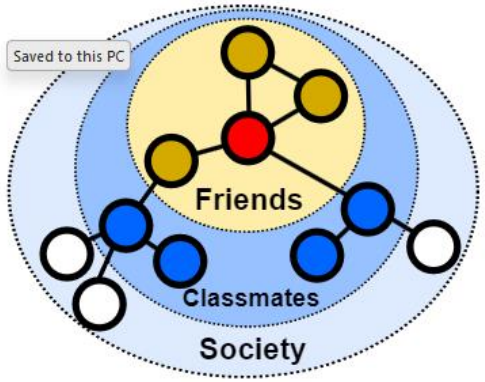


Short random walk is not sufficient in large scale graph

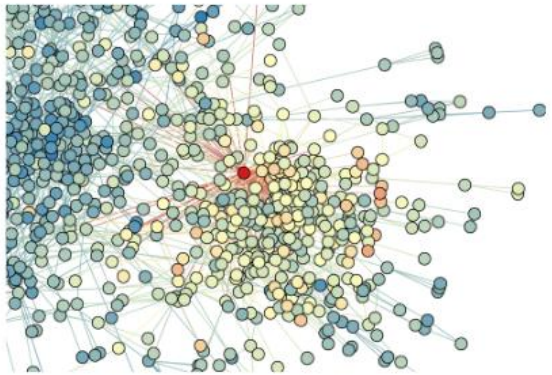
Bryan Perozzi et al: DeepWalk: Online Learning of Social Representations.

Don’t Walk – Skip! Online Learning of Multi-scale Network Embeddings

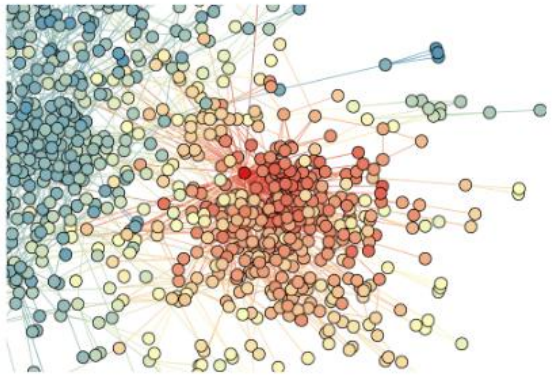
- **Problem**: DeepWalk learn a single global representation that conflates information across all scales.
  - Not sufficient in large scale graph.
- **Idea**: Multiple Scales of Random Walks at different scales to explicitly deal with large graph.
- **Solutions**: Propose WalkLets algorithm with skipping mechanism.



(a) A student (in red) is a member of several increasing larger social communities.



(b) WALKLETS Fine Representation



(c) WALKLETS Coarse Representation

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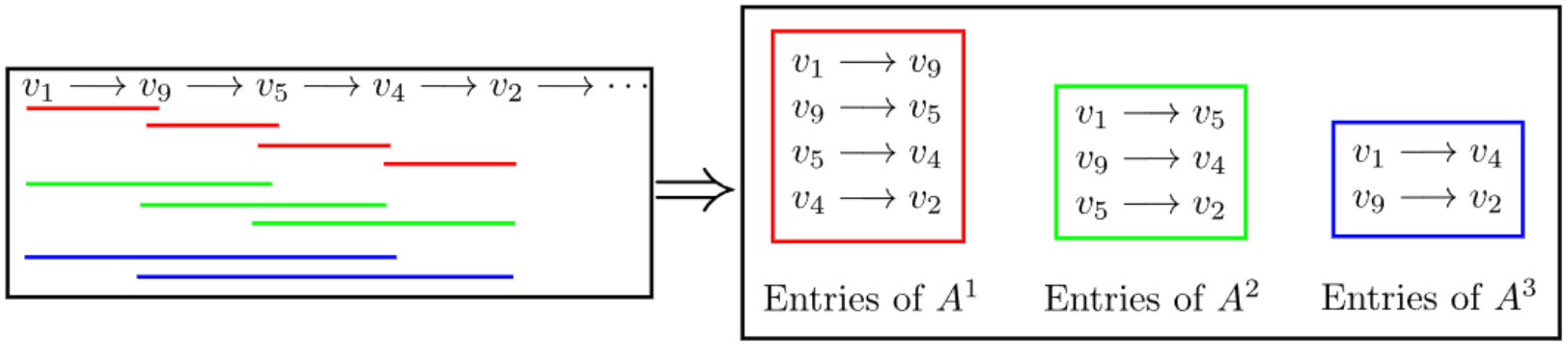
WalkLets: Algorithm

- Generates truncated random walks on the graph, but "skips" over nodes at different scales.
  - results in multiple "corpora" of node co-occurrences at different scales
- Using skip-gram models to learns separate embeddings from each of these corpora.
  - learns multiple embeddings capturing relationships at different scales explicitly.
- Optimization by Stochastic Gradient Descent.



Random walk, rooted at v_1

WALKLETS corpus of skipped random walks

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WalkLets: Optimization using Stochastic Gradient Descent

- Optimize embeddings to maximize likelihood of random walk co-occurrences.

$$J = -\sum_{v_i, v_j \in C_k} \log \Pr(v_i | v_j)$$

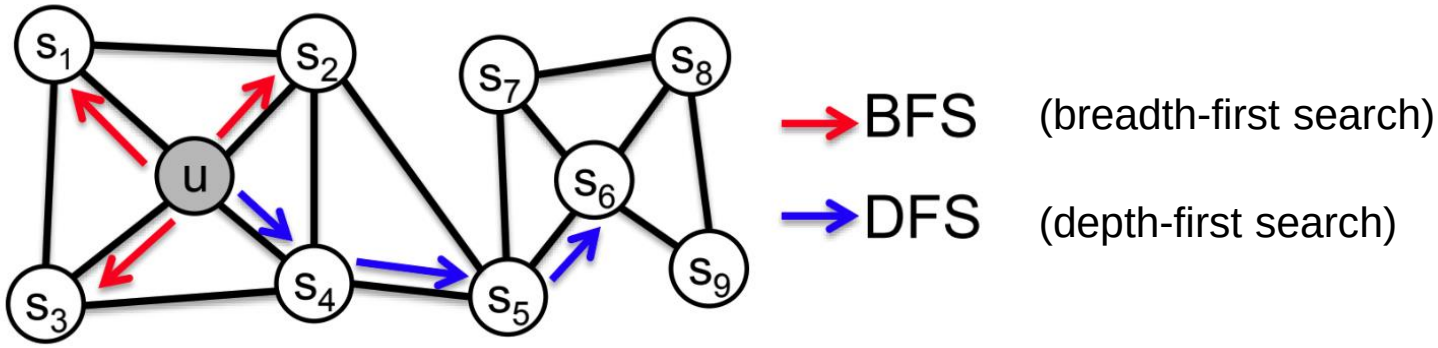
- (Stochastic) Gradient Descent: a simple way to minimize J.
- **SGD Algorithm:** evaluate it for each individual training example
  - Initialize z_u at some randomized value for all nodes u.
  - Iterative until J converges:
    - Sample a node u, for all v calculate the derivative $\frac{\partial J^{(u)}}{\partial z_v}$.
    - For all v, update:

$$z_v \leftarrow z_v - \eta \frac{\partial \mathcal{L}^{(u)}}{\partial z_v}$$

Learning rate

Node2vec: Biased Walks

- **Idea**: Use flexible, **biased random walks** that can trade-off between local and global views of the network (Grover and Leskovec, 2016).
- Two classic strategies to define a neighborhood $N_R(\boldsymbol{u})$ of a given node u



- Walk of length ($N_R(\boldsymbol{u})$ of size 3):

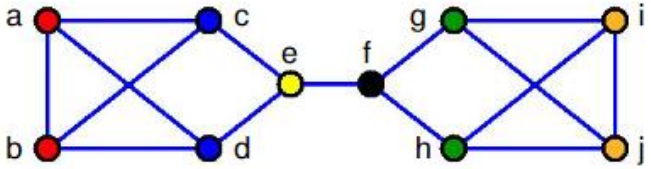
$$N_{BFS}(u) = \{s_1, s_2, s_3\}$$ **Local view**

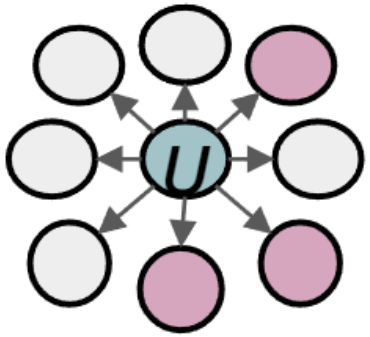
$$N_{DFS}(u) = \{s_4, s_5, s_6\}$$ **Global view**

node2vec: Scalable Feature Learning for Networks

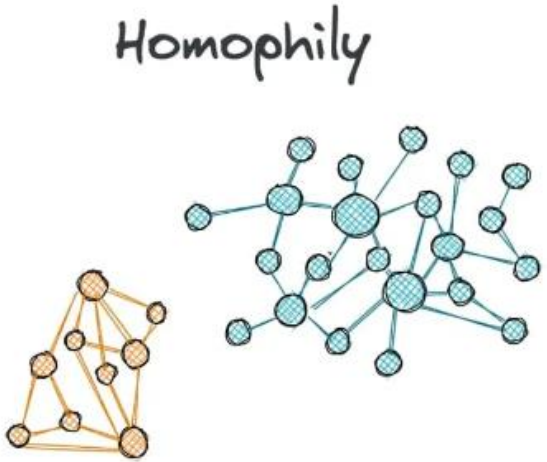
Node2vec: Homophily with Interpolating BFS and DFS

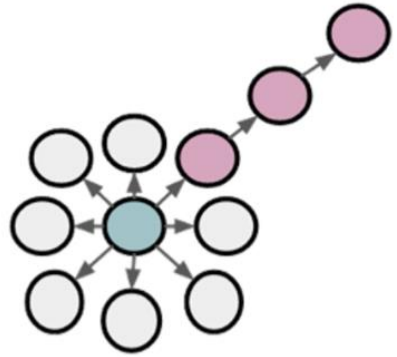
- **Structural Equivalence:** if and only if they have the same structure.
- **Homophily:** tendency of individuals to associate and bond with similar others.
  - Neighborhoods sampled by **BFS** corresponding to **structural** equivalences.
  - **DFS** explore macro-view of the network, which infers communities: **homophily** equivalence.





BFS





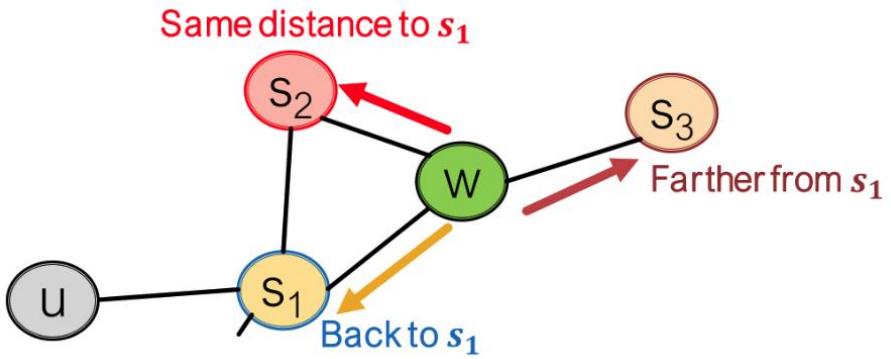
DFS

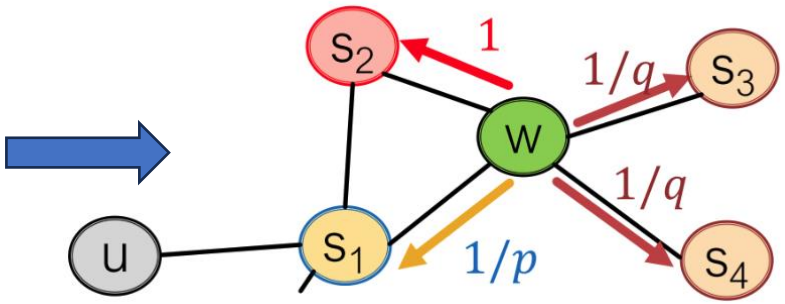
- Biased fixed-length random walk R that given a node u generates neighborhood $N_R(u)$.
  - Two parameters of random walks:
    - Return parameter p: Return to the previous node.
    - In-out parameter q: Moving outwards (DFS) vs. inwards (BFS) from the previous node.

SERGEY IVANOV: GML Newsletter: Homophily, Heterophily, and Oversmoothing for GNNs

Node2vec: Biased Random Walk

- Biased 2nd-order random walks explore network neighborhood.
- Walker just traversed edge (s_1, w) and is at w, now he/she can go using a bias probability:





1/p, 1, 1/q are unnormalized probs.
p: return parameter.
q: "walk away" parameter.

- BFS-like walk: Low value of p
- DFS-like walk: Low value of q

	Target t	Prob.	Dist. (s_1, t)
w →	s_1	$1/p$	0
	s_2	1	1
	s_3	$1/q$	2
	s_4	$1/q$	2

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LINE: Large-scale Information Network Embedding

- **Motivation**:
  - Preserving network proximities: LINE seeks to preserve both the **first-order proximity** (direct connections between nodes) and **second-order proximity** (shared neighborhood structures) in the learned embeddings.
  - Scalable objective functions:
    - consider first-order and second-order proximities separately.
    - different network types: directed, undirected, weighted or unweighted.
  - An edge-sampling algorithm is proposed to help stochastic gradient descent on weighted edges.

LINE: First-order Proximity and Preserving the First-order Proximity

- First-order proximity: local pairwise proximity between two connected nodes.
- For each node pair (v_i, v_j)
  - if $(v_i, v_j) \in E$, the first-order proximity between v_i and v_j is w_{ij}.
  - otherwise, the first-order proximity between v_i and v_j is 0.
- Given an undirected edge (v_i, v_j), the joint probability of v_i and v_j:

$$p_1(v_i, v_j) = \frac{1}{1 + \exp(-\vec{u}_i^T \cdot \vec{u}_j)}$$

$\vec{u}_i$:Embedding of node v_i

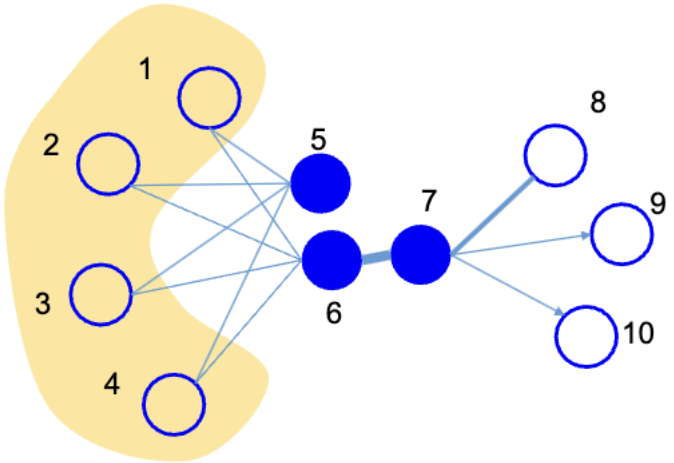
$$\hat{p}_1(v_i, v_j) = \frac{w_{ij}}{\sum_{(i',j')} w_{i'j'}}$$

- Objective:

KL-divergence

$$O_1 = d(\hat{p}_1(\cdot,\cdot), p_1(\cdot,\cdot))$$

$$\propto -\sum_{(i,j)\in E} w_{ij} \log p_1(v_i, v_j)$$



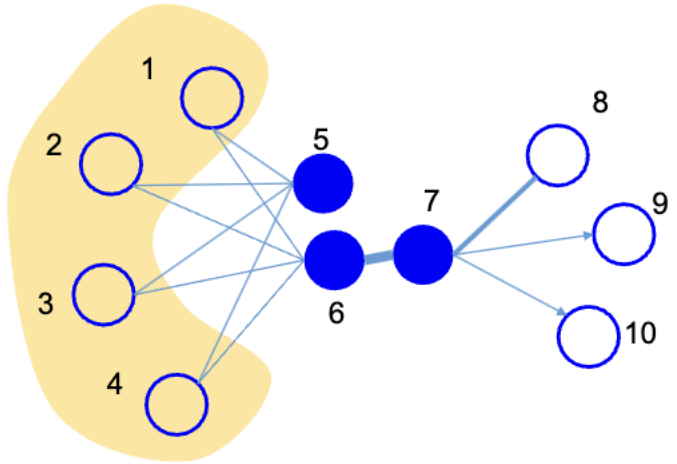
First-order: node 6 and 7

Jian Tang et al.: Asymmetric Transitivity Preserving Graph Embedding

LINE: Second-order Proximity

- Second-order proximity: captures the 2-step relations between each pair of nodes.
- For each node pair (v_i, v_j)
  - determining by the number of common neighbors shared by the two nodes.

$$\hat{p}_u = (w_{u1}, w_{u2}, \dots, w_{u|V|})$$
$$\hat{p}_v = (w_{v1}, w_{v2}, \dots, w_{v|V|})$$



Node **5** and **6** have a large second-order proximity

$\hat{p}_5 = (1,1,1,1,0,0,0,0,0,0)$

$\hat{p}_6 = (1,1,1,1,0,0,1,0,0,0)$

Jian Tang et al.: Asymmetric Transitivity Preserving Graph Embedding

LINE: Preserving the Second-order Proximity

- Given an undirected edge (v_i, v_j), the joint probability of v_i and v_j:

$$p_2(v_j|v_i) = \frac{\exp(\vec{u}_j'^T \cdot \vec{u}_i)}{\sum_{k=1}^{|V|} \exp(\vec{u}_k'^T \cdot \vec{u}_i)},$$

$\vec{u}_i$:Embedding of node v_i when i is a source node.

$\overrightarrow{u_i'}$:Embedding of node v_i when i is a target node.

$$\hat{p}_2(v_j|v_i) = \frac{w_{ij}}{\sum_{k \in V} w_{ik}}$$

- Objective:

λ_i: Prestige of node in the network $\lambda_i = \sum_j w_{ij}$

$$O_2 = \sum_{i \in V} \lambda_i d(\hat{p}_2(\cdot|v_i), p_2(\cdot|v_i)),$$

$$\propto -\sum_{(i,j) \in E} w_{ij} \log p_2(v_j|v_i).$$

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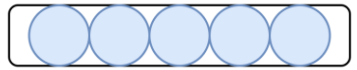
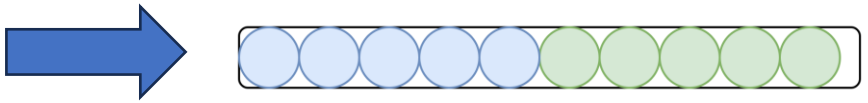
LINE: Preserving both the Proximity

- Concatenate the embeddings individually learned by the two proximity:

First-order:





Second-order:

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LINE: Optimization

- Stochastic Gradient Descent + Negative Sampling.
  - Randomly sample an edge and multiple negative edges.
- The gradient w.r.t the embedding with edge (i,j)

$$\frac{\partial O_2}{\partial \vec{u}_i} = w_{ij} \cdot \frac{\partial \log p_2(v_j|v_i)}{\partial \vec{u}_i}$$

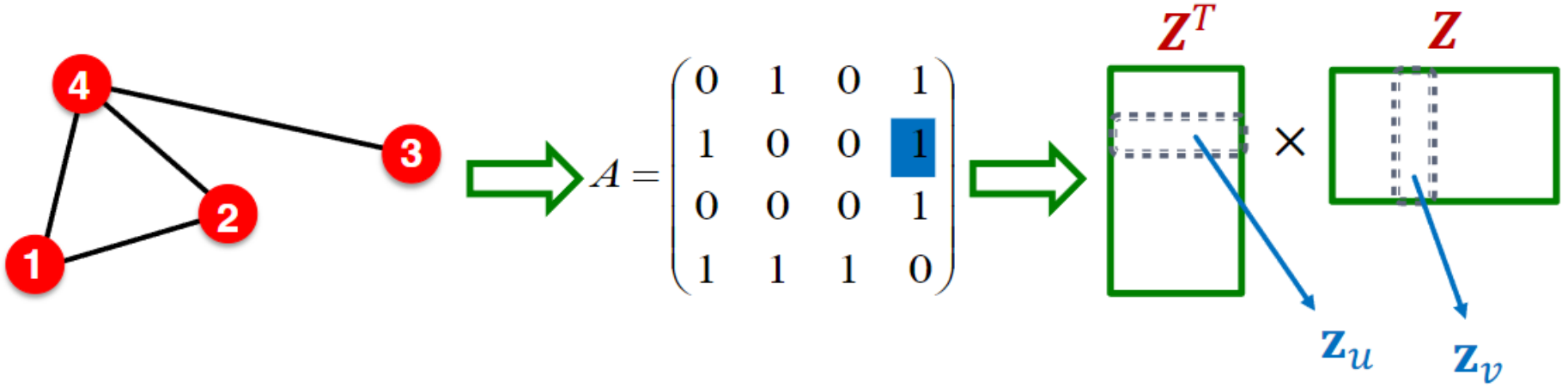
Multiplied by the weight of the edge w_{ij}

- Problematic when the weights of the edges diverge
  - The scale of the gradients with different edges diverges.
- **Solution:** Edge sampling
  - Sample the edges according to their weights and treat the edges as binary.
- Complexity: $\Theta(dK|E|)$
  - Linear to the dimension d, number of negative samples K, and number of edges E.

Adjacency-based Approaches

- One of the simplest and most intuitive approaches to defining similarity:
  - adjacency between two nodes v and u.
- Similarity: Two nodes are adjacent to one another within the structure of the graph.

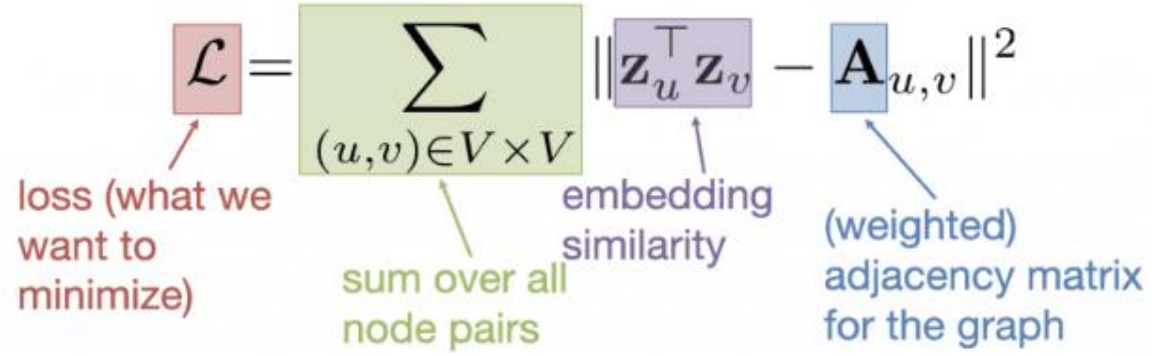
$$\boldsymbol{z}_v^T \boldsymbol{z}_u = A_{u,v} \; or \; \boldsymbol{Z}^T \boldsymbol{Z} = A$$



https://snap-stanford.github.io/cs224w-notes/machine-learning-with-networks/node-representation-learning

Adjacency-based Approaches

- Encoding: Find the embedding matrix **Z** that minimizes the loss function **L**



- Solution:
  - Option 1: Use stochastic gradient descent (SGD) as a general optimization method.
  - Option 2: Solve matrix decomposition solvers (e.g., SVD or QR decomposition routines).
    - Matrix Factorization-based.

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

- Let A be an m × n adjacency matrix. The factorization of A takes the form

$$A = USV^T$$

where U is a $m \times m$ orthogonal matrix, V^T is a $n \times n$ orthogonal matrix and S is a $m \times n$ diagonal matrix.

- Factorizing to low-rank approximations based on minimizing the sum-squared distance using **Singular Value Decomposition**.
- To decompose:
  - Evaluate the n eigenvectors v_i and eigenvalues λ_i of $A^T A$.
  - Make a matrix V from the normalized vectors v_i.
  - Make a diagonal matrix S from the square roots of the eigenvalues

$$\sigma_i = \sqrt{\lambda_i} \quad \text{and} \quad \sigma_1 \geq \sigma_2 \geq \sigma_3 \ldots$$

  - Find U: $A = USV^T \Rightarrow US = AV \Rightarrow U = AVS^{-1}$.

Asymmetric Transitivity Preserving Graph Embedding

- **Ideas**: Critical property in directed graph - Asymmetric Transitivity.
- Transitivity is Asymmetric in directed graph.
- **Challenge**: incorporate asymmetric transitivity in graph embedding.
- **Problem**: metric space is symmetric.

Asymmetric transitivity

Matrix space

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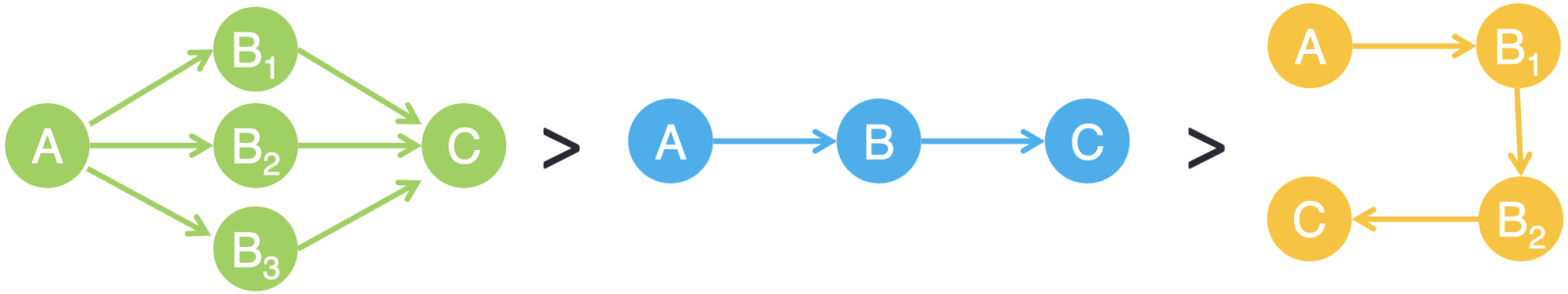
Asymmetric Transitivity Preserving Graph Embedding

- **High-order Proximity with asymmetric transitivity:**
  - Asymmetry: not symmetric in directed graph.
  - Transitivity:
    - More directed paths, larger similarity.
    - Shorter paths, larger similarity



  - Compare A -> C similarity: Katz Index.

$$\mathbf{S}^{Katz} = \sum_{l=1}^{+\infty} (\beta \cdot A)^l$$

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Asymmetric Transitivity Preserving Graph Embedding

- **Preserve high-order proximity embedding:**
  - Katz Index modified:

$$\boldsymbol{S}^{Katz} = \sum_{l=1}^{+\infty} (\beta \cdot A)^l = (I - \beta \cdot A)^{-1} \cdot (\beta \cdot A)$$

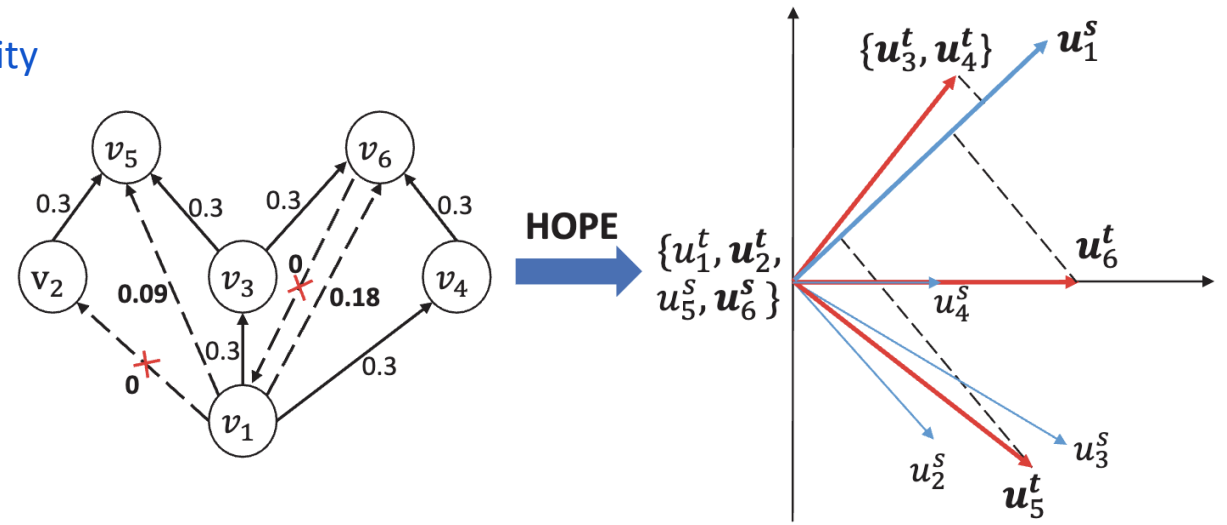
  - Objective:

Embedding similarity

$$\min_{U_s, U_t} \|\boldsymbol{S} - U_s \cdot U_t^T\|_F^2$$

$$\boldsymbol{S} = M_g^{-1} \cdot M_l$$

where M_g, M_l are polynomial of adjacency matrix or proximity measurements: Katz, Adamic Adar, PageRank, Common Neighbors.



- Solving by **Generalized Singular Value Decomposition**: decompose $\boldsymbol{S}$ without calculating it.
  - Linear complexity w.r.t. the volume of data (i.e. edge number).

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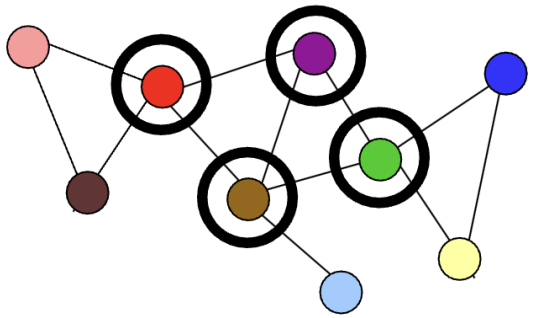
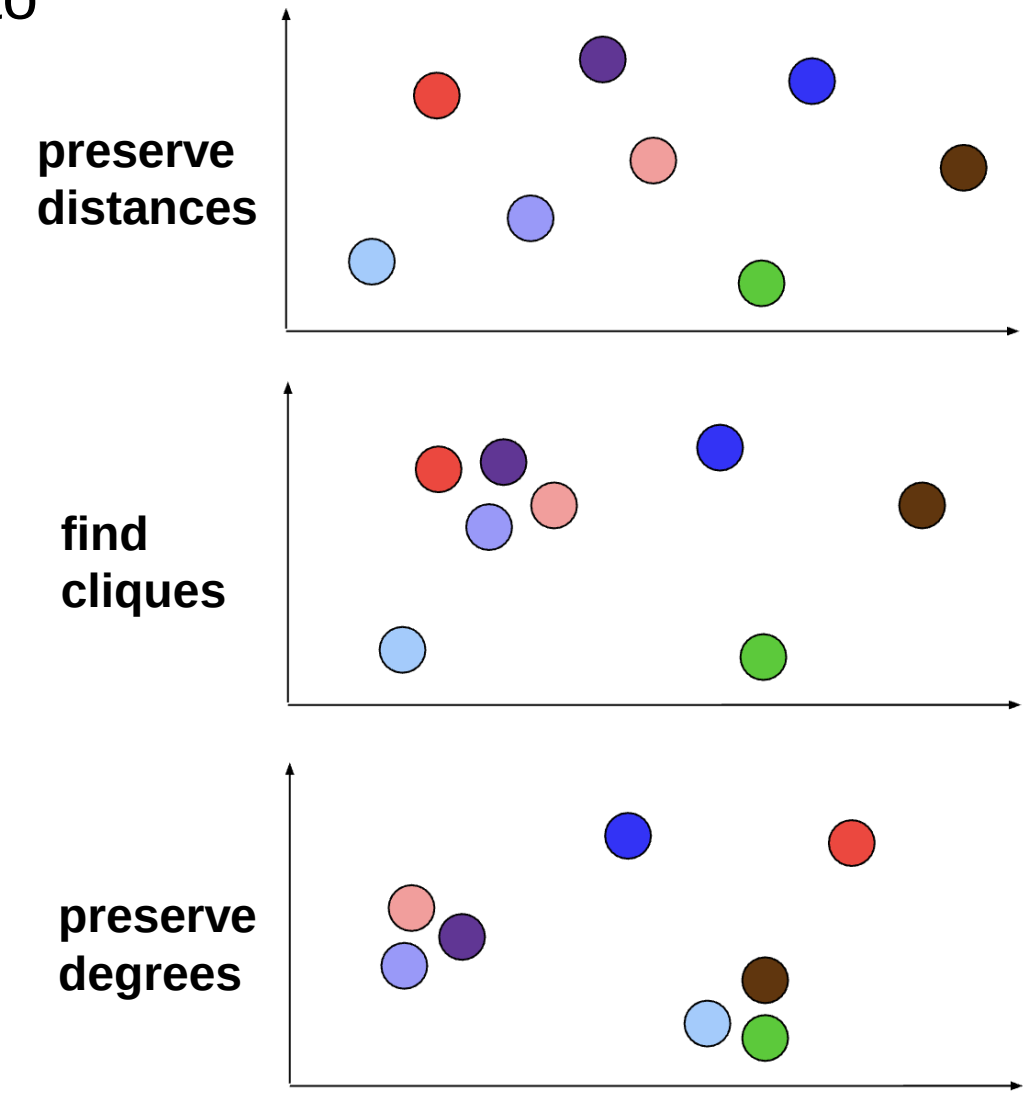
Node Representations and Structural Identity

- Network embedding: map network nodes into Euclidean space.
- Structural Identity:
  - Nodes in networks have specific roles
    - E.g., individuals, web pages, proteins, etc
  - Structural identity: identification of nodes based on network structure (no other attribute)
    - often related to role played by node
  - **Automorphism**: strong structural equivalence



Red, Green: automorphism.
Purple, Brown: structurally similar.



Leonardo F. R. Ribeiro et al: struc2vec: Learning Node Representations from Structural Identity

struc2vec: Learning Node Representations from Structural Identity

- **Ideas:** based on structural identity.
- Structural similarity does not depend on hop distance
  - neighbor nodes can be different, far away nodes can be similar.
- Structural identity as a hierarchical concept
  - depth of similarity varies.
- Flexible four step procedure
  - operational aspect of steps are flexible.

struc2vec: Step 1 - Structural Similarity

- $g(D_1,D_2)$: distance between two ordered sequences
  - cost of pairwise alignment: max(a, b) / min(a, b) - 1.
  - optimal alignment by Dynamic Time Warping (DTW) in our framework

$s(R_0(u)) = 4$ $s(R_1(u)) = 1,3,4,4$ $s(R_2(u)) = 2,2,2,2$

$s(R_0(v)) = 3$ $s(R_1(v)) = 4,4,4$ $s(R_2(v)) = 1,2,2,2,2$

$g(.\ ,\ .) = 0.33$ $g(.\ ,\ .) = 3.33$ $g(.\ ,\ .) = 1$

- $f_k(u,v)$: structural distance between nodes u and v considering first k rings
  - $f_k(u,v) = f_{k-1}(u,v) + g(s(R_k(u)), s(R_k(v)))$.

$f_0(u,v) = 0.33$ $f_1(u,v) = 3.66$ $f_2(u,v) = 4.66$

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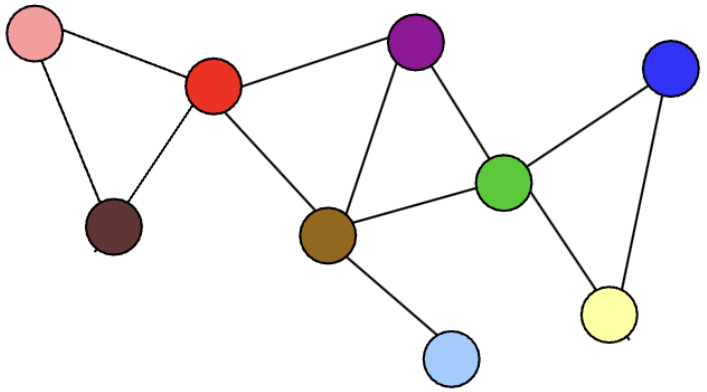
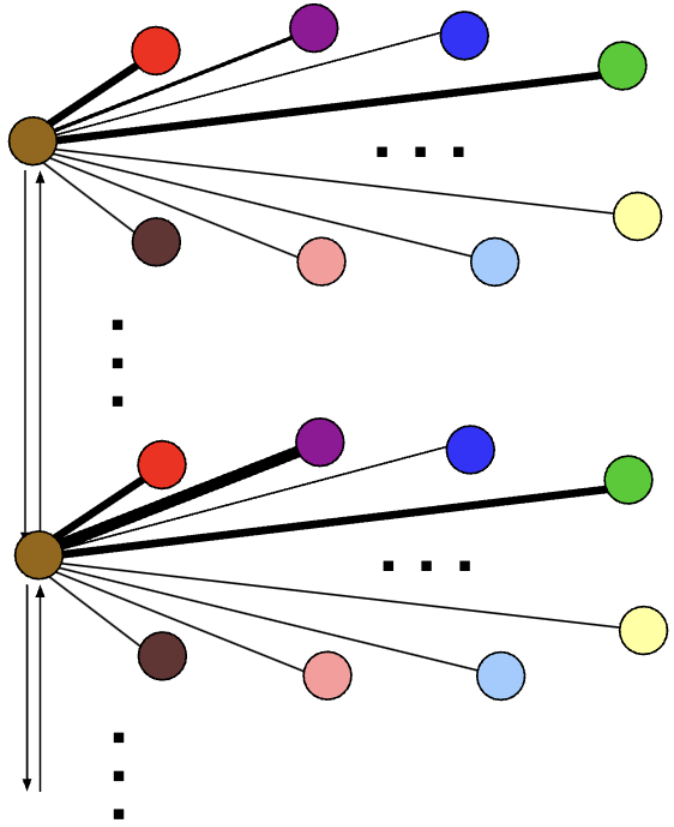
struc2vec: Step 2 - Multi-layer graph

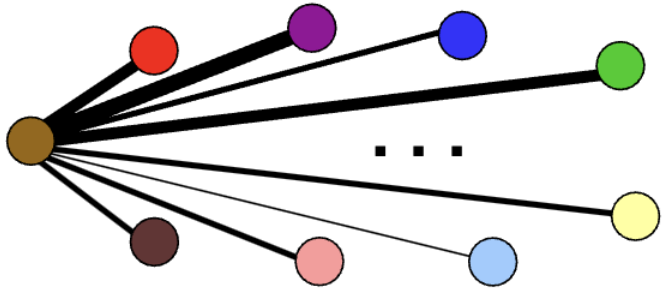
- Encodes structural similarity between all node pairs.



$$w(u_k, u_{k+1}) = \log(\Gamma_k(u) + e), \quad k = 0, \ldots, k^* - 1$$
$$w(u_k, u_{k-1}) = 1, \quad k = 1, \ldots, k^*$$



- Each layer is weighted complete graph
  - corresponds to similarity hierarchies. $\Gamma_k(u) = \sum_{v \in V} \mathbb{1}(w_k(u, v) > \overline{w_k})$
- Edge weights in layer k
  - $w_k(u, v) = e^{-f_k(u,v)}, \quad k = 0, \ldots, k^*$
- Connect corresponding nodes in adjacent layers



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struc2vec: Step 3 - Generate Context

- Context generated by biased random walk (same as Node2vec)
  - walking on multi-layer graph.
- Walk in current layer with probability p:
  - choose neighbor according to edge weight.
  - RW prefers more similar nodes.
- Change layer with probability 1-p
  - choose up/down according to edge weight.
  - RW prefer layer with less similar neighbors.

$$p_k(u,v) = \frac{e^{-f_k(u,v)}}{Z_k(u)}$$

where $Z_k(u)$ is the normalization factor for vertex u in layer k,

$$Z_k(u) = \sum_{\substack{v \in V \\ v \neq u}} e^{-f_k(u,v)}$$

$$p_k(u_k, u_{k+1}) = \frac{w(u_k, u_{k+1})}{w(u_k, u_{k+1}) + w(u_k, u_{k-1})}$$
$$p_k(u_k, u_{k-1}) = 1 - p_k(u_k, u_{k+1})$$

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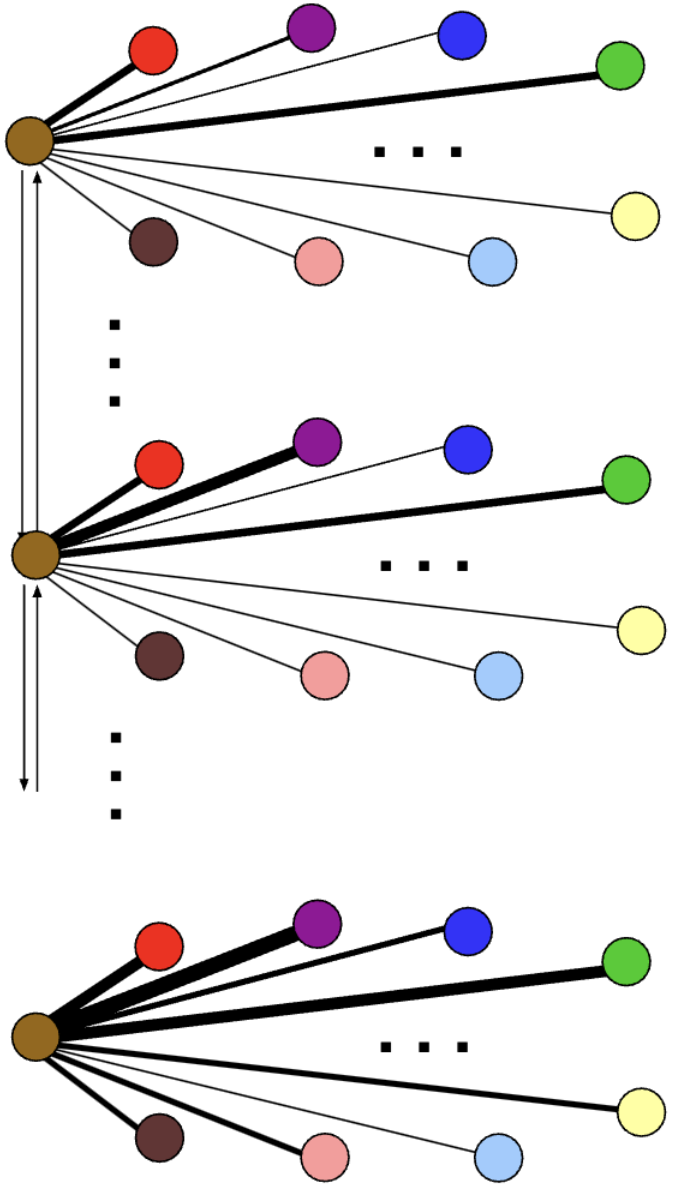
struc2vec: Step 4 – Learn Representation

- For each node, generate set of independent and relative short random walks
  - context for node; sentences of a language.

- Train a neural network to learn latent representation for nodes
  - maximize probability of nodes within context
  - Skip-gram (Hierarchical Softmax) adopted.



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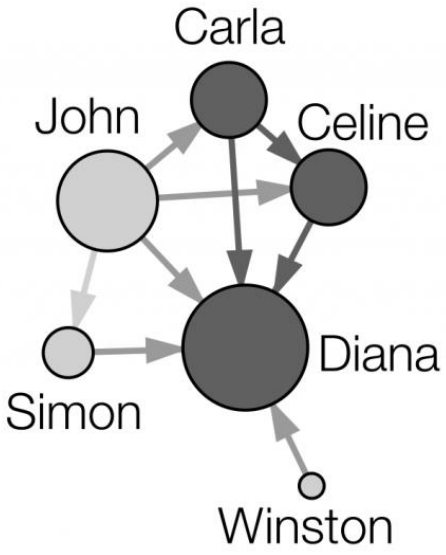
struc2vec: Optimization

- Reduce time to generate/store multi-layer graph and context for nodes:
  - Option 1: Reduce length of degree sequences
    - use pairs (degree, number of occurrences).
  - Option 2: Reduce number of edges in multi-layer graph
    - only log n neighbors per node.
  - Option 3: Reduce number of layers in multi-layer graph
    - fixed (small) number of layers.
  - Scales quasi-linearly
    - over 1 million nodes.

Leonardo F. R. Ribeiro et al: struc2vec: Learning Node Representations from Structural Identity

role2vec: Learning Role-based Graph Embeddings

- **Ideas**: struc2vec and conventional methods (DeepWalk, Node2vec) learn in node representation.
  - Role2Vec learns embeddings for "node types/roles" determined by node attributes/features.
- **Solution**: "attributed random walks"
  - maps nodes to node types/roles using node attributes like motif counts, degrees etc.
  - generates attributed random walks over the node types instead of node IDs.
  - Finally, it learns embeddings for the node types rather than individual nodes.



Nodes

Id,Label,Attribute
1,John,1
2,Carla,2
3,Simon,1
4,Celine,2
5,Winston,1
6,Diana,2

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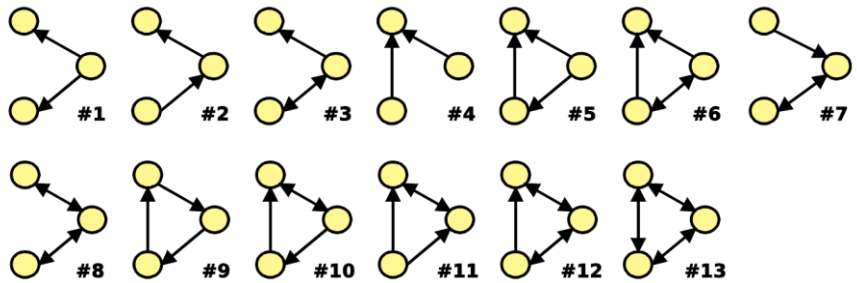
- Given a network, most of the time, some subgraphs are “overrepresented”.
- A connected graph that has many occurrences in a network is called a motif of the network.
- Assume set of occurrences G' in G is $occ_G(H)$.
  - cardinality of $occ_G(H)$ in G is frequent.
  - How to know if G' is frequent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

role2vec: Algorithms

- **Input**: Graph G, node attribute matrix X, embedding dimension D, number of walks per node R, walk length L, context window size ω.
- If X is not available, extract structural features like motif counts from the graph structure itself and use those as node attributes in X.
- Apply logarithmic binning to the node attribute values in X. Map nodes to node types/roles using a function $\phi(x)$ that takes the node attribute vector x as input.
  - two types of ϕ functions:
    - a) Simple functions like concatenation of attribute values.
    - b) Low-rank matrix factorization of X.
- Precompute random walk transition probabilities π. Generate R attributed random walks of length L for each node, using the node type mapping ϕ instead of node IDs.
- Learn embeddings using stochastic gradient descent on the attributed random walks, optimizing the probability of observing the context node types in the walks.
- **Output**: Learned embeddings for each node type w $\in$ W, where W is the set of node types found by ϕ.

Nesreen K. Ahmed et al: Learning Role-based Graph Embeddings

role2vec: Different from Previous Methods

- Mostly same as Node2Vec, except their work are considered in terms of node attribute, not node representation.

- There are many advantage from node attributed embedding:
  - Embeddings generalize to new nodes/graphs (inductive learning).
  - Better captures structural node roles.
  - Space-efficient as it learns fewer embeddings for node types instead of all nodes.
  - Supports attributed graphs.

Nesreen K. Ahmed et al: Learning Role-based Graph Embeddings

From Homogeneous to Heterogeneous Network Embedding: Problem

- Previous works are considering homogeneous network.
  - only one type of nodes and edges.
  - real world is ubiquitous. For example: social media websites like Facebook contain a set of node types, such as users, posts, groups and, tags.
  - special case of heterogeneous network.
- Input: a heterogeneous information network $\mathrm{G} = (V, E, T)$. T is object relation type.
- Output: $\boldsymbol{X} \in R^{|V| \times d}, d \ll |V|, d$-dim vector $\boldsymbol{X}_v$ for each node V.

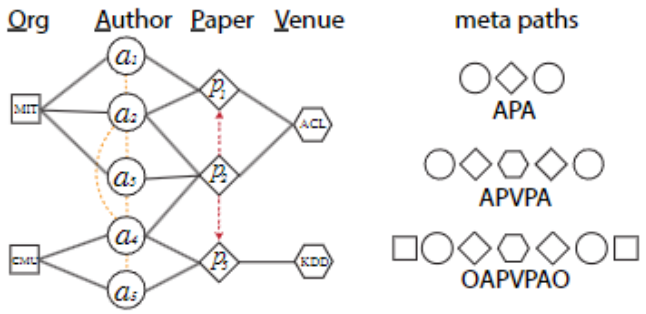
Latent representation vector

https://blog.reachsumit.com/posts/2023/05/shallow-heterogeneous-graphs-rep/

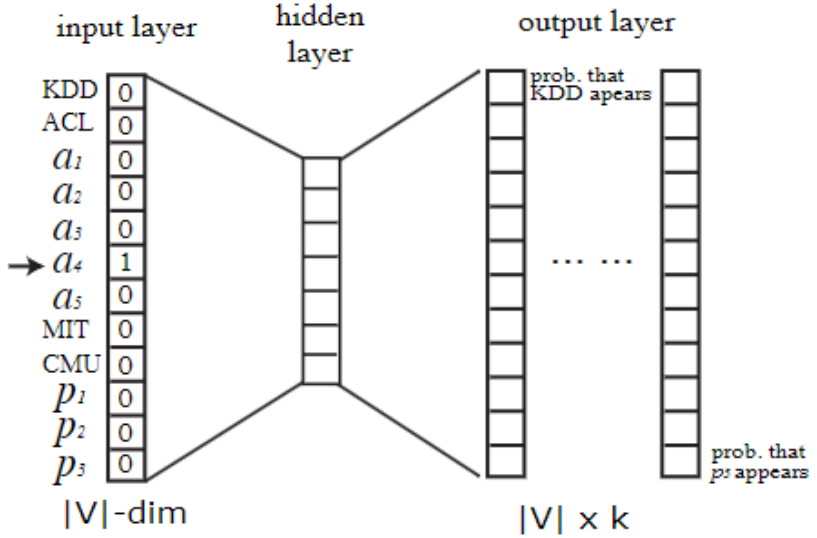
Heterogeneous Network Embedding: Challenges

- How do we effectively preserve the concept of “node-context” among multiple types of nodes?
  - e.g., users, posts, groups and, tags in social heterogeneous networks.
  - or authors, papers, & venues in academic heterogeneous networks.
- Can we directly apply homogeneous network embedding architectures to heterogeneous networks?
- It is also difficult for conventional meta-path-based methods to model similarities between nodes without connected meta-paths.

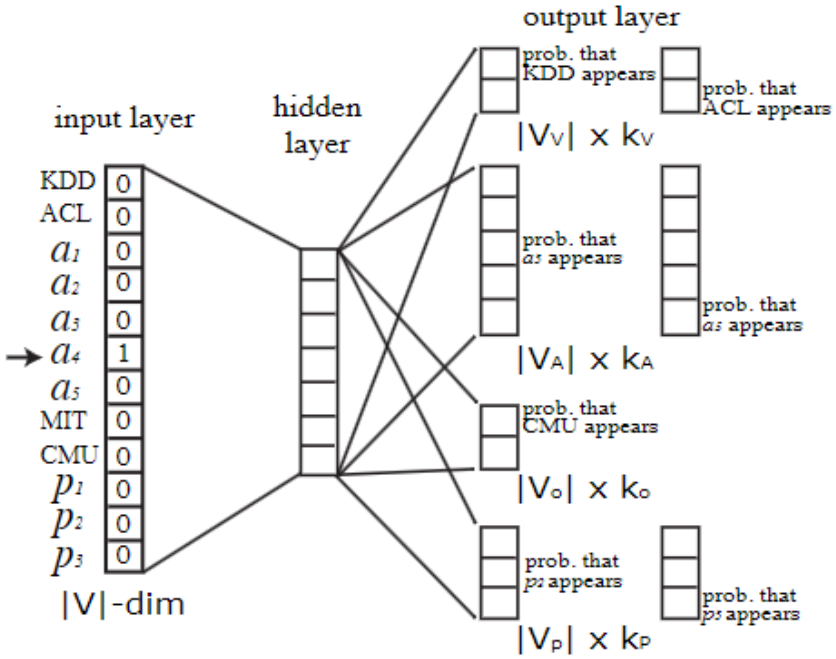
- **Solution**: meta-path based random walk (inspired by DeepWalk and Node2Vec)
  - metapath2vec and metapath2vec++.
- **Goal**: to generate paths that can capture both the semantic and structural correlations between different types of nodes, facilitating the transformation of heterogeneous network structures into skip-gram.



Heterogenous network



Skip-gram in metapath2vec



Skip-gram in metapath2vec++

Yuxiao Dong et al:"metapath2vec: Scalable representation learning for heterogeneous networks." *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, 2017.

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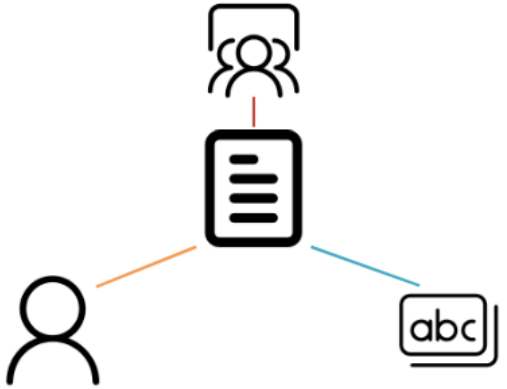
- Network schema $S = (V, R)$ of graph G
  - directed graph defined over node types V and with edges as relations from R



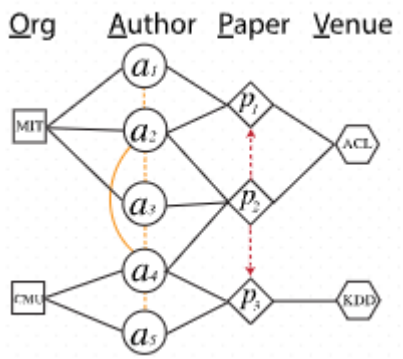
- meta-path: based on network schema S.
  - Denoted as $V_1 \xrightarrow{R_1} V_2 \xrightarrow{R_2} \cdots V_t \xrightarrow{R_t} V_{t+1} \cdots \xrightarrow{R_{l-1}} V_l$
  - Node types $V_1, V_2, \ldots, V_l \in V$ and edge type $R_1, R_2, \ldots, R_{l-1} \in R$

- Each meta-path captures the proximity between the nodes on its two ends from a particular semantic perspective.

https://blog.reachsumit.com/posts/2023/05/shallow-heterogeneous-graphs-rep/

- **Metapath2Vec**:
- Given a meta-path scheme:

$$V_1 \xrightarrow{R_1} V_2 \xrightarrow{R_2} \cdots V_t \xrightarrow{R_t} V_{t+1} \cdots \xrightarrow{R_{l-1}} V_l$$



- The transition probability at step i is defined as:

$$p(v^{i+1}|v_t^i, \mathcal{P}) = \begin{cases} \frac{1}{|N_{t+1}(v_t^i)|} & (v^{i+1}, v_t^i) \in E, \phi(v^{i+1}) = t+1 \\ 0 & (v^{i+1}, v_t^i) \in E, \phi(v^{i+1}) \neq t+1 \\ 0 & (v^{i+1}, v_t^i) \notin E \end{cases}$$

- Recursive guidance for random walkers, i.e.,

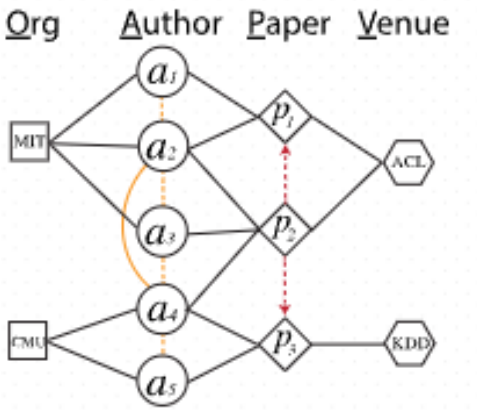
$$p(v^{i+1}|v_t^i) = p(v^{i+1}|v_1^i), \text{ if } t = l$$

- **Metapath2Vec**:
- Given a meta-path scheme (Example):

OAPVPAO

- In a traditional random walk procedure, the next step of a walker on node a4 transitioned from node CMU can be all types of nodes surrounding it - a2,a3, a5, p2, p3, and CMU.

- Under the meta-path scheme ‘OAPVPAO’, for example, the walker is biased towards paper nodes (P) given its previous step on an organization node CMU (O), following the semantics of this meta-path.



Yuxiao Dong et al:"metapath2vec: Scalable representation learning for heterogeneous networks." *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, 2017.
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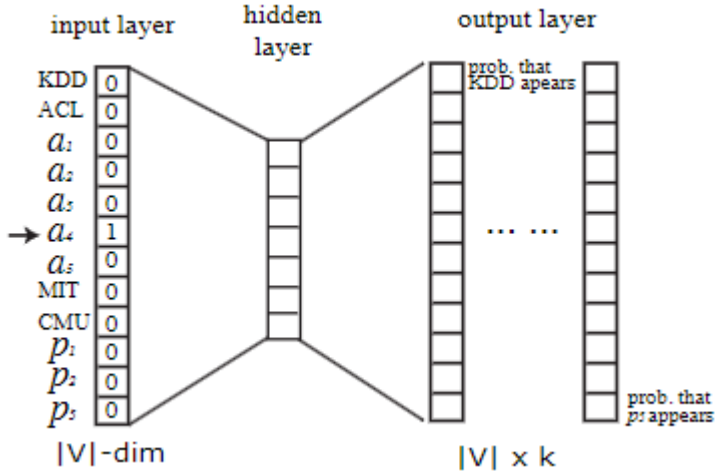
- Softmax in Metapath2Vec

$$p(c_t|v;\theta) = \frac{e^{X_{c_t} \cdot X_v}}{\sum_{u \in V} e^{X_u \cdot X_v}},$$

Not consider node type

- The potential issue of skip-gram for heterogeneous network embedding:
  - To predict the context node c_t (type t) given a node v, metapath2vec encourages all types of nodes to appear in this context position.



Yuxiao Dong et al:"metapath2vec: Scalable representation learning for heterogeneous networks." *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, 2017.

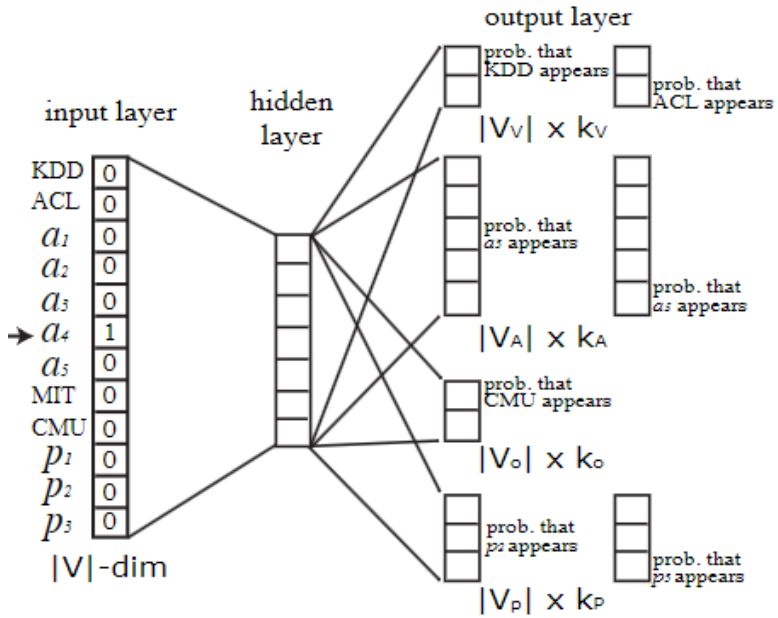
- **Metapath2Vec++**: Heterogeneous Skip-Gram
- Objective function (heterogeneous negative sampling):

$$O(\mathrm{X}) = \log \sigma(X_{c_t} \cdot X_v) + \sum_{m=1}^{M} \mathbb{E}_{u_t^m \sim P_t(u_t)} [\log \sigma(-X_{u_t^m} \cdot X_v)]$$

- Softmax in Metapath2Vec++

$$p(c_t | v; \theta) = \frac{e^{X_{c_t} \cdot X_v}}{\sum_{u_t \in V_t} e^{X_{u_t} \cdot X_v}}$$

Consider node type t



- Stochastic gradient descent

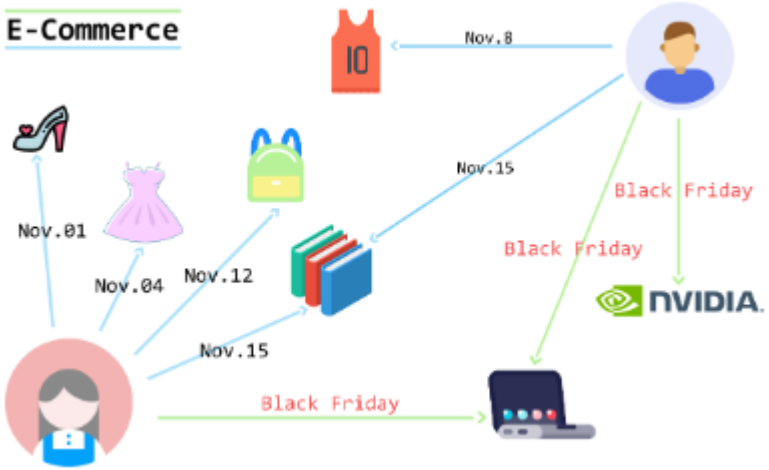
$$\frac{\partial O(\mathrm{X})}{\partial X_{u_t^m}} = (\sigma(X_{u_t^m} \cdot X_v - \mathbb{I}_{c_t}[u_t^m]))X_v$$

$$\frac{\partial O(\mathrm{X})}{\partial X_v} = \sum_{m=0}^{M} (\sigma(X_{u_t^m} \cdot X_v - \mathbb{I}_{c_t}[u_t^m]))X_{u_t^m}$$

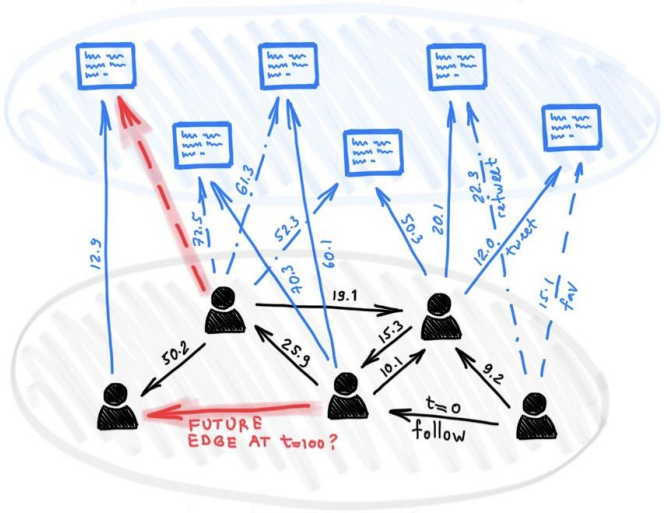
Yuxiao Dong et al:"metapath2vec: Scalable representation learning for heterogeneous networks." *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, 2017.

Dynamic Network Embedding

- Previous random walk methods – Node2Vec, WalkLet, LINE, Struc2Vec, Role2Vec, Metapath2Vec, etc – are relied on static graph.
- However, the networks in the real world are dynamic
  - evolving over time.



An illustration of user-item graph.



An illustration of social graph.

Guotong Xue et al:"Dynamic Network Embedding Survey."

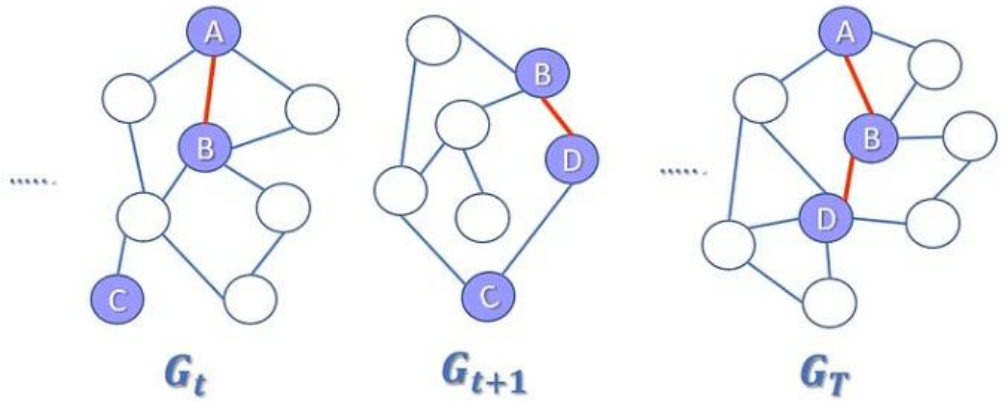
Dynamic Network Embedding: Problem and Challenges

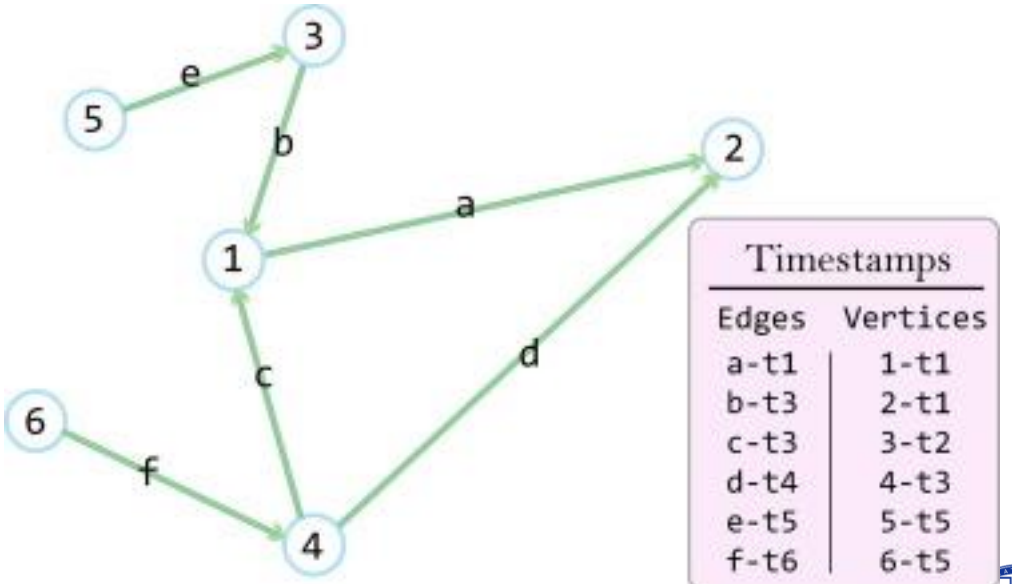
- **Problem**: Learning dynamic node representations.
- **Challenges**:
  - Time-varying graph structures: links and node can emerge and disappear; communities are changing all the time.
    - requires the node representations capture both structural proximity (as in static cases) and their temporal evolution.
    - Time intervals of events are uneven.
  - Causes of the change: can come from different aspects, e.g.in co-authorship network, research community & career stage perspectives.
    - requires modeling multi-faceted variations.

Zhiping Xiao:"Dynamic Graph Representation Learning."

Dynamic Network Embedding: Problem and Challenges

- **2 ways to model dynamic**: discrete model and continuous model.
  - Discrete model: sequence of network snapshots within a given time interval
    - $G = \{G_1, \ldots, G_T\}$, where T is the number of snapshots. Each snapshot $G_t = (V_t, E_t)$ is a static network recorded at time t.
  - Continuous model: a network with edges and nodes annotated with timestamps
    - We have $G = (V_T, E_T, \Im)$ where $\Im : V, E \rightarrow \mathbb{R}^+$ is a function that maps each edge and node to a corresponding timestamp.





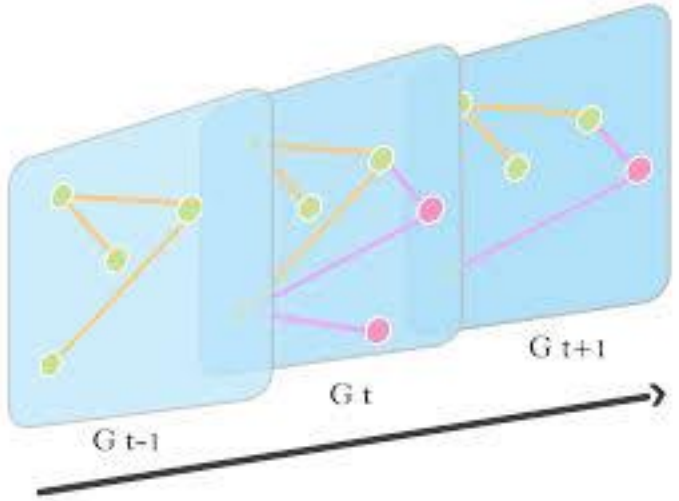
Timestamps

Edges	Vertices
a-t1	1-t1
b-t3	2-t1
c-t3	3-t2
d-t4	4-t3
e-t5	5-t5
f-t6	6-t5

Zhiping Xiao:"Dynamic Graph Representation Learning."

dynnode2vec: Scalable Dynamic Network Embedding

- **Motivation**: Networks in the real world are always evolving
  - new users (new vertices) in social networks, new citations (new edges) in citation networks.
  - Users may delete friends (delete edges) or some users may leave the network (delete nodes).
- The static graph embedding methods are not capable of dealing with the critical challenge involved in dynamic networks.
  - **Disadvantage**: embedding vectors for each timestamp are in different spaces.
    - Leading to learn embedding vectors separately is a time-consuming process.
- **Solution**: dynnode2vec method to modify the node2vec method
  - employing the previous learned embedding vectors as initials weights for the skip-gram model.



Sedigheh Mahdavi et al:"dynnode2vec: Scalable Dynamic Network Embedding."

dynnode2vec: Scalable Dynamic Network Embedding

- Given a dynamic graph as a sequence $G_1, G_2, \ldots, G_T$ from timestamp 1 to T.
- Each graph at time t is defined as $G_t = (V_t, E_t)$
- **Evolving Random Walk Generation:**
  - only generates random walks for the set of "evolving nodes" (ΔV_t) that have changed between consecutive timestamps t and t+1:

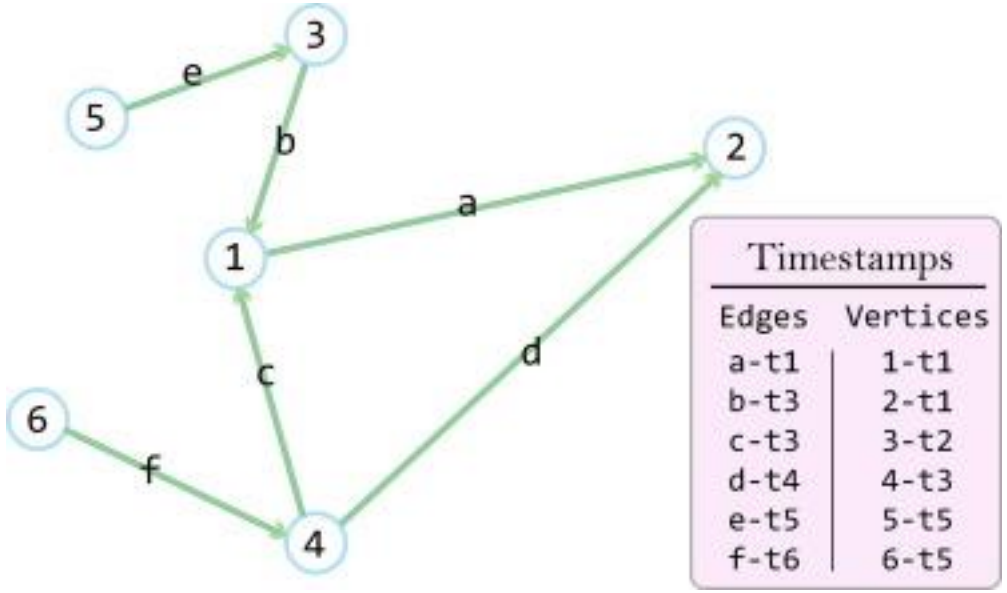
$$\Delta V_t = V_{add} \cup \{v_i \in V_t | \exists e_i = (v_i, v_j) \in (E_{add} \cup E_{del})\}$$

    - Change: new nodes added, existing nodes deleted, or edges added/removed for existing nodes).
- Dynamic Skip-gram Model:
  - initializes the skip-gram model at timestamp t with the pre-trained embedding vectors from the previous timestamp t-1.
  - vocabulary is updated based on the new evolving random walks, and Skip-gram t is retrained using only the new evolving random walks on the evolving node set ΔV_t.

Sedigheh Mahdavi et al:"dynnode2vec: Scalable Dynamic Network Embedding."

Continuous-Time Dynamic Network Embeddings

- **Motivation**: traditional methods often treat dynamic network as a sequence of static snapshots, which loss important temporal information.
- **Solution**: treat network as a continuous-time dynamic network, capturing the exact times of interaction.



Timestamps

Edges	Vertices
a-t1	1-t1
b-t3	2-t1
c-t3	3-t2
d-t4	4-t3
e-t5	5-t5
f-t6	6-t5

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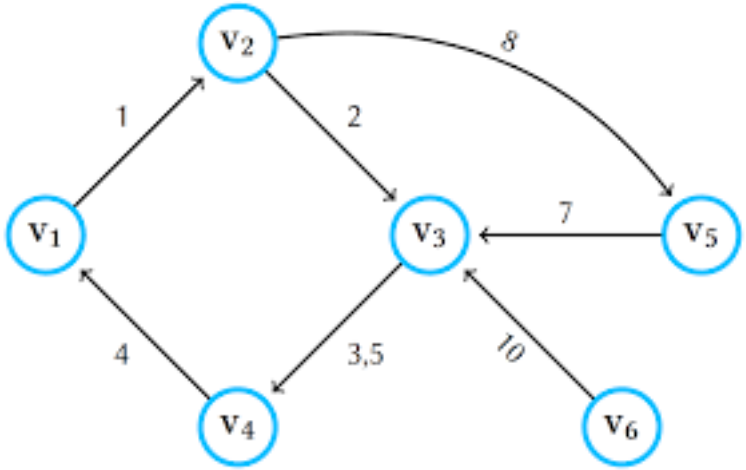
Continuous-Time Dynamic Network Embeddings

- A continuous-time dynamic network is defined as $G = (V, E_T, \Im)$.
  - V: set of nodes.
  - $E_T \subseteq V \times V \times R^+$: set of temporal edges between vertices in V.
  - $\Im: \mathrm{E} \rightarrow \mathrm{R}^+$: a function that maps each edge to a corresponding timestamp.

- Temporal walk:
  - A temporal walk from v_1 to v_k in G is a sequence of vertices $\langle v_1, v_2, \ldots, v_k \rangle$ such that
    - $\langle v_i, v_{i+1} \rangle$ for $1 \leq i < k$ and
    - $\Im(v_i, v_{i+1}) \leq \Im(v_{i+1}, v_{i+2})$ for $1 \leq i < (k-1)$



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- **Temporal random walk**:
- The set of temporal neighbors of a node v at time t:

$$\Gamma_t(v) = \{(w, t') \mid e = (v, w, t') \in E_T \wedge \mathcal{T}(e) > t\}$$

- Unbiased selection: each temporal neighbor w of node v at time t is selected

$$\Pr(w) = 1/|\Gamma_t(v)|$$

- Biased selection: sampling the next node in a temporal walk via temporally weighted distribution based on

$$\Pr(w) = \frac{\exp[\tau(w) - \tau(v)]}{\sum_{w' \in \Gamma_t(v)} \exp[\tau(w') - \tau(v)]}$$

→ **Exponential decay: selecting a neighbor decreases exponentially with time**

$$\Pr(w) = \frac{\delta(w)}{\sum_{w' \in \Gamma_t(v)} \delta(w')}$$

→ **Linear decay: sorts temporal neighbors in descending order time-wise.**

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Continuous-Time Dynamic Network Embeddings

- Temporal context windows: To handle the temporal nature of walks - a walk to run out of temporally valid edges to traverse.
  - A walk must have a minimum length ω and can extend up to a maximum length L. The number of context windows is defined

$$\beta = \sum_{i=1}^{k} |\mathcal{S}_{t_i}| - \omega + 1$$

- Learning time-preserving embeddings: maximize the likelihood of observing temporal context windows given the embeddings

$$\max_{f} \log \Pr\left(W_T = \{v_{i-\omega}, \cdots, v_{i+\omega}\} \setminus v_i \mid f(v_i)\right)$$

⇒ Utilizing stochastic gradient descent.

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