Heterogeneous and Dynamic Graph Representation Learning

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Remind the Node Embeddings

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

$$\text{similarity}(u, v) \approx \mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u$$

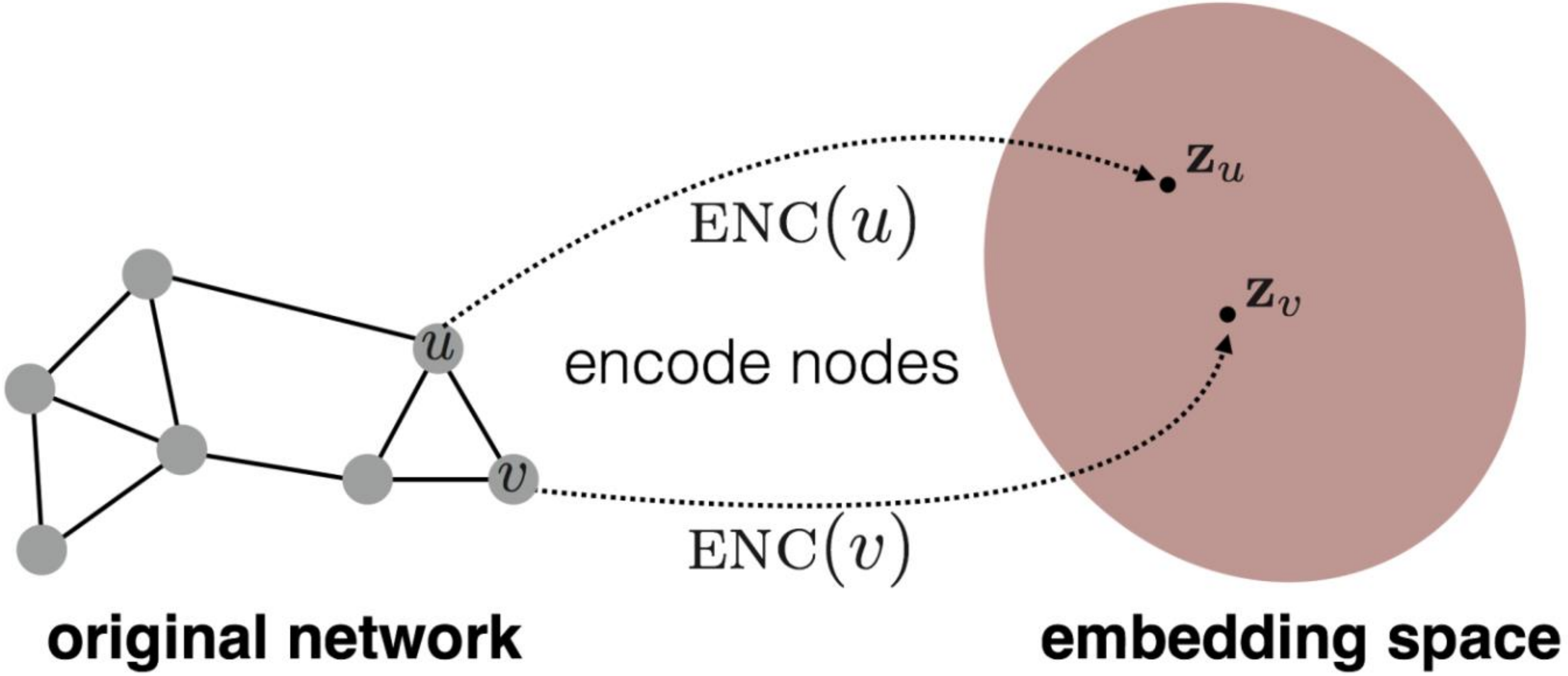
in the original network

Similarity of the embedding

We need to define:

ENC(u)

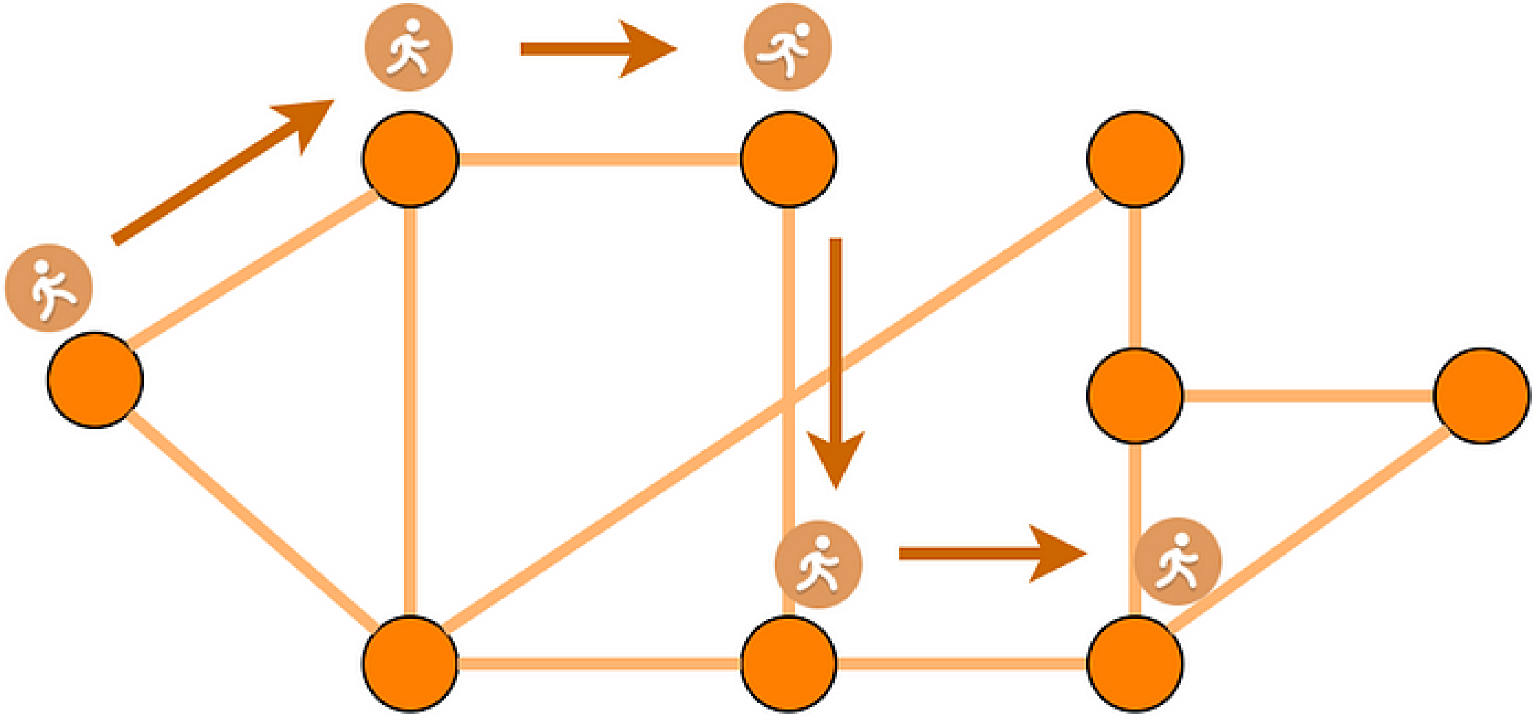
Similarity(u, v)


$\mathbf{z}_u$
ENC(u)
$\mathbf{z}_v$
u
encode nodes
v
ENC(v)
original network
embedding space

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

Random Walk

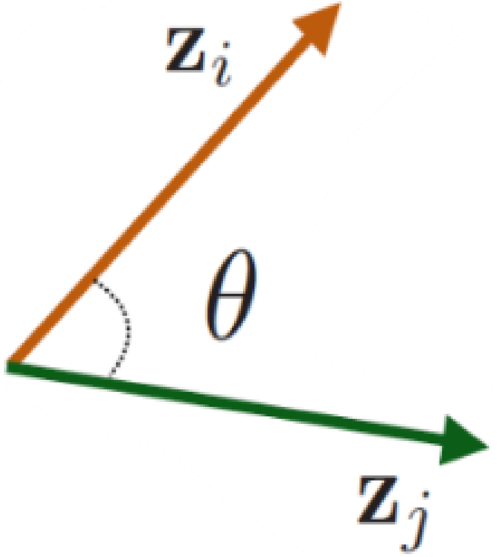
- Given a graph and a starting point, we select a neighbour of it at random, and move to this neighbour
- Then, we select a neighbor of this point at random, and move to it,…
- The random sequence of nodes visited this way is **a random walk on the graph**



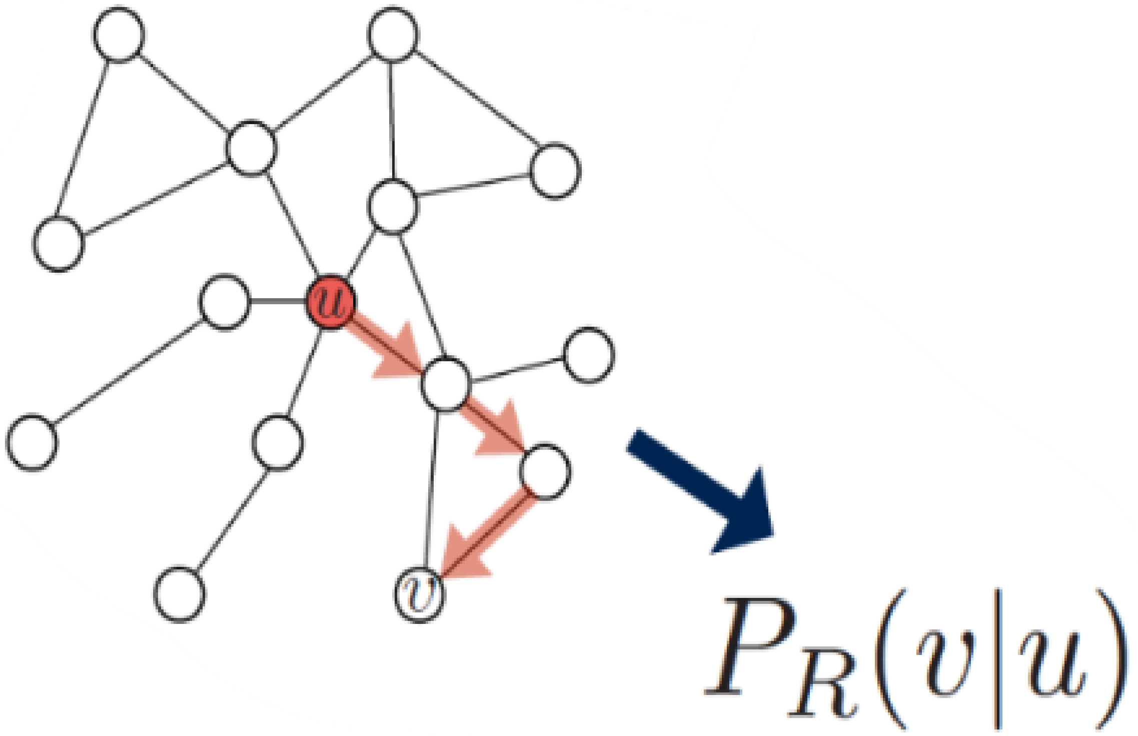
https://medium.com/analytics-vidhya/an-intuitive-explanation-of-deepwalk-84177f7f2b72

Random Walk Embeddings

- 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

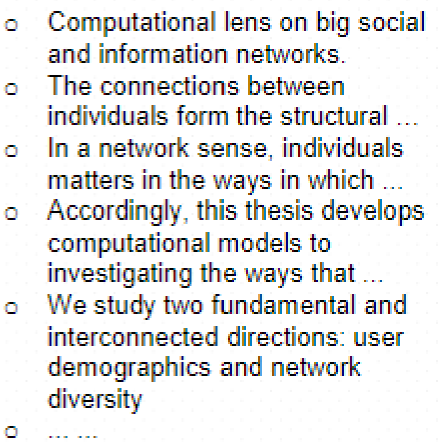


$$\mathbf{z}_u^{\mathrm{T}}\mathbf{z}_v \approx$$



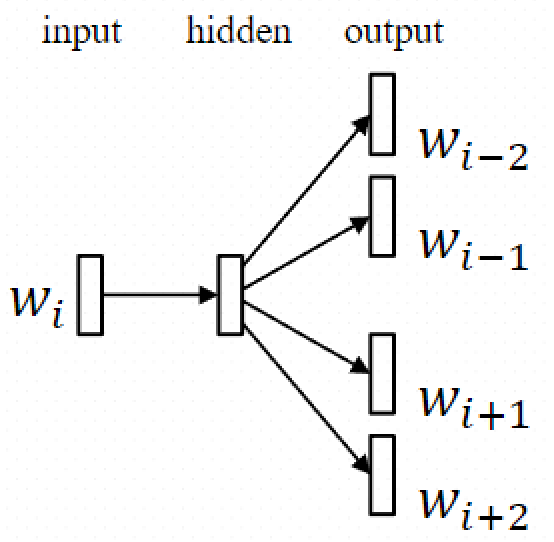
Word Embedding in NLP

- Input: a text corpus $D = \{W\}$
- Output: $\boldsymbol{X} \in R^{|W| \times d}, d \ll |W|, d$-dim vector $\boldsymbol{X}_w$ for each word w



- Computational lens on big social and information networks.
- The connections between individuals form the structural ...
- In a network sense, individuals matters in the ways in which ...
- Accordingly, this thesis develops computational models to investigating the ways that ...
- We study two fundamental and interconnected directions: user demographics and network diversity
- ... ...

Sentences



Word2vec

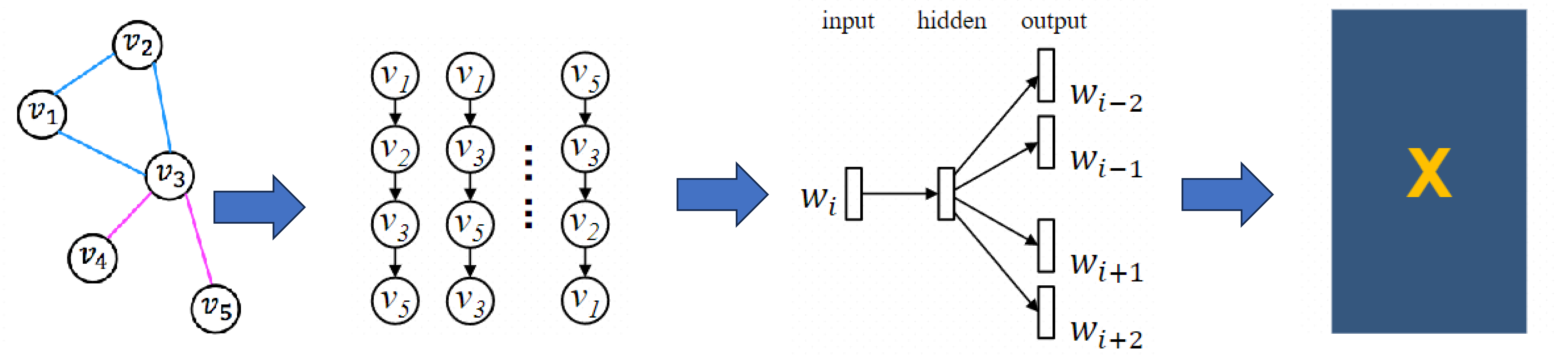
Latent representation vector

- Geographically close words: a word and its context words -- in a sentence or document exhibit interrelations in human natural language

T. Mikolov, I Sutskever, K Chen, GS Corrado, J Dean. Distributed representations of words and phrases and their compositionality. In NIPS '13, pp. 3111-31119

DeepWalk

- Input: a network $\mathrm{G} = (V, E)$
- Output: $\boldsymbol{X} \in R^{|V|\times d}, d \ll |V|, d$-dim vector $\boldsymbol{X}_v$ for each node V


v_2
v_1
v_3
v_4
v_5
v_1 v_2 v_3 v_5
v_1 v_3 v_5 v_3
v_5 v_3 v_2 v_1
input
hidden
output
w_i
w_{i-2}
w_{i-1}
w_{i+1}
w_{i+2}
X

Random walk paths (sentences)

Word2vec (Skip-gram)

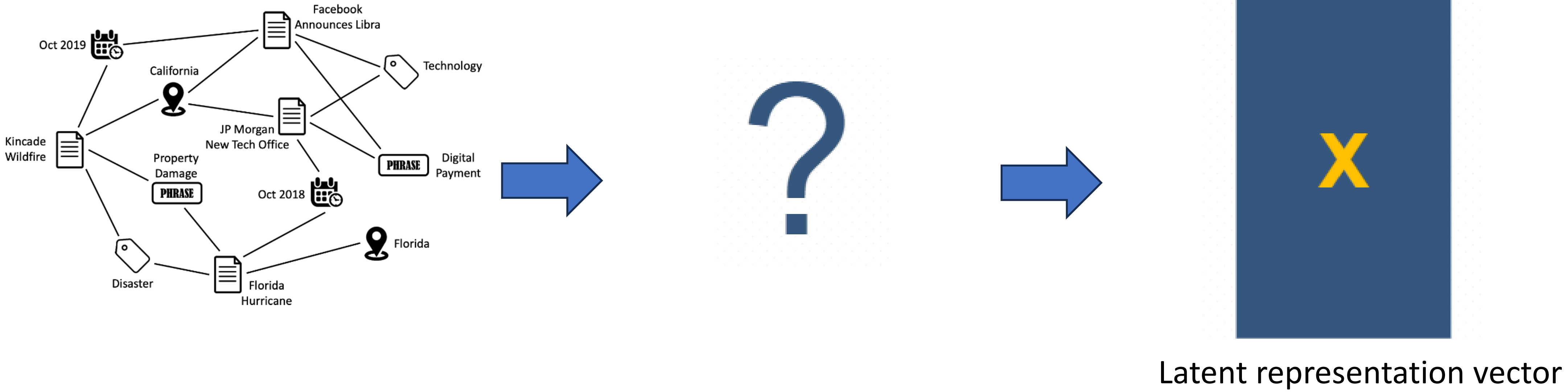
Latent representation vector

- Employ random walks on the graph to discover the structure

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

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


Oct 2019
Facebook Announces Libra
Technology
California
JP Morgan New Tech Office
Kincade Wildfire
Property Damage
PHRASE
Digital Payment
PHRASE
Oct 2018
Florida
Disaster
Florida Hurricane
?
X
Latent representation vector

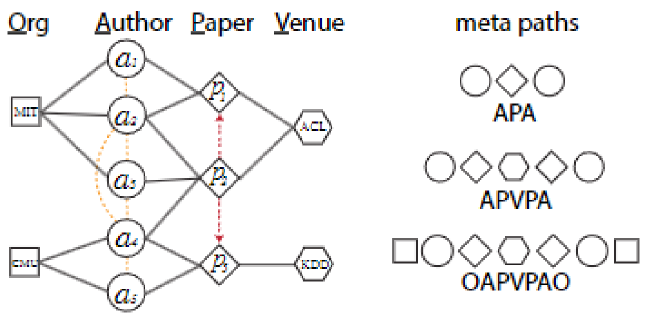
https://blog.reachsumit.com/posts/2023/05/shallow-heterogeneous-graphs-rep/

Heterogeneous Network Embedding: Challenges

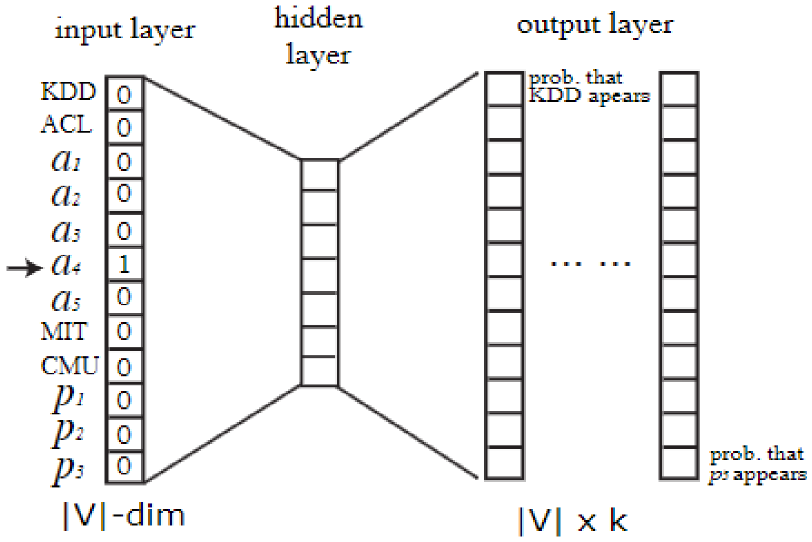
- How do we effectively preserve the concept of “node-context” among multiple types of nodes?
  - E.g., users, posts, groups and, tags in social heterogeneous networks
  - Or authors, papers, & venues in academic heterogeneous networks
- Can we directly apply homogeneous network embedding architectures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

Metapath2Vec: Scalable Representation Learning for Heterogeneous Networks

- **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


Org
Author
Paper
Venue
MIT
CMU
a_1
a_2
a_3
a_4
a_5
p_1
p_2
p_3
ACL
KDD
meta paths
APA
APVPA
OAPVPAO

Heterogenous network


input layer
hidden layer
output layer
KDD
ACL
a_1
a_2
a_3
a_4
a_5
MIT
CMU
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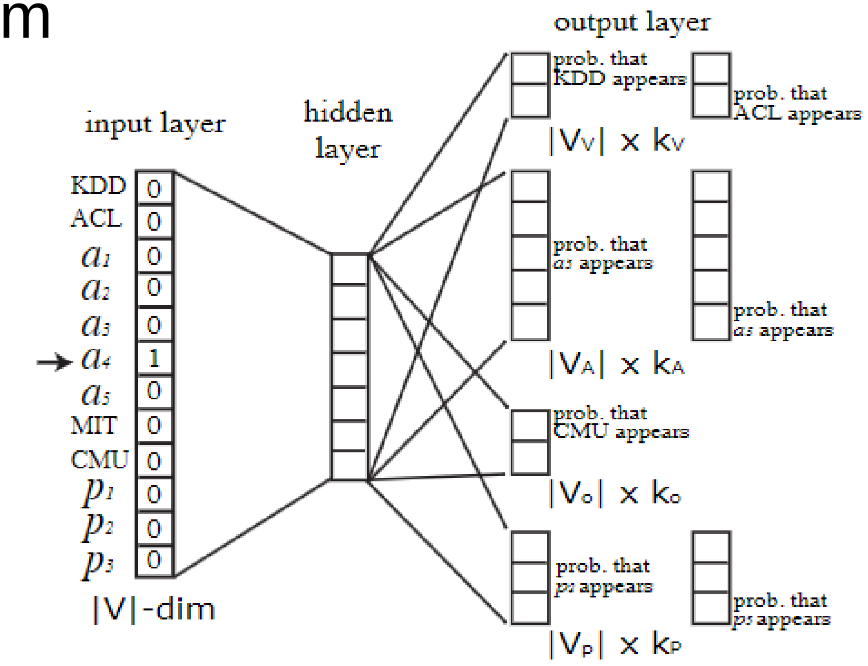
prob. that KDD apears
… …
prob. that p_3 appears
|V|-dim
|V| x k

Skip-gram in metapath2vec


input layer
hidden layer
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KDD
ACL
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a_3
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a_5
MIT
CMU
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p_3
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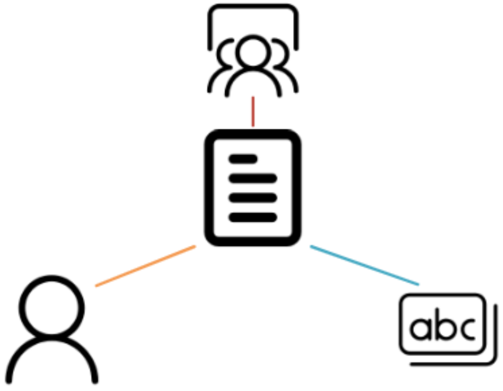
|V|-dim
prob. that KDD appears
prob. that ACL appears
$|V_V| \times k_V$
prob. that a_3 appears
prob. that a_5 appears
$|V_A| \times k_A$
prob. that CMU appears
$|V_O| \times k_O$
prob. that p_2 appears
prob. that p_3 appears
$|V_P| \times k_P$

Skip-gram in metapath2vec++

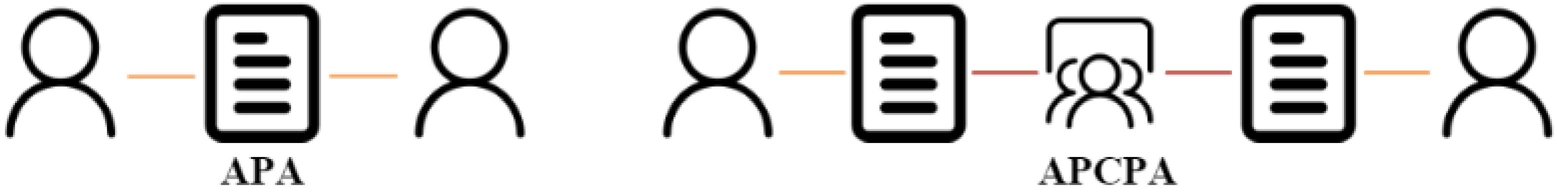
Yuxiao Dong et al:"metapath2vec: Scalable representation learning for heterogeneous networks." *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, 2017.

Metapath2Vec: Scalable Representation Learning for Heterogeneous Networks

- 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 $R_1, R_2, \ldots, R_{l-1} \in R$



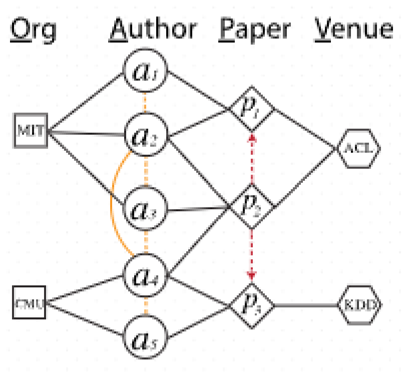
- Each meta-path captures the proximity between the nodes on its two ends from a particular semantic perspective

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

Metapath2Vec: Scalable Representation Learning for Heterogeneous Networks

- 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.,

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

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.

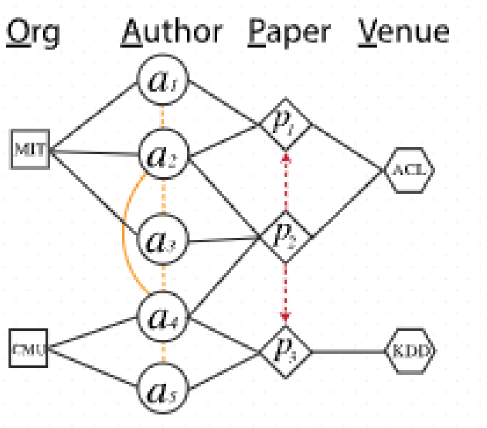
Metapath2Vec: Scalable Representation Learning for Heterogeneous Networks

- 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.

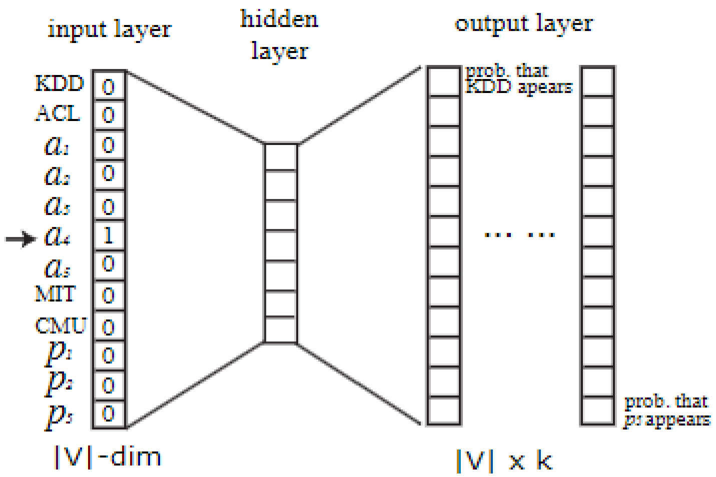
Metapath2Vec: Scalable Representation Learning for Heterogeneous Networks

- 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:
  - Predict the context node c_t (type t) given a node v, metapath2vec encourages all types of nodes to appear in this context position


input layer
hidden layer
output layer
KDD
ACL
a_1
a_2
a_3
a_4
a_5
MIT
CMU
p_1
p_2
p_3
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0
prob. that KDD apears
… …
prob. that p_3 appears
|V|-dim
|V| x k

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Metapath2Vec: Scalable Representation Learning for Heterogeneous Networks

- **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++

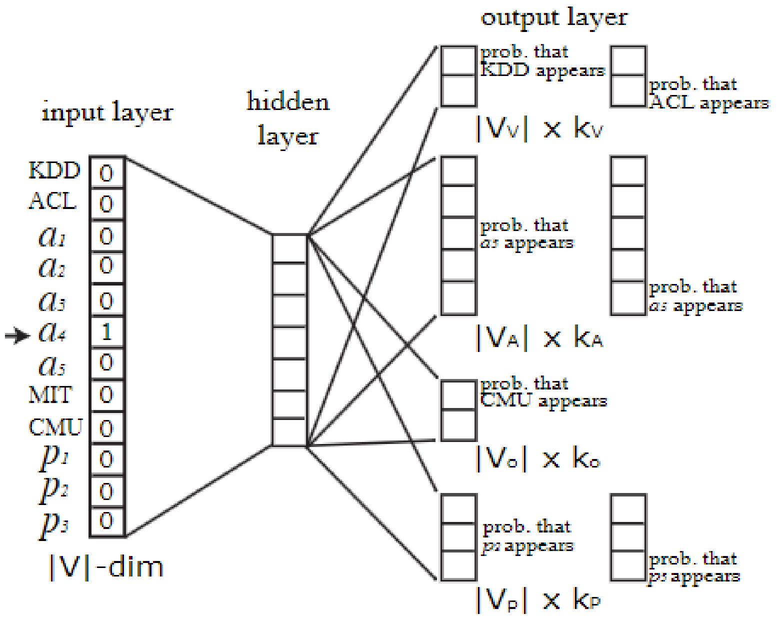
$$p(c_t|v;\theta) = \frac{e^{X_{c_t} \cdot X_v}}{\sum_{\underline{u_t \in V_t}} e^{X_{u_t} \cdot X_v}}$$

Consider node type t

- Stochastic gradient descent

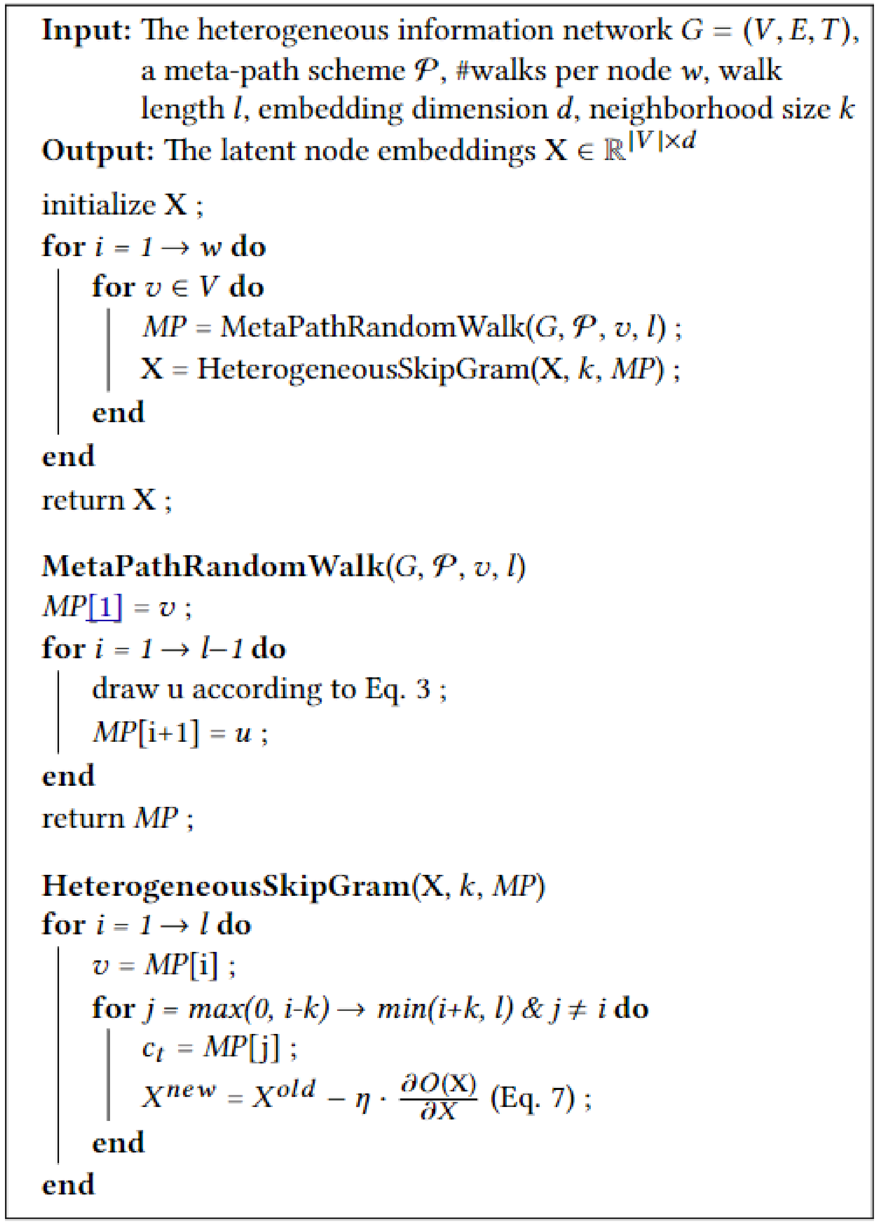
$$\frac{\partial O(\mathrm{X})}{\partial X_{u_t^m}} = (\sigma(X_{u_t^m} \cdot X_v - \mathbb{I}_{c_t}[u_t^m]))X_v$$

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


output layer
prob. that KDD appears
prob. that ACL appears
|V_V| x k_V
input layer
hidden layer
KDD
ACL
a1
a2
a3
a4
a5
MIT
CMU
p1
p2
p3
0
0
0
0
0
1
0
0
0
0
0
0
|V|-dim
prob. that a3 appears
prob. that a5 appears
|V_A| x k_A
prob. that CMU appears
|V_O| x k_O
prob. that p2 appears
prob. that p3 appears
|V_P| x k_P

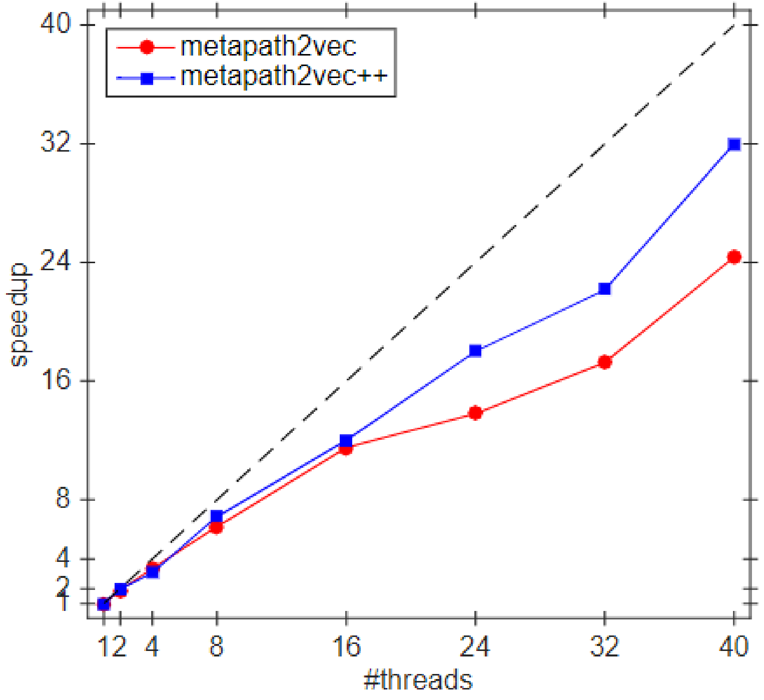
Yuxiao Dong et al:"metapath2vec: Scalable representation learning for heterogeneous networks." *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, 2017.

Metapath2Vec: Metapath2Vec++ Algorithm



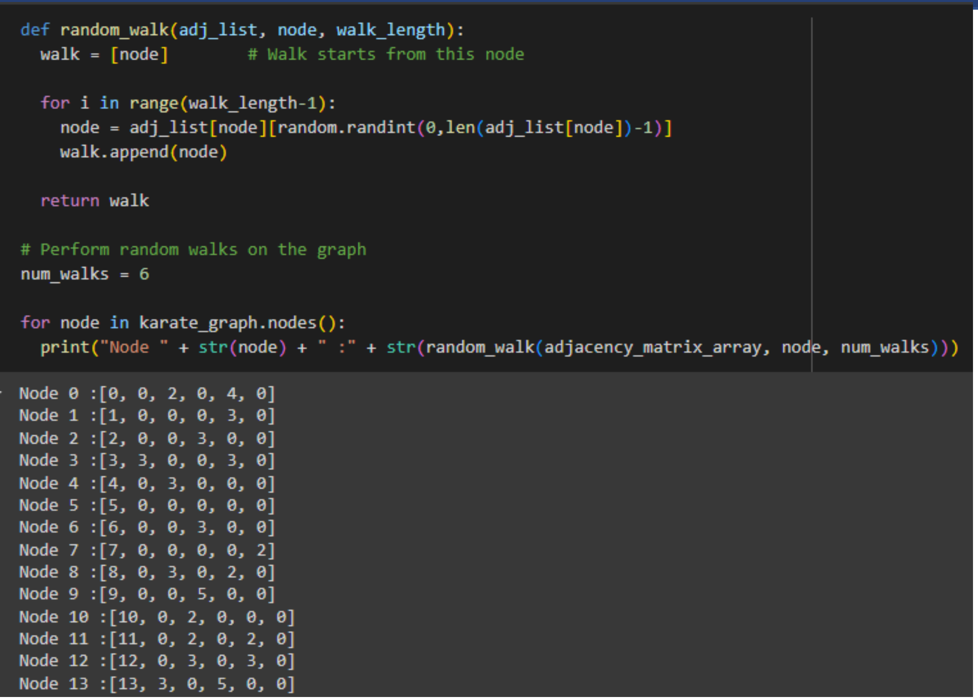
```
Input: The heterogeneous information network $G = (V, E, T)$,
       a meta-path scheme $\mathcal{P}$, #walks per node $w$, walk
       length $l$, embedding dimension $d$, neighborhood size $k$
Output: The latent node embeddings $\mathbf{X} \in \mathbb{R}^{|V| \times d}$

initialize X ;
for $i = 1 \rightarrow w$ do
    for $v \in V$ do
        $MP$ = MetaPathRandomWalk($G, \mathcal{P}, v, l$) ;
        X = HeterogeneousSkipGram(X, $k$, $MP$) ;
    end
end
return X ;

MetaPathRandomWalk($G, \mathcal{P}, v, l$)
$MP[1] = v$ ;
for $i = 1 \rightarrow l-1$ do
    draw u according to Eq. 3 ;
    $MP[i+1] = u$ ;
end
return $MP$ ;

HeterogeneousSkipGram(X, $k$, $MP$)
for $i = 1 \rightarrow l$ do
    $v = MP[i]$ ;
    for $j = max(0, i-k) \rightarrow min(i+k, l)$ & $j \neq i$ do
        $c_t = MP[j]$ ;
        $X^{new} = X^{old} - \eta \cdot \frac{\partial O(X)}{\partial X}$ (Eq. 7) ;
    end
end
```

- ➢ Every sub-procedure is easy to parallelize
- ➢ 24-32X speedup by using 40 cores



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.

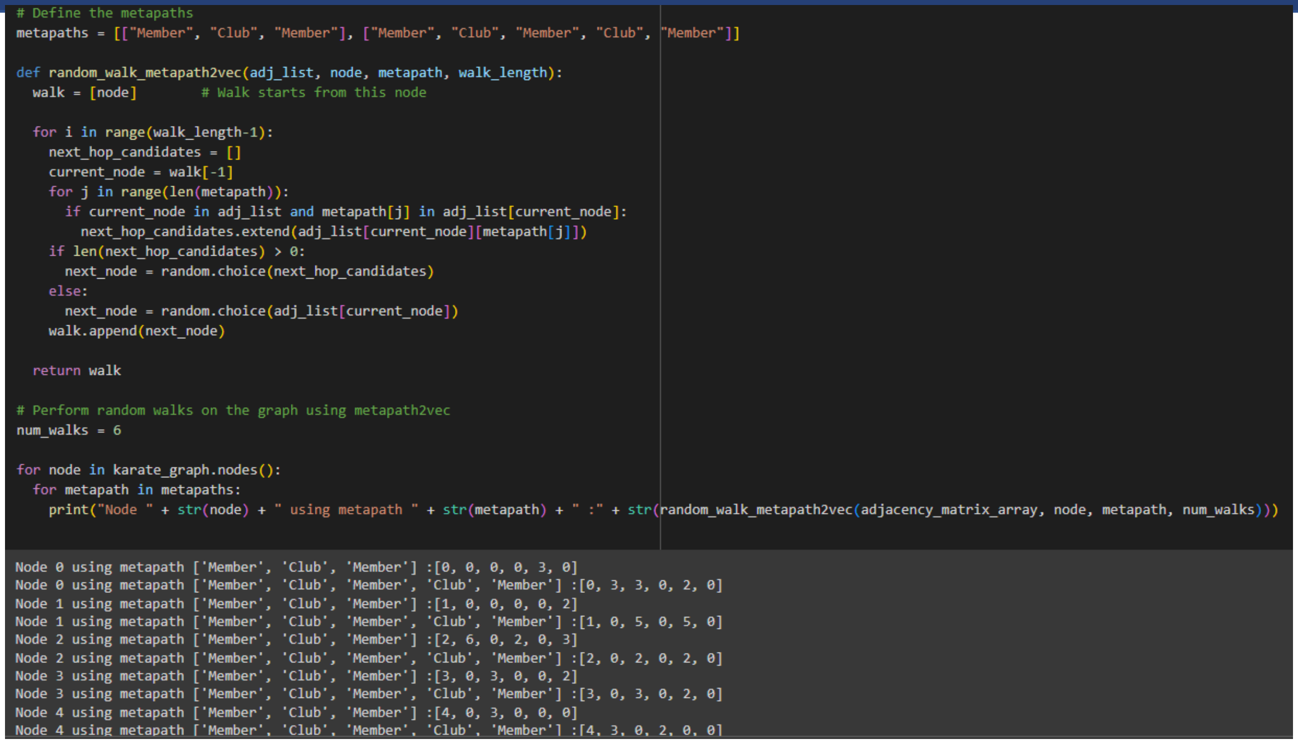
Sample code of Random Walk of DeepWalk and Metapath2Vec in Karate Graph



```
def random_walk(adj_list, node, walk_length):
  walk = [node]         # Walk starts from this node

  for i in range(walk_length-1):
    node = adj_list[node][random.randint(0,len(adj_list[node])-1)]
    walk.append(node)

  return walk

# Perform random walks on the graph
num_walks = 6

for node in karate_graph.nodes():
  print("Node " + str(node) + " :" + str(random_walk(adjacency_matrix_array, node, num_walks)))
```

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

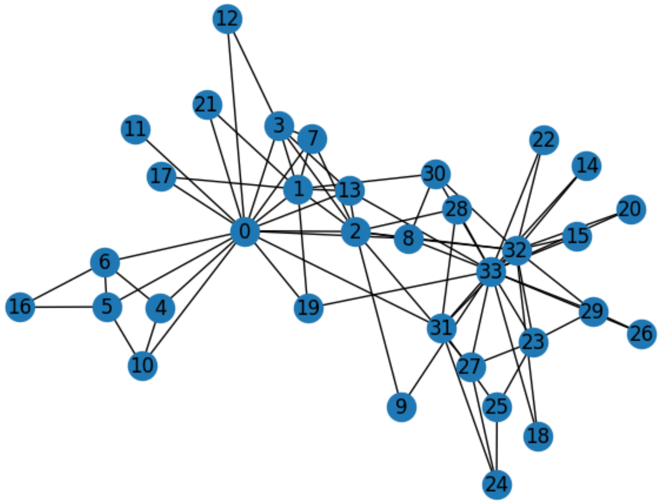
Deep Walk



```
# Define the metapaths
metapaths = [["Member", "Club", "Member"], ["Member", "Club", "Member", "Club", "Member"]]

def random_walk_metapath2vec(adj_list, node, metapath, walk_length):
  walk = [node]         # Walk starts from this node

  for i in range(walk_length-1):
    next_hop_candidates = []
    current_node = walk[-1]
    for j in range(len(metapath)):
      if current_node in adj_list and metapath[j] in adj_list[current_node]:
        next_hop_candidates.extend(adj_list[current_node][metapath[j]])
    if len(next_hop_candidates) > 0:
      next_node = random.choice(next_hop_candidates)
    else:
      next_node = random.choice(adj_list[current_node])
    walk.append(next_node)

  return walk

# Perform random walks on the graph using metapath2vec
num_walks = 6

for node in karate_graph.nodes():
  for metapath in metapaths:
    print("Node " + str(node) + " using metapath " + str(metapath) + " :" + str(random_walk_metapath2vec(adjacency_matrix_array, node, metapath, num_walks)))
```

```
Node 0 using metapath ['Member', 'Club', 'Member'] :[0, 0, 0, 0, 3, 0]
Node 0 using metapath ['Member', 'Club', 'Member', 'Club', 'Member'] :[0, 3, 3, 0, 2, 0]
Node 1 using metapath ['Member', 'Club', 'Member'] :[1, 0, 0, 0, 0, 2]
Node 1 using metapath ['Member', 'Club', 'Member', 'Club', 'Member'] :[1, 0, 5, 0, 5, 0]
Node 2 using metapath ['Member', 'Club', 'Member'] :[2, 6, 0, 2, 0, 3]
Node 2 using metapath ['Member', 'Club', 'Member', 'Club', 'Member'] :[2, 0, 2, 0, 2, 0]
Node 3 using metapath ['Member', 'Club', 'Member'] :[3, 0, 3, 0, 0, 2]
Node 3 using metapath ['Member', 'Club', 'Member', 'Club', 'Member'] :[3, 0, 3, 0, 2, 0]
Node 4 using metapath ['Member', 'Club', 'Member'] :[4, 0, 3, 0, 0, 0]
Node 4 using metapath ['Member', 'Club', 'Member', 'Club', 'Member'] :[4, 3, 0, 2, 0, 0]
```

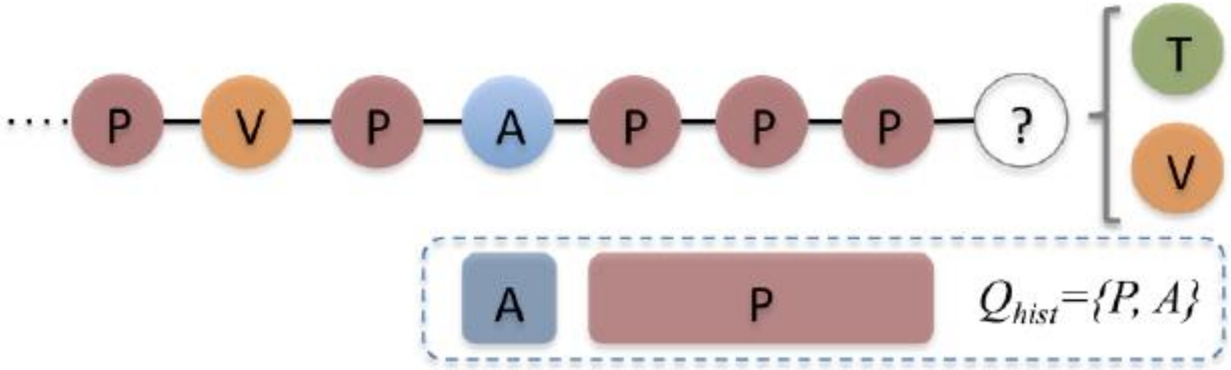
Metapath2Vec



Meta-path Limitation

- Meta-paths must be manually customized based on task and dataset, hence requiring domain knowledge
- They fail to capture more complex relationships such as motifs, i.e. patterns of interconnections occurring in complex networks at numbers that are significantly higher than those in randomized networks
- The usage of meta-path is limited to the discrete space. So, if two vertices are not structurally connected in the graph, metapath-based methods cannot capture their relations

- **Solution**: propose JUST, which performs random walks by probabilistically deciding whether to "jump" to a different node type or "stay" in the same node type
  - No rely on predefined meta-paths
  - **Balance** between **homogeneous** edges (same node type) and **heterogeneous** edges (across node types)
  - balances the node distribution over different node types by controlling the jumping behavior



Rana Hussein et al:"Are Meta-Paths Necessary? Revisiting Heterogeneous Graph Embeddings."

Are Meta-Paths Necessary? Revisiting Heterogeneous Graph Embeddings

- Perform random walks on the heterogeneous graph, but probabilistically decide at each step
  - **Jump** to a target domain q: uniformly sampling one node from those in a target domain q connected to v_i via heterogeneous edge

$$V_{jump}^{q}(v_i) = \{v | (v_i, v) \in E_{he} \vee (v_i, v) \in E_{he}, \phi(v) = q$$

  - **Stay** in the current domain: uniformly sampling one node from those connected to vi via homogeneous edges

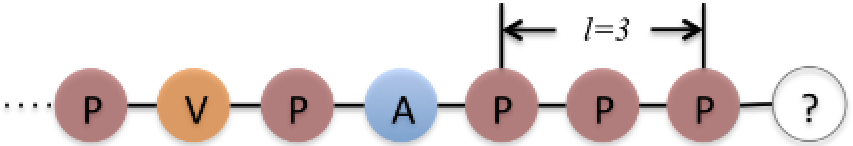
$$V_{stay}(v_i) = \{v | (v_i, v) \in E_{ho} \vee (v_i, v) \in E_{ho}$$

Rana Hussein et al:"Are Meta-Paths Necessary? Revisiting Heterogeneous Graph Embeddings."

Are Meta-Paths Necessary? Revisiting Heterogeneous Graph Embeddings

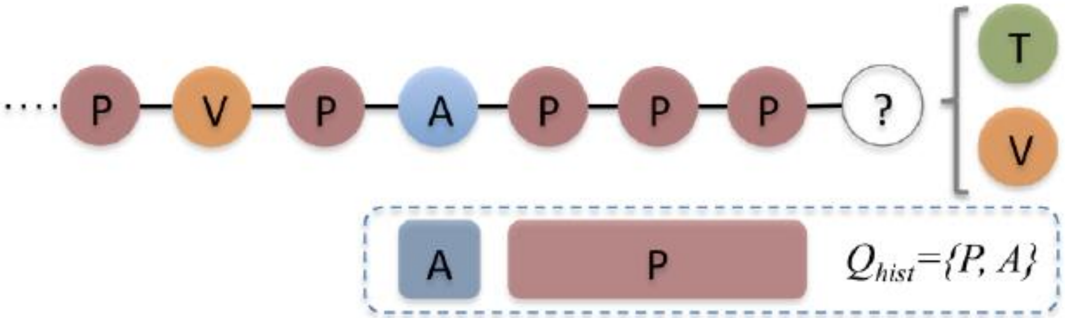
- **Probability** for stay or jump is controlled by an exponential decay function:
  - Stay:

$$Pr_{stay}(v_i) = \begin{cases} 0, \text{ if } V_{stay}(v_i) = \emptyset \\ 1, \text{ if } \{V^{q}_{jump}(v_i) | q \in Q, q \neq \phi(v_i)\} = \emptyset \\ \alpha^{l}, \ otherwise \end{cases}$$



  - Jump:

$$Q_{Jump}(v_i) = \begin{cases} \{q | q \in Q \wedge q \notin Q_{hist}, V^{q}_{jump}(v_i) \neq \emptyset\}, \text{ if not empty} \\ \{q | q \in Q, q \neq \phi(v_i), V^{q}_{jump}(v_i) \neq \emptyset\}, \ otherwise \end{cases}$$



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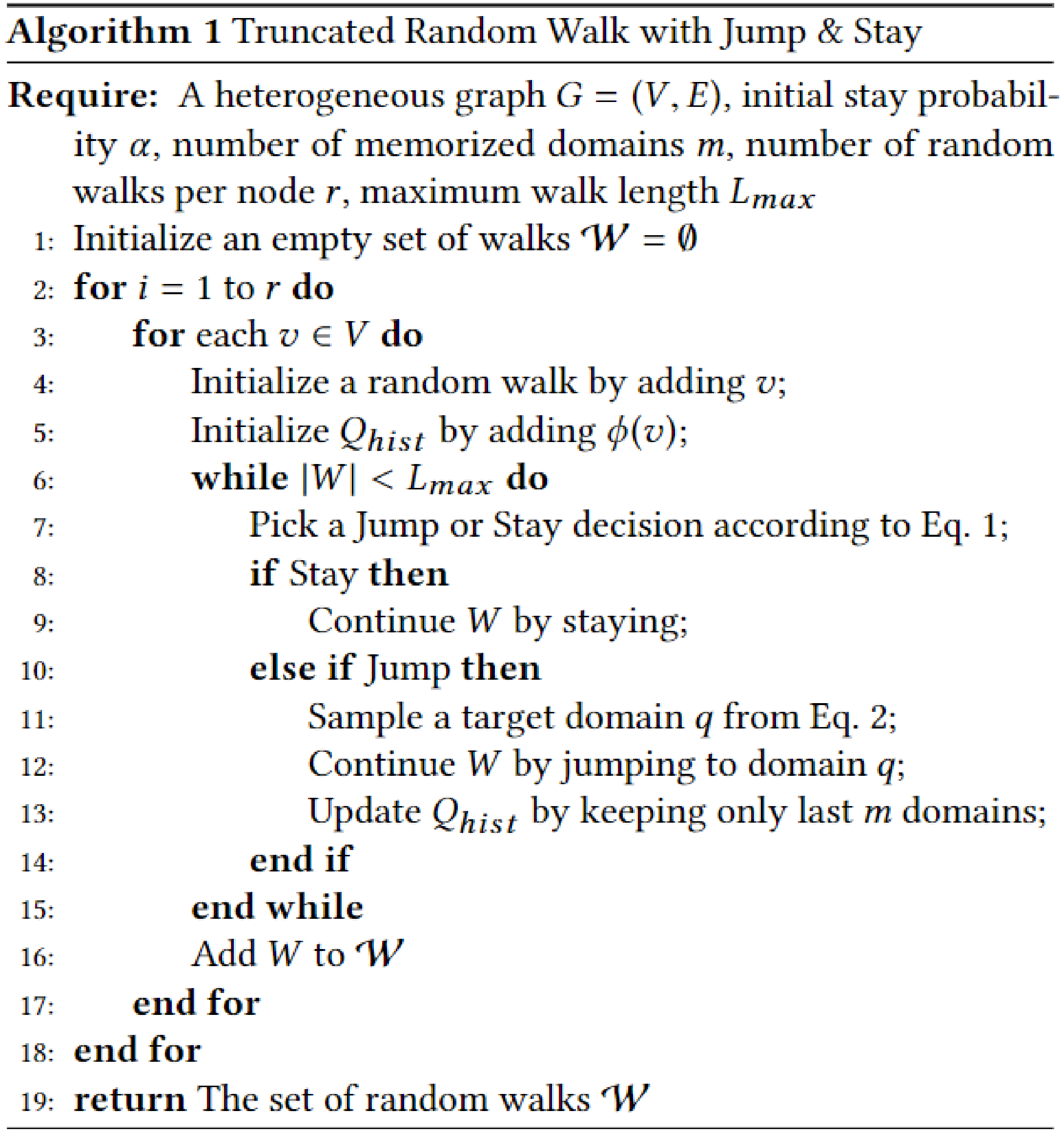
Are Meta-Paths Necessary? Revisiting Heterogeneous Graph Embeddings



Algorithm 1 Truncated Random Walk with Jump & Stay

```
Require: A heterogeneous graph $G = (V, E)$, initial stay probability $\alpha$, number of memorized domains $m$, number of random walks per node $r$, maximum walk length $L_{max}$
Initialize an empty set of walks $\mathcal{W} = \emptyset$
for $i = 1$ to $r$ do
    for each $v \in V$ do
        Initialize a random walk by adding $v$;
        Initialize $Q_{hist}$ by adding $\phi(v)$;
        while $|W| < L_{max}$ do
            Pick a Jump or Stay decision according to Eq. 1;
            if Stay then
                Continue $W$ by staying;
            else if Jump then
                Sample a target domain $q$ from Eq. 2;
                Continue $W$ by jumping to domain $q$;
                Update $Q_{hist}$ by keeping only last $m$ domains;
            end if
        end while
        Add $W$ to $\mathcal{W}$
    end for
end for
return The set of random walks $\mathcal{W}$
```

- Apply Skip-gram model same as metapth2vec
- Different with Metapath2Vec:
  - Decide probabilistically whether to "jump" across node types via a heterogeneous edge or "stay" in the same node type via a homogeneous edge
  - When jumping, select the target node type probabilistically while trying to avoid recently visited node types

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BHIN2vec: Balancing the Type of Relation in Heterogeneous Information Network

- **Motivation**: Random walk produces an imbalanced training of heterogeneous networks
  - The major relation types take a large portion of training samples
  - Dominate the training and minor relation types will hardly be learned
- **Idea**: Formulate heterogeneous network embedding as a multi-task learning problem, where each task corresponds to a relation type in the network.
  - Allow handling the imbalance by focusing on under-trained relation types
- **Solution**: Introduce an inverse training ratio tensor that quantifies how well each relation type is represented in the embedding space based on the task losses
  - Propose a biased random walk strategy that uses the inverse training ratios to generate walks containing more of the under-trained relation types

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BHIN2vec: Balancing the Type of Relation in Heterogeneous Information Network

- **Biased random walk generator**:
  - Determine the type for the next node by sampling and do another sampling for the next node that has the sampled type
- A stochastic matrix to store transition probabilities between node types

$$P_{ij} = p\left(t_j | t_i\right) \text{ such that } \sum_i P_{ij} = 1$$

- For k steps:

$$(P^k)_{ij} = p\left(t_j | t_i, k\right)$$

Seonghyeon Lee et al:"BHIN2vec: Balancing the Type of Relation in Heterogeneous Information Network."

BHIN2vec: Balancing the Type of Relation in Heterogeneous Information Network

- **From inverse training ratio tensor to stochastic matrix**:
  - Sample more of less-trained relations so that the less-trained relations would be reflected more in the embedding space
- Perturbation approach with uniform probability:

$$P_{uni_{xy}} = \begin{cases} \frac{1}{degree(t_x)} & \text{if } (t_x, t_y) \in E_{meta} \\ 0 & \text{otherwise} \end{cases}$$

- Probability to move from t_i to t_j in k steps

$$L_{stochastic} = \sum_{i=0}^{k-1} \left| P^{i+1} - \left(P_{uni}^{i+1} + \alpha \left(I_i - 1\right)\right)\right|_F^2$$

Perturbation parameter

- Update stochastic matrix: update nonzero values and clip the values between zero and one
  - Preserve the property in the stochastic matrix

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BHIN2vec: Balancing the Type of Relation in Heterogeneous Information Network

- **Skip-gram model**: Learn embedding table Q where $f(v_i) = Q[i]$
- The skip-gram loss for one random walk w

$$L = -\sum_{i=1}^{l}\sum_{j=1}^{k} \log p\left(w_{i+j} \mid w_i\right) = -\sum_{i=1}^{l}\sum_{j=1}^{k} \log \frac{e^{f(w_{i+j})^{\top} f(w_i)}}{\sum_{v_n}^{V} e^{f(v_n)^{\top} f(w_i)}}.$$

Negative log-likelihood (Softmax function)

Take m samples

$$L = -\sum_{i=1}^{l}\sum_{j=1}^{k}\left(L_p\left(w_{i+j}, w_i\right) + \sum_{v_o}^{N_V} L_n\left(v_o, w_i\right)\right)$$

$$L_p\left(v_c, v_s\right) = \log \sigma\left(f\left(v_c\right)^{\top} f\left(v_s\right)\right)$$

$$L_n\left(v_c, v_s\right) = \log \sigma\left(-f\left(v_c\right)^{\top} f\left(v_s\right)\right),$$

Sigmoid function

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BHIN2vec: Skip-gram model

- Multi-task setting: Possible task set is defined

$$\mathfrak{J}_{possible} = \left\{ J_{xyz} \mid \left(A^{z}\right)_{xy} > 0 \right\}$$

$$A = \text{the adjacency matrix of } G_{meta}$$

- Balance in multitasks:

$$L\left[J_{xyz}\right] = -\frac{\sum_{i=1}^{l}\left(L\left[J_{xyz}\right]_{p}\left(w_{i+z+1}, w_{i}\right) + \sum_{v_o}^{N_V} L\left[J_{xyz}\right]_{n}\left(v_{o}, w_{i}\right)\right)}{\sum_{i=1}^{l}\left(\mathbb{I}\left[J_{xyz}\right]\left(w_{i+z+1}, w_{i}\right) + \sum_{v_o}^{N_V} \mathbb{I}\left[J_{xyz}\right]\left(v_{o}, w_{i}\right)\right)}$$

$$L\left[J_{xyz}\right]_{p}\left(v_{c}, v_{s}\right) = \begin{cases} L_{p}\left(v_{c}, v_{s}\right) & \text{if } \phi\left(v_{c}\right) = t_{y} \wedge \phi\left(v_{s}\right) = t_{x} \\ 0 & \text{otherwise} \end{cases}$$

$$L\left[J_{xyz}\right]_{n}\left(v_{c}, v_{s}\right) = \begin{cases} L_{n}\left(v_{c}, v_{s}\right) & \text{if } \phi\left(v_{c}\right) = t_{y} \wedge \phi\left(v_{s}\right) = t_{x} \\ 0 & \text{otherwise} \end{cases}$$

$$\mathbb{I}\left[J_{xyz}\right]\left(v_{c}, v_{s}\right) = \begin{cases} 1 & \text{if } \phi\left(v_{c}\right) = t_{y} \wedge \phi\left(v_{s}\right) = t_{x} \\ 0 & \text{otherwise} \end{cases}$$

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BHIN2vec: Skip-gram model

- The inverse training ratios (some relation types are not contained in a random walk by chance)

$$\tilde{L}\left[J_{xyz}\right](t) = L\left[J_{xyz}\right]/L_{initial}\left[J_{xyz}\right]$$
$$r\left[J_{xyz}\right](t) = \tilde{L}\left[J_{xyz}\right](t)/\mathbb{E}_{\mathcal{J}_{possible}}\left[\tilde{L}[J](t)\right],$$

- The tasks that always not occur in a random walk

$$I_{zxy}(t) = \begin{cases} r[J_{xyz}](t) & \text{if } J_{xyz} \in \mathcal{J}_{possible} \\ 1 & \text{otherwise} \end{cases}$$

- Heterogeneous skip-gram model: Sample negative nodes which have the same type with positive node

$$L_p(v_c, v_s) = \log\sigma\left(\left(\sqrt{r} \odot f(v_c)\right)^{\top}\left(\sqrt{r} \odot f(v_s)\right)\right)$$
$$L_n(v_c, v_s) = \log\sigma\left(-\left(\sqrt{r} \odot f(v_c)\right)^{\top}\left(\sqrt{r} \odot f(v_s)\right)\right)$$
$$r = f_R\left(k, \phi(v_c), \phi(v_s)\right)$$

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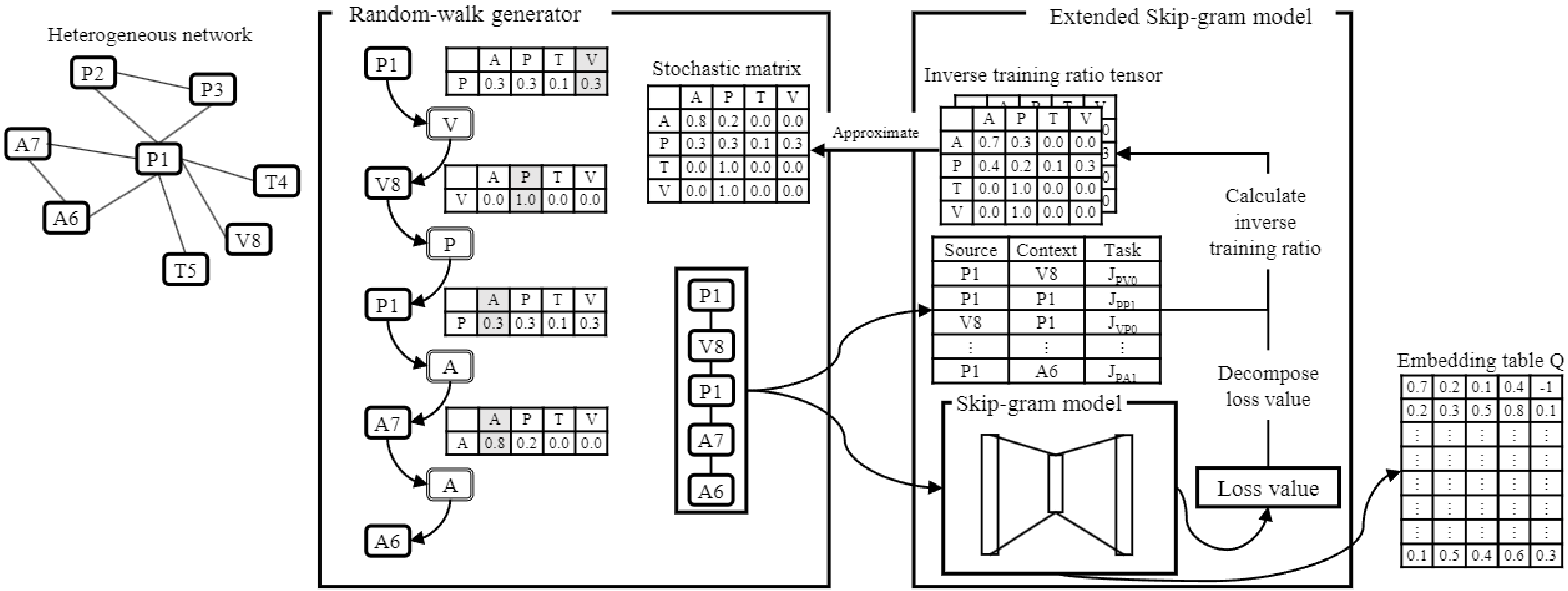
BHIN2vec: Algorithm's Diagram


Heterogeneous network
P2
P3
A7
P1
T4
A6
V8
T5
Random-walk generator
P1
V
V8
P
P1
A
A7
A
A6
Stochastic matrix
P1
V8
P1
A7
A6
Approximate
Extended Skip-gram model
Inverse training ratio tensor
Calculate inverse training ratio
Skip-gram model
Decompose loss value
Loss value
Embedding table Q

	A	P	T	V
P	0.3	0.3	0.1	0.3

	A	P	T	V
V	0.0	1.0	0.0	0.0

	A	P	T	V
P	0.3	0.3	0.1	0.3

	A	P	T	V
A	0.8	0.2	0.0	0.0

Stochastic matrix

	A	P	T	V
A	0.8	0.2	0.0	0.0
P	0.3	0.3	0.1	0.3
T	0.0	1.0	0.0	0.0
V	0.0	1.0	0.0	0.0

Inverse training ratio tensor

	A	P	T	V
A	0.7	0.3	0.0	0.0
P	0.4	0.2	0.1	0.3
T	0.0	1.0	0.0	0.0
V	0.0	1.0	0.0	0.0

Source	Context	Task
P1	V8	J_{PV0}
P1	P1	J_{PP1}
V8	P1	J_{VP0}
⋮	⋮	⋮
P1	A6	J_{PA1}

Embedding table Q

0.7	0.2	0.1	0.4	-1
0.2	0.3	0.5	0.8	0.1
⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮	⋮
0.1	0.5	0.4	0.6	0.3

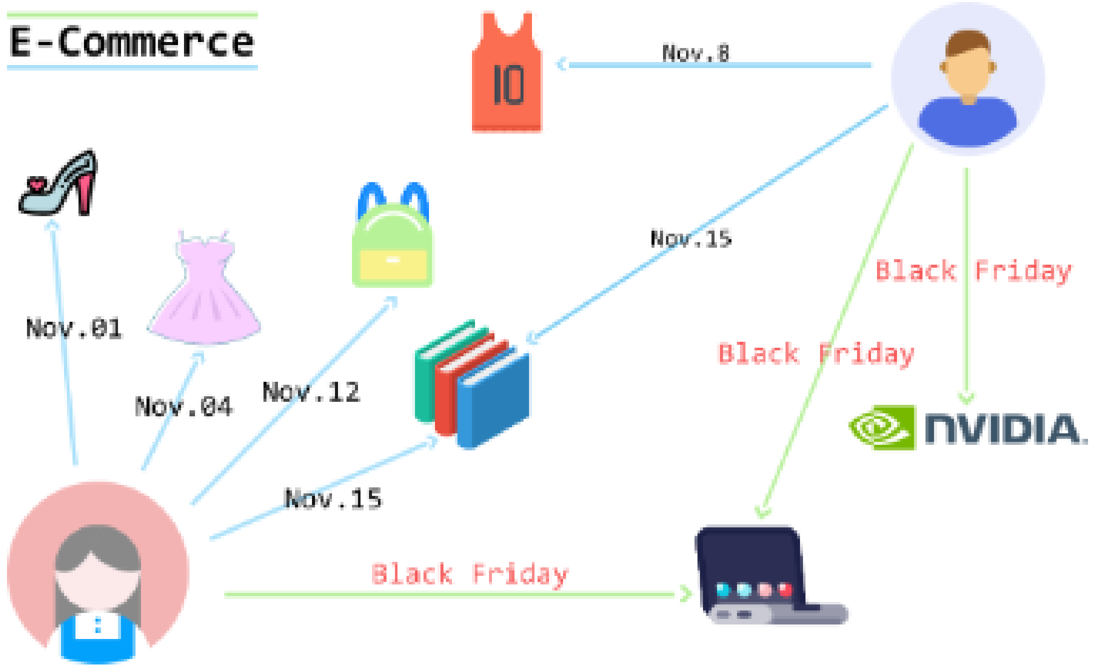
Biased Random Walk

Skip-gram model

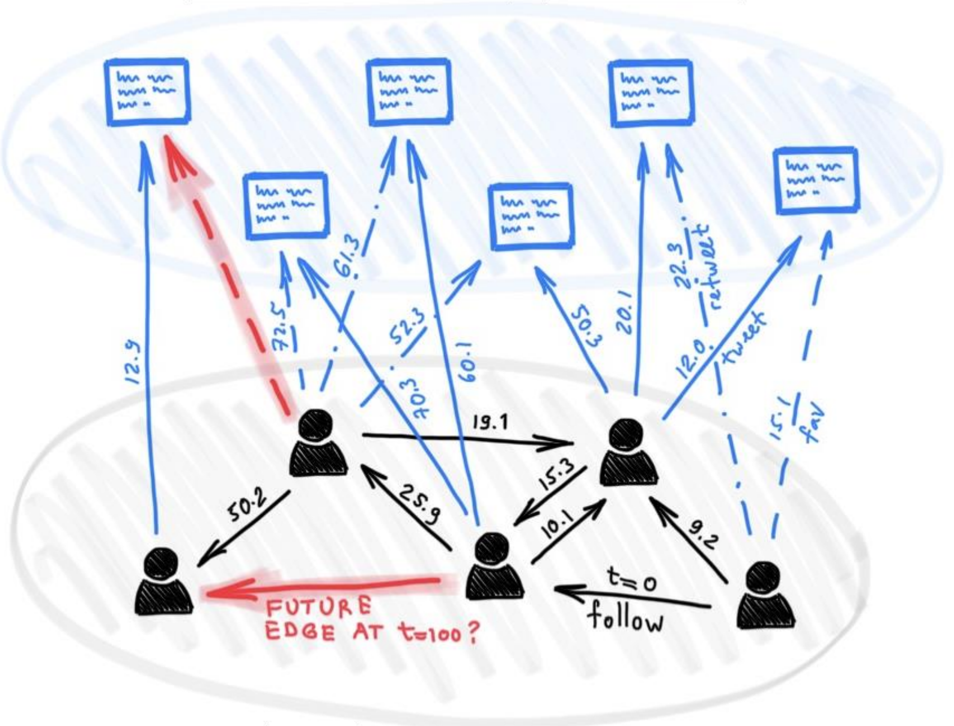
Seonghyeon Lee et al:"BHIN2vec: Balancing the Type of Relation in Heterogeneous Information Network."

Dynamic Network Embedding

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


E-Commerce
Nov.8
Nov.15
Black Friday
Black Friday
Nov.01
Nov.04
Nov.12
Nov.15
Black Friday
10
NVIDIA

An illustration of user-item graph


12.9
72.5
61.3
52.3
70.3
60.1
50.3
20.1
22.3
retweet
12.0
tweet
15.1
fav
19.1
50.2
25.9
15.3
10.1
9.2
t=0
follow
FUTURE
EDGE AT t=100?

An illustration of social graph

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

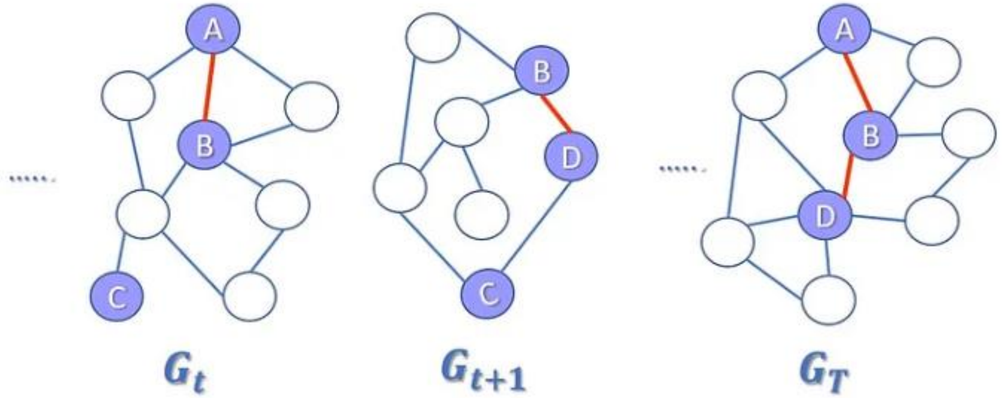
Dynamic Network Embedding: Problem and Challenges

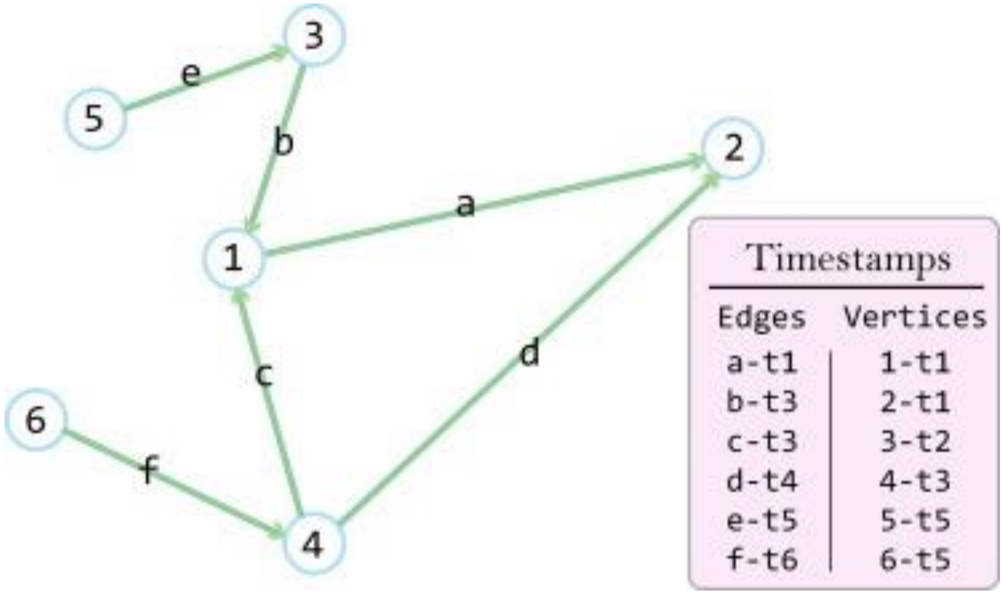
- **Problem**: Learning dynamic node representations
- **Challenges**:
  - Time-varying graph structures: Links and node can emerge and disappear; communities are changing all the time
    - Require the node representations capture both structural proximity (as in static cases) and their temporal evolution
    - 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
    - Require 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
    - $G = \{G_1, \dots, G_T\}$, 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 $\Im : V, E \to \mathbb{R}^+$ is a function that maps each edge and node to a corresponding timestamp





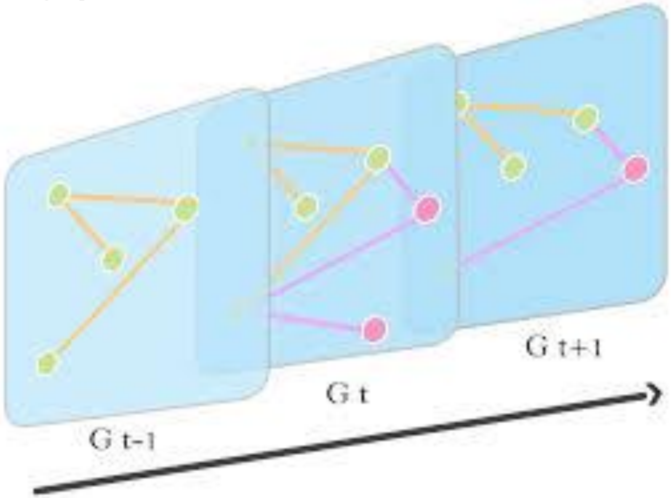
Timestamps

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 nodes) 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
    - Lead to learn embedding vectors separately is a time-consuming process
- **Solution**: dynnode2vec method to modify the node2vec method
  - Employ 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:

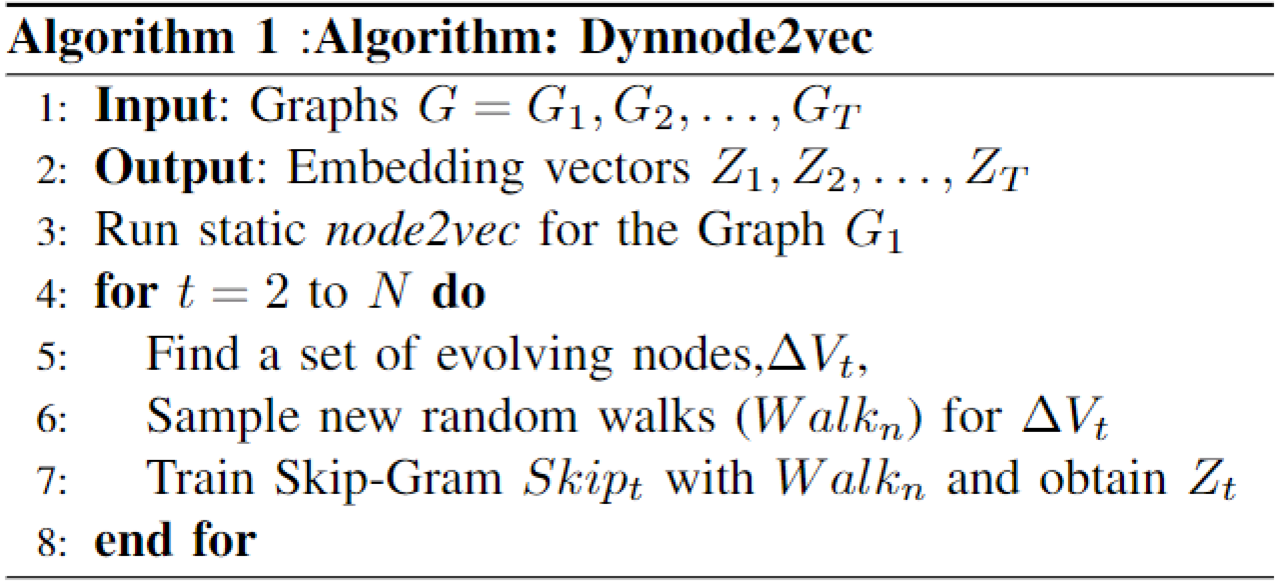
$$\Delta V_t = V_{add} \cup \{v_i \in V_t | \exists e_i = (v_i, v_j) \in (E_{add} \cup E_{del})\}$$

    - Change: New nodes added, existing nodes deleted, or edges added/removed for existing nodes)
- Dynamic Skip-gram Model:
  - Initialize 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."

dynnode2vec: Algorithm

- Run static node2vec on the initial graph G_1 to get embedding vectors Z_1
- For each subsequent timestamp t=2 to T:
  - a) Find evolving node set ΔV_t
  - b) Sample new random walks only for ΔV_t
  - c) Train Skip-gram using new walks, initialized with Skip-gram t-1
  - d) Obtain embedding vectors Z_t



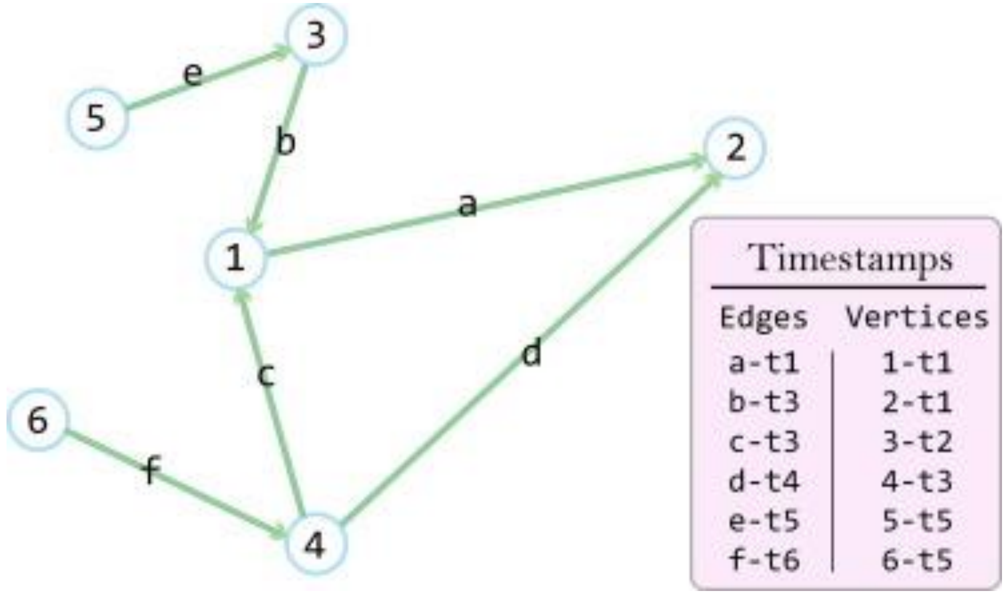
Algorithm 1 :Algorithm: Dynnode2vec

```
**Input**: Graphs $G = G_1, G_2, \dots, G_T$
**Output**: Embedding vectors $Z_1, Z_2, \dots, Z_T$
Run static *node2vec* for the Graph $G_1$
**for** $t = 2$ to $N$ **do**
    Find a set of evolving nodes,$\Delta V_t$,
    Sample new random walks ($Walk_n$) for $\Delta V_t$
    Train Skip-Gram $Skip_t$ with $Walk_n$ and obtain $Z_t$
**end for**
```

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

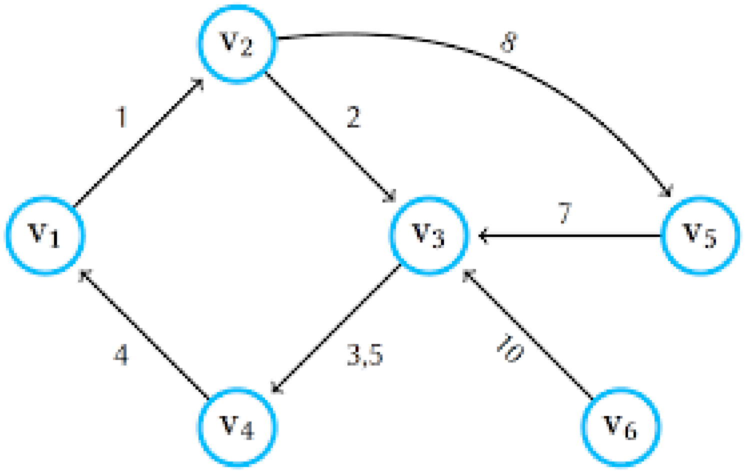
Edges	Vertices
a-t1	1-t1
b-t3	2-t1
c-t3	3-t2
d-t4	4-t3
e-t5	5-t5
f-t6	6-t5

Giang Hoang Nguyen et al: "Continuous-Time Dynamic Network Embeddings"

Continuous-Time Dynamic Network Embeddings

- A continuous-time dynamic network is defined as $G = (V, E_T, \mathfrak{I})$
  - V: set of nodes
  - $E_T \subseteq V \times V \times R^{+}$: set of temporal edges between vertices in V
  - $\mathfrak{I}: \mathrm{E} \rightarrow \mathrm{R}^{+}$: 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 nodes $\langle v_1, v_2, \ldots, v_k \rangle$ such that
    - $\langle v_i, v_{i+1} \rangle$ for $1 \leq i < k$ and
    - $\mathfrak{I}(v_i, v_{i+1}) \leq \mathfrak{I}(v_{i+1}, v_{i+2})$ for $1 \leq i < (k-1)$



Giang Hoang Nguyen et al: "Continuous-Time Dynamic Network Embeddings"

Continuous-Time Dynamic Network Embeddings

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

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

- 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

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

Exponential decay: selecting a neighbor decreases exponentially with time

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

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

Giang Hoang Nguyen et al: "Continuous-Time Dynamic Network Embeddings"

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

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

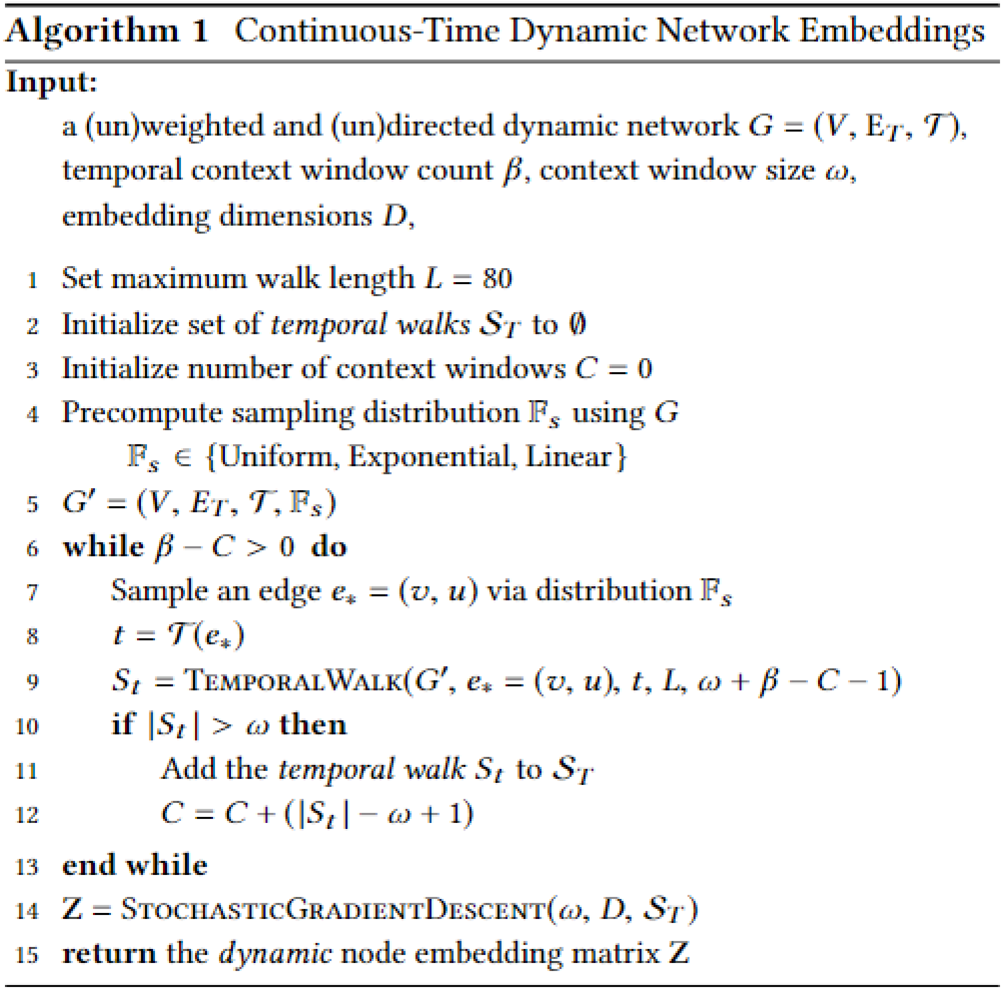
- Learning time-preserving embeddings: maximize the likelihood of observing temporal context windows given the embeddings

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

➡ Utilizing stochastic gradient descent

Giang Hoang Nguyen et al: "Continuous-Time Dynamic Network Embeddings"

Continuous-Time Dynamic Network Embeddings: Algorithm

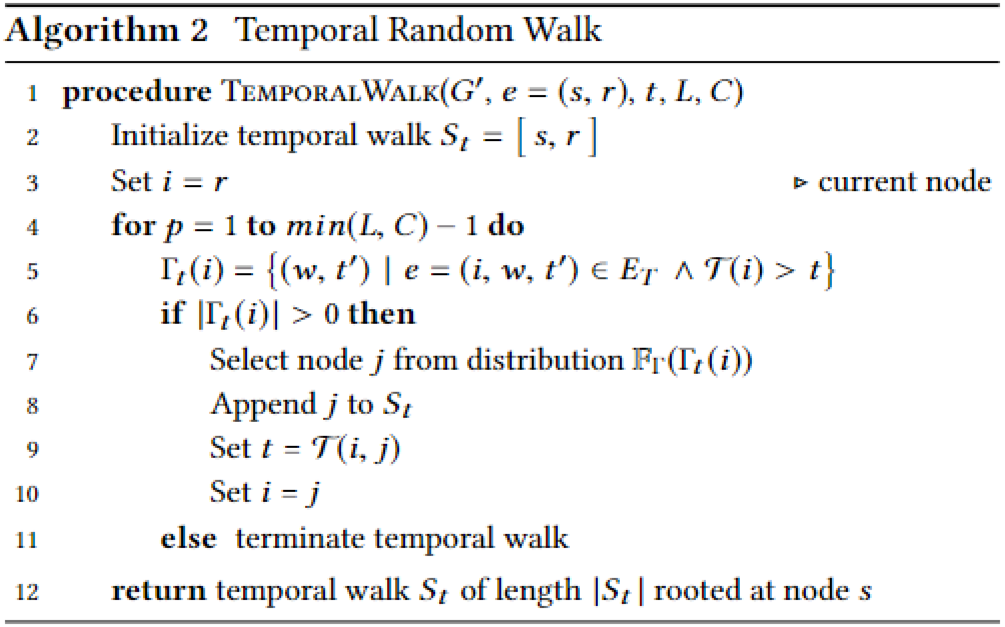


Algorithm 1 Continuous-Time Dynamic Network Embeddings

Input:

```
a (un)weighted and (un)directed dynamic network $G = (V, E_T, \mathcal{T})$,
temporal context window count $\beta$, context window size $\omega$,
embedding dimensions $D$,

Set maximum walk length $L = 80$
Initialize set of temporal walks $\mathcal{S}_T$ to $\emptyset$
Initialize number of context windows $C = 0$
Precompute sampling distribution $\mathbb{F}_s$ using $G$
    $\mathbb{F}_s \in \{$Uniform, Exponential, Linear$\}$
$G' = (V, E_T, \mathcal{T}, \mathbb{F}_s)$
while $\beta - C > 0$ do
    Sample an edge $e_* = (v, u)$ via distribution $\mathbb{F}_s$
    $t = \mathcal{T}(e_*)$
    $S_t$ = TemporalWalk($G'$, $e_* = (v, u)$, $t$, $L$, $\omega + \beta - C - 1$)
    if $|S_t| > \omega$ then
        Add the temporal walk $S_t$ to $\mathcal{S}_T$
        $C = C + (|S_t| - \omega + 1)$
end while
$\mathbf{Z}$ = StochasticGradientDescent($\omega$, $D$, $\mathcal{S}_T$)
return the dynamic node embedding matrix $\mathbf{Z}$
```



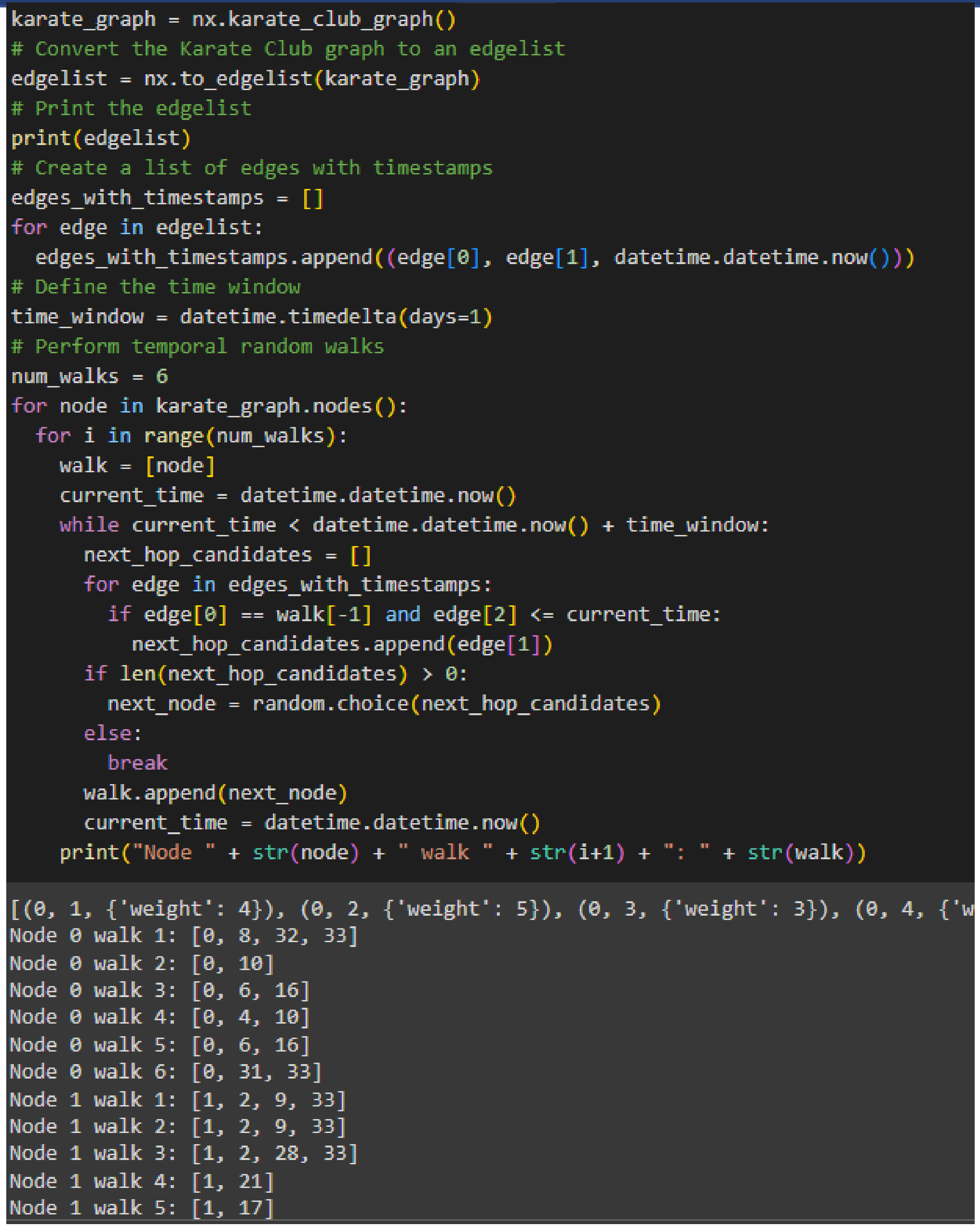
Algorithm 2 Temporal Random Walk

```
procedure TemporalWalk($G'$, $e = (s, r)$, $t$, $L$, $C$)
    Initialize temporal walk $S_t = [\, s, r \,]$
    Set $i = r$                                        ▷ current node
    for $p = 1$ to $min(L, C) - 1$ do
        $\Gamma_t(i) = \{(w, t') \mid e = (i, w, t') \in E_T \wedge \mathcal{T}(i) > t\}$
        if $|\Gamma_t(i)| > 0$ then
            Select node $j$ from distribution $\mathbb{F}_\Gamma(\Gamma_t(i))$
            Append $j$ to $S_t$
            Set $t = \mathcal{T}(i, j)$
            Set $i = j$
        else terminate temporal walk
    return temporal walk $S_t$ of length $|S_t|$ rooted at node $s$
```

- Initialize parameters and precompute sampling distributions
- Sample temporal walks using the specified distributions
- Use stochastic gradient descent to optimize the embeddings

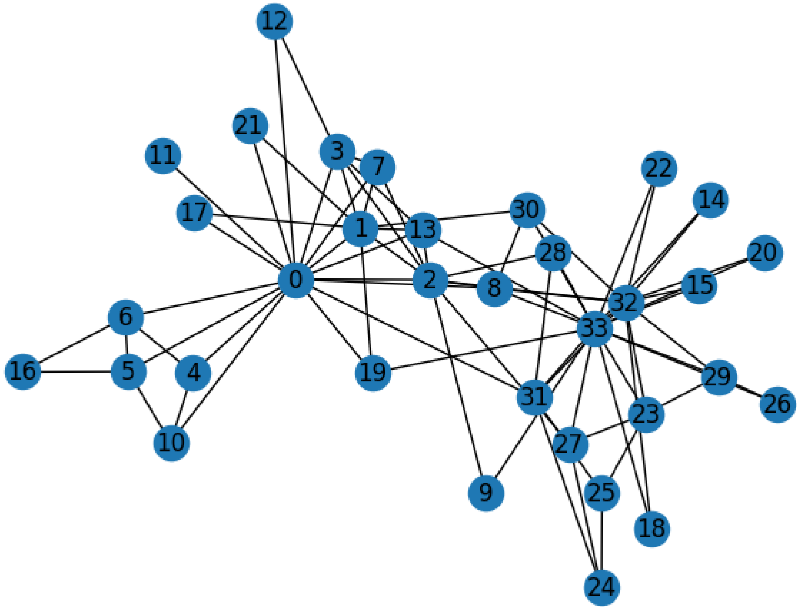
Giang Hoang Nguyen et al: "Continuous-Time Dynamic Network Embeddings"

Sample code of Temporal Random Walk in Karate Graph



```
karate_graph = nx.karate_club_graph()
# Convert the Karate Club graph to an edgelist
edgelist = nx.to_edgelist(karate_graph)
# Print the edgelist
print(edgelist)
# Create a list of edges with timestamps
edges_with_timestamps = []
for edge in edgelist:
  edges_with_timestamps.append((edge[0], edge[1], datetime.datetime.now()))
# Define the time window
time_window = datetime.timedelta(days=1)
# Perform temporal random walks
num_walks = 6
for node in karate_graph.nodes():
  for i in range(num_walks):
    walk = [node]
    current_time = datetime.datetime.now()
    while current_time < datetime.datetime.now() + time_window:
      next_hop_candidates = []
      for edge in edges_with_timestamps:
        if edge[0] == walk[-1] and edge[2] <= current_time:
          next_hop_candidates.append(edge[1])
      if len(next_hop_candidates) > 0:
        next_node = random.choice(next_hop_candidates)
      else:
        break
      walk.append(next_node)
      current_time = datetime.datetime.now()
    print("Node " + str(node) + " walk " + str(i+1) + ": " + str(walk))
```

```
[(0, 1, {'weight': 4}), (0, 2, {'weight': 5}), (0, 3, {'weight': 3}), (0, 4, {'w
Node 0 walk 1: [0, 8, 32, 33]
Node 0 walk 2: [0, 10]
Node 0 walk 3: [0, 6, 16]
Node 0 walk 4: [0, 4, 10]
Node 0 walk 5: [0, 6, 16]
Node 0 walk 6: [0, 31, 33]
Node 1 walk 1: [1, 2, 9, 33]
Node 1 walk 2: [1, 2, 9, 33]
Node 1 walk 3: [1, 2, 28, 33]
Node 1 walk 4: [1, 21]
Node 1 walk 5: [1, 17]
```



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