

Metapath2vec

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SML² Lab, University of Trento, Italy

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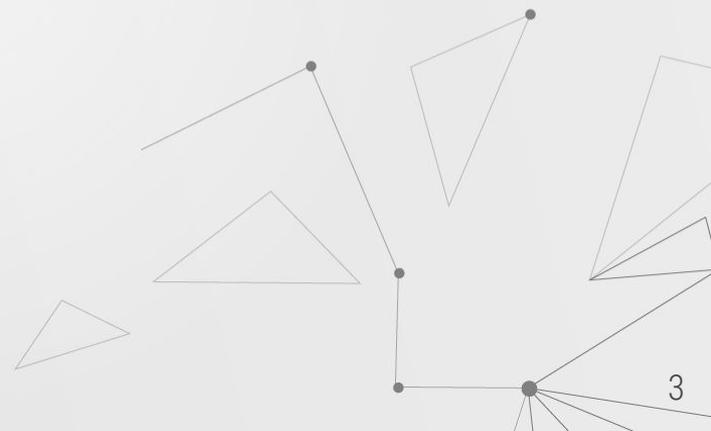
04 Training
(my laptop not powerful enough 😊)

05 Load a pre trained model

06

01 Metapath

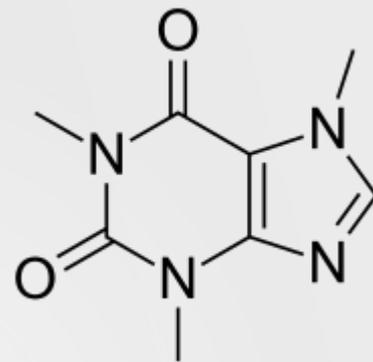
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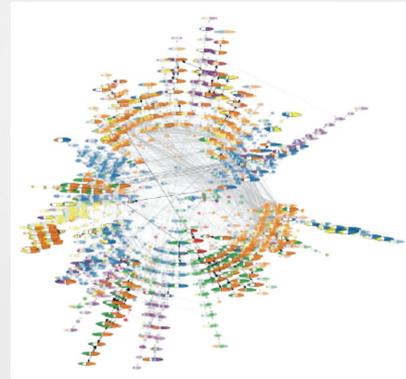
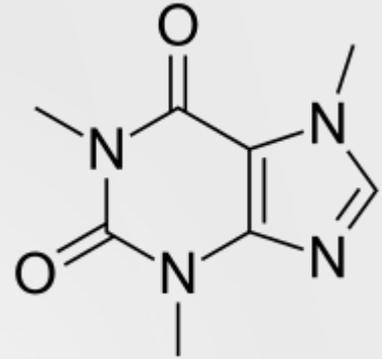
- **Molecules**
- CiteSeer
- Cora



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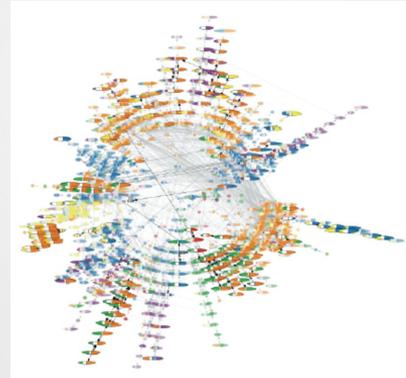
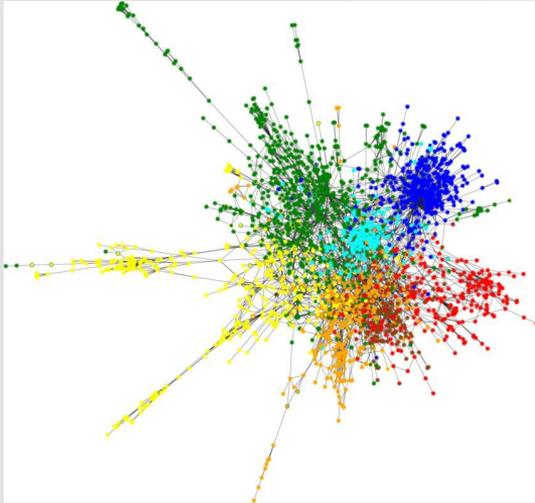
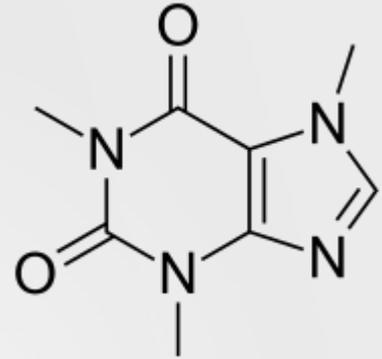
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- **Cora**



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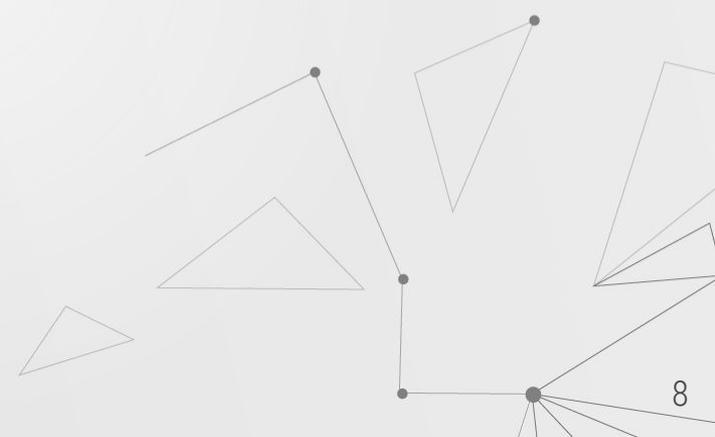
What are **heterogeneous** graph?



01 Metapath

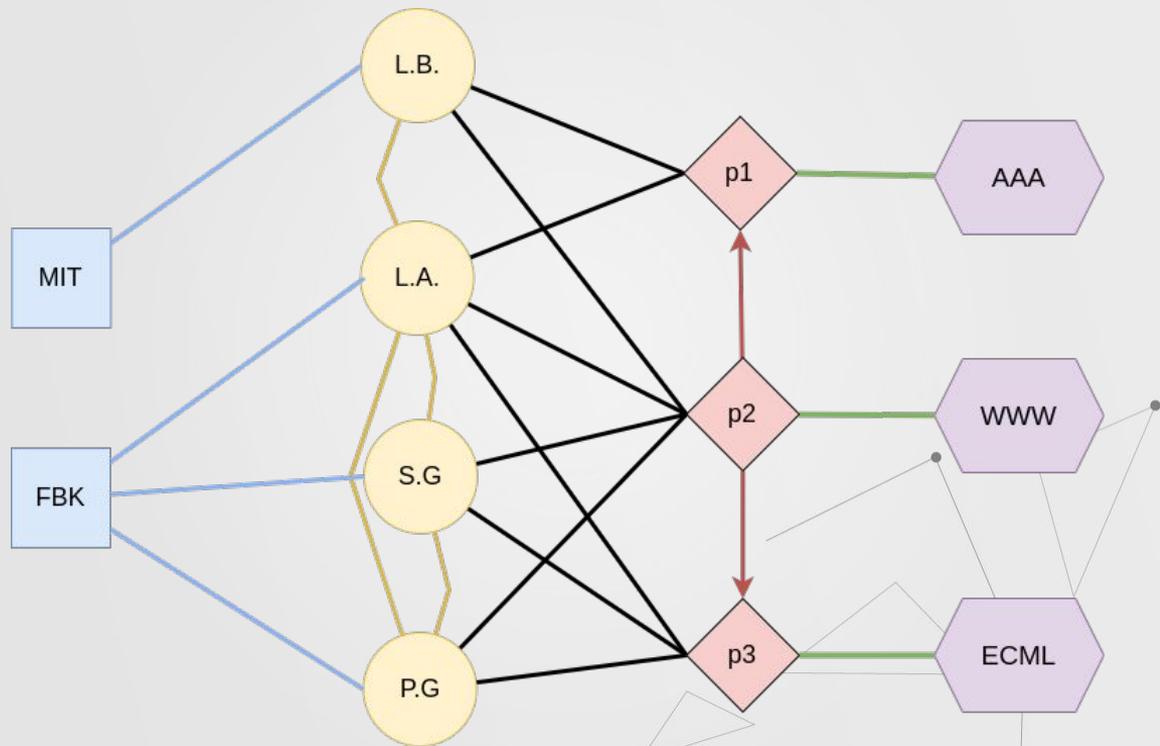
What are **heterogeneous** graph?

An heterogeneous graph is a graph in witch nodes and edges have differents types.



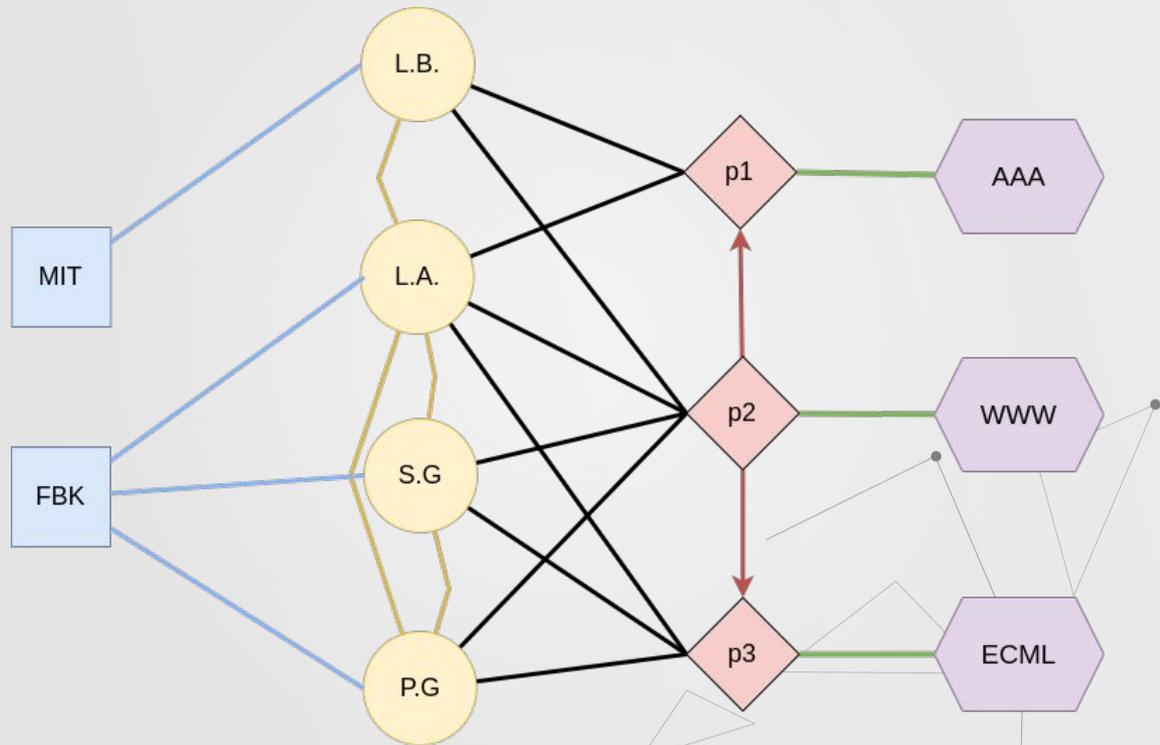
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For instance:



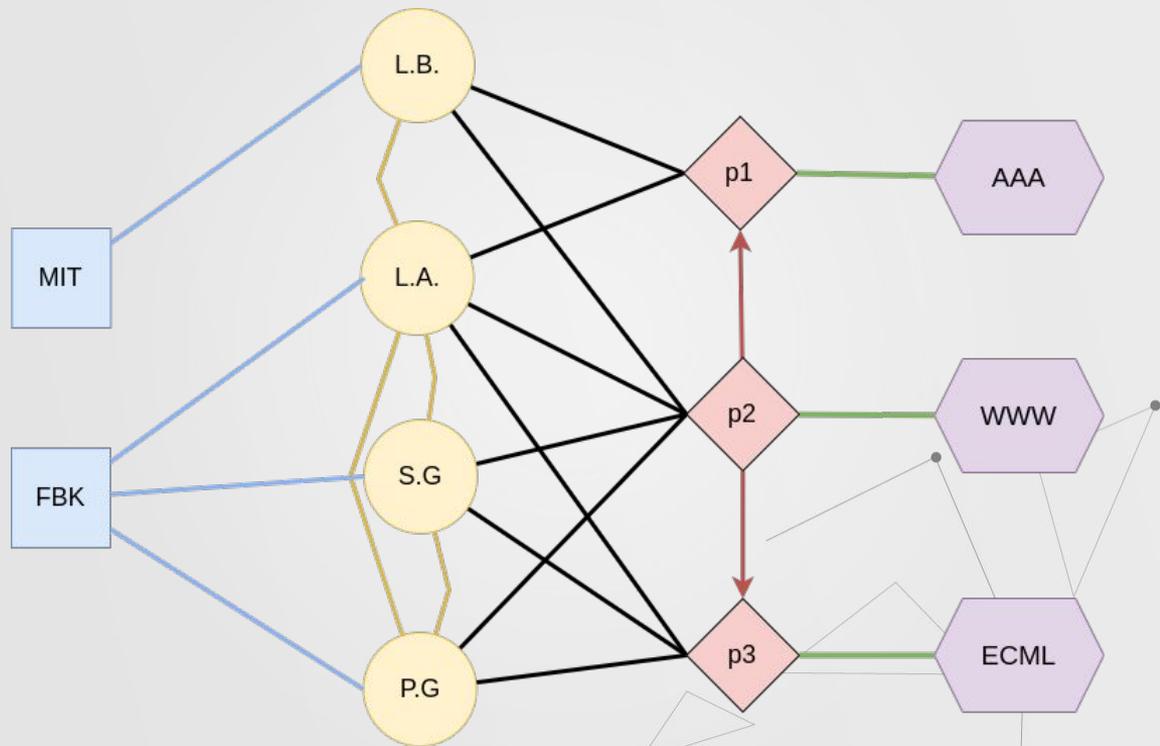
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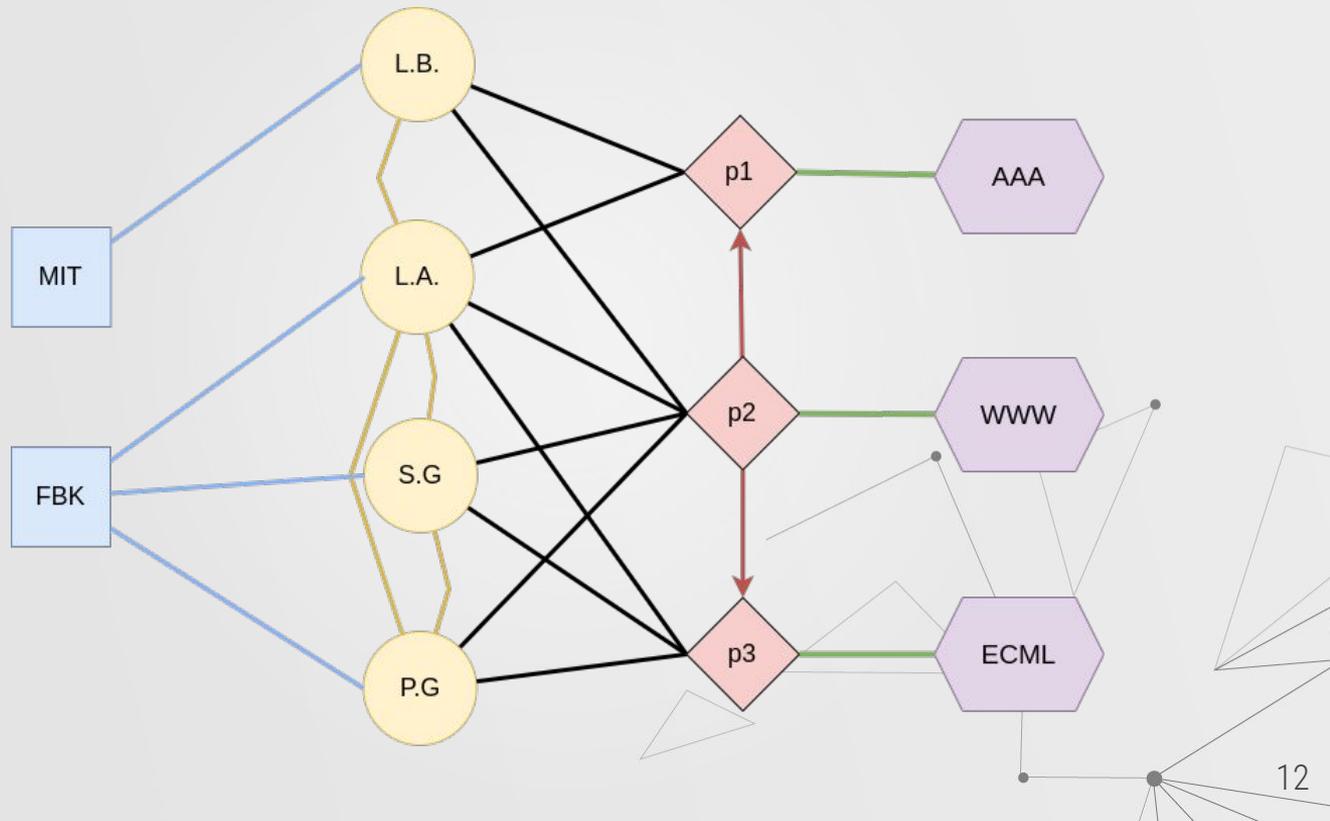
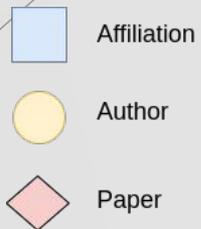
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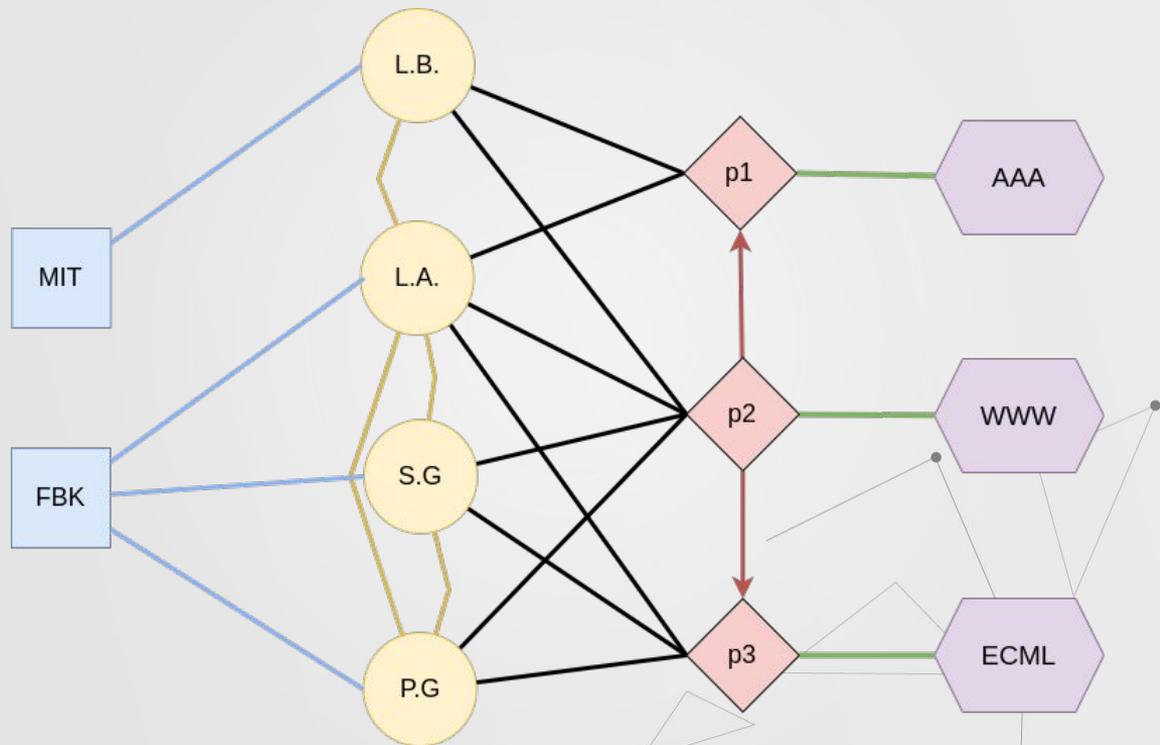
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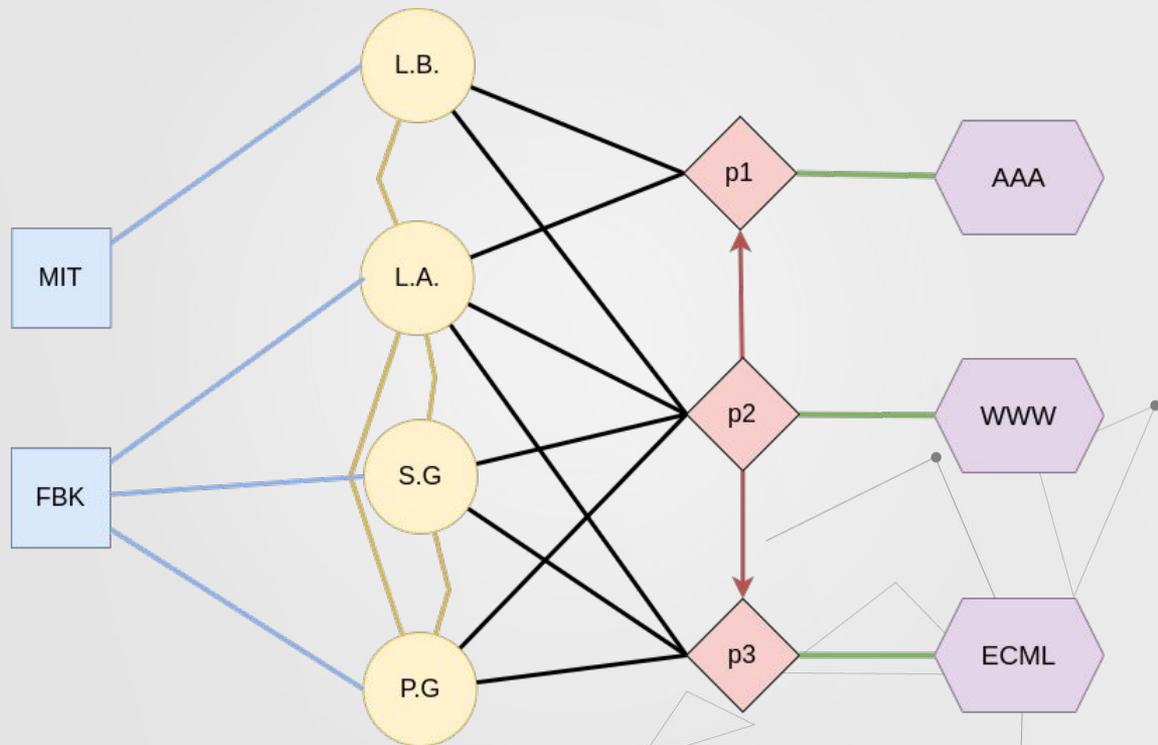
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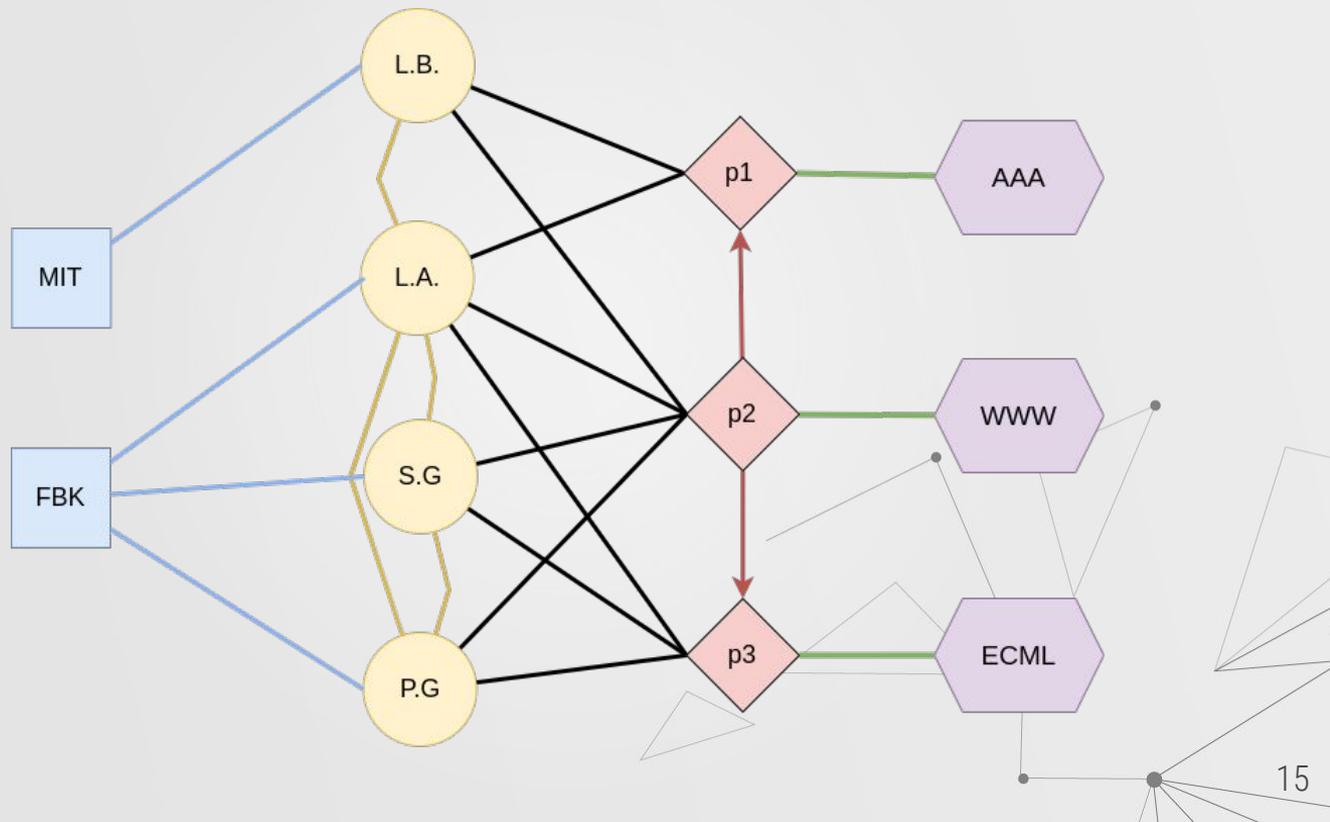
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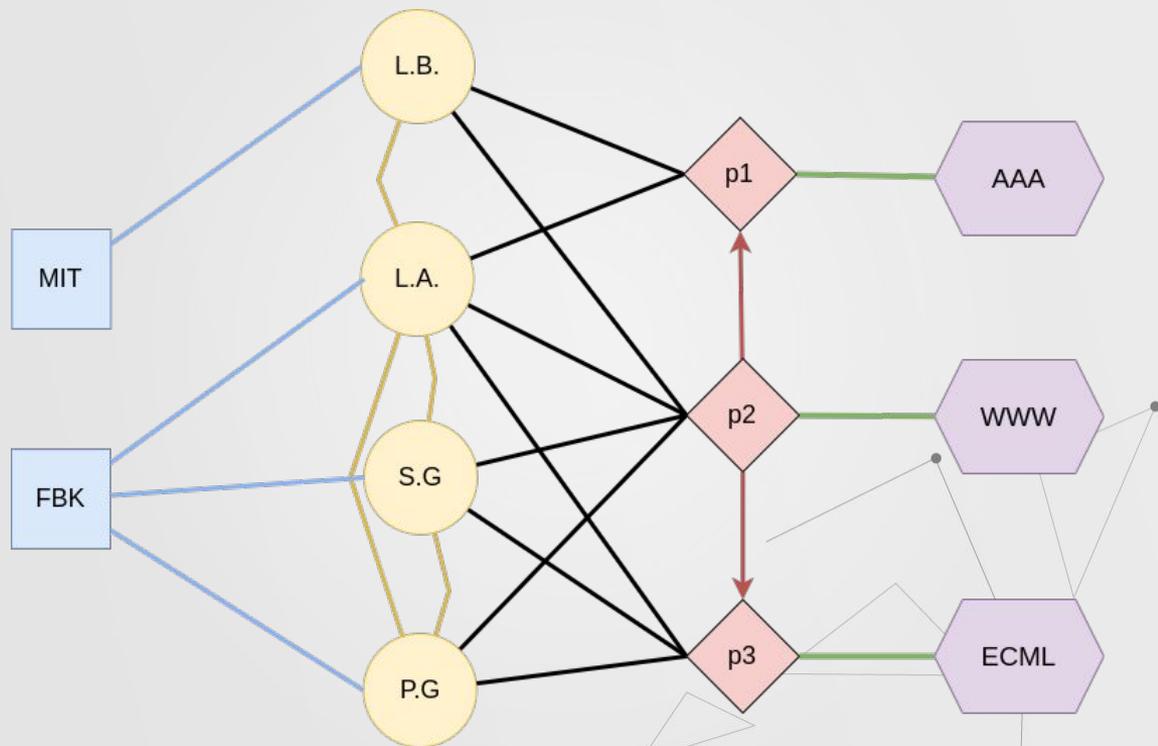
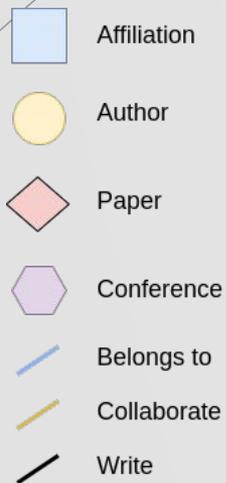
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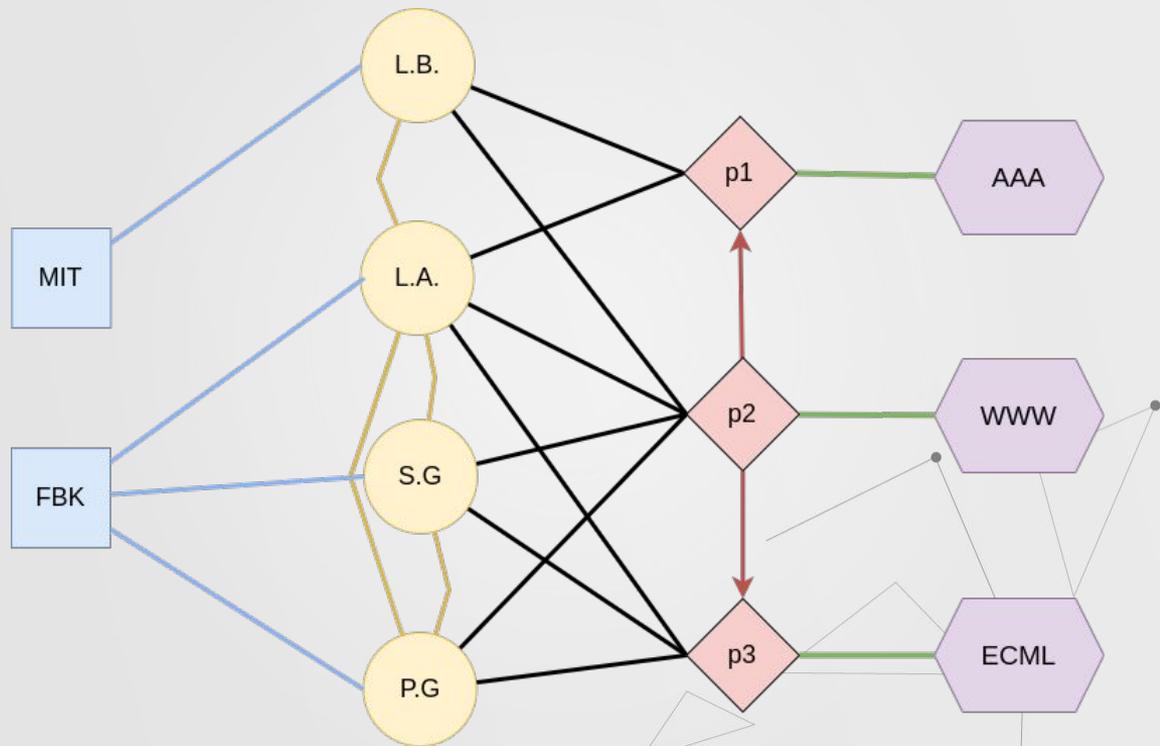
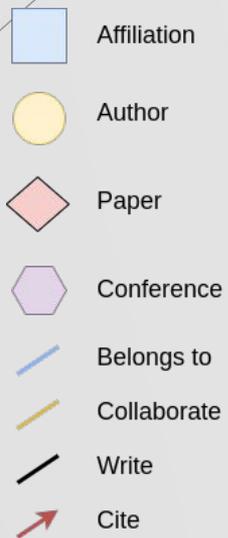
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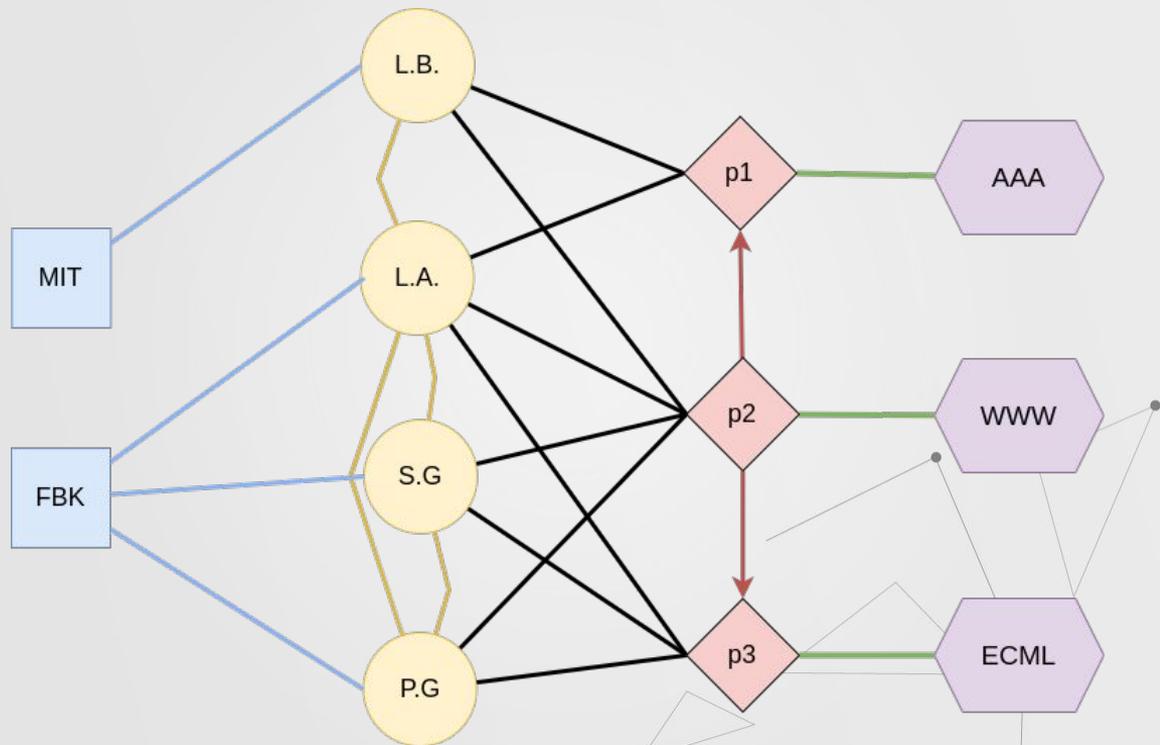
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A **meta path** in a heterogeneous graphs, is a path following a specific meta path scheme P .

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Def:

A **meta path scheme** P is defined as a path that is denoted in the form of :

$$V_1 \xrightarrow{r_1} V_2 \xrightarrow{r_2} V_3 \xrightarrow{r_3} V_4 \xrightarrow{r_4} \dots V_{l-1} \xrightarrow{r_{l-1}} V_l$$

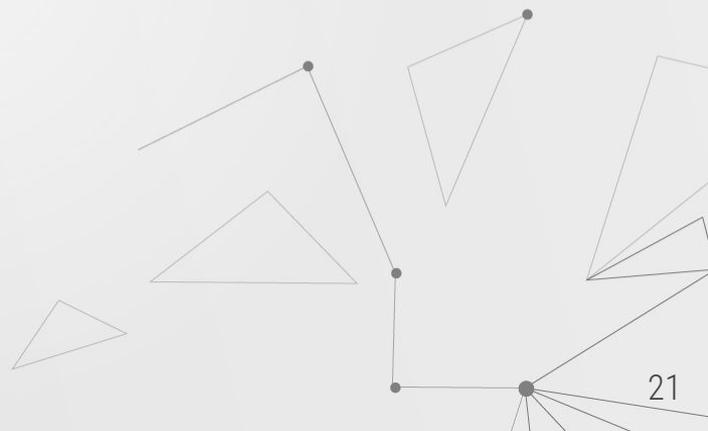
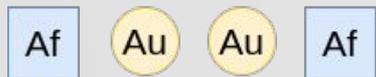
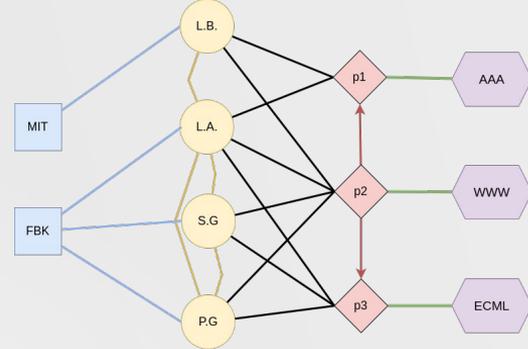
Wherein

$$R = R_1 \cdot R_2 \cdot R_3 \cdot \dots \cdot R_{l-1}$$

Defines the composite relations between nodes types V_1 and V_l

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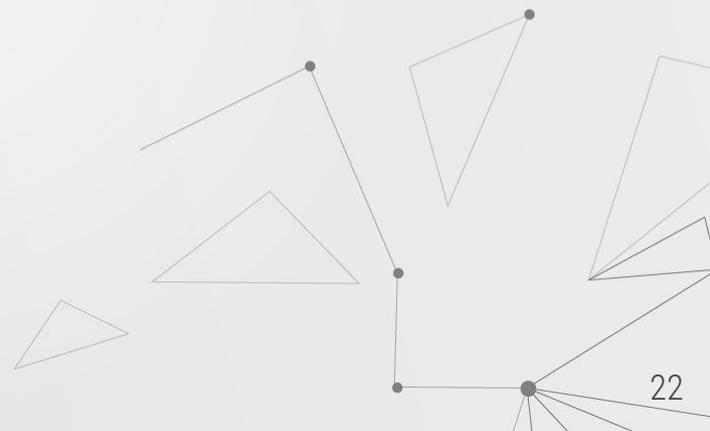
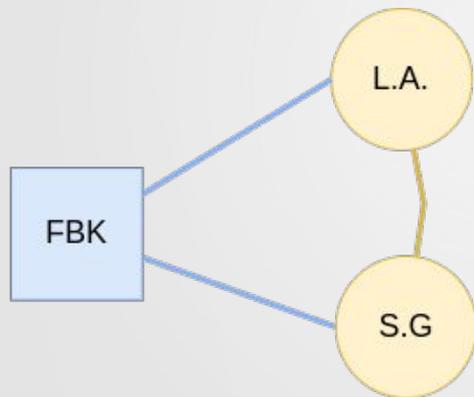
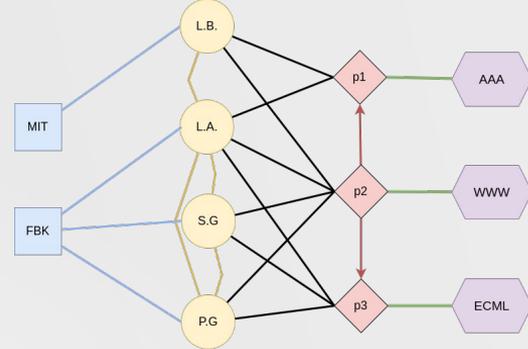
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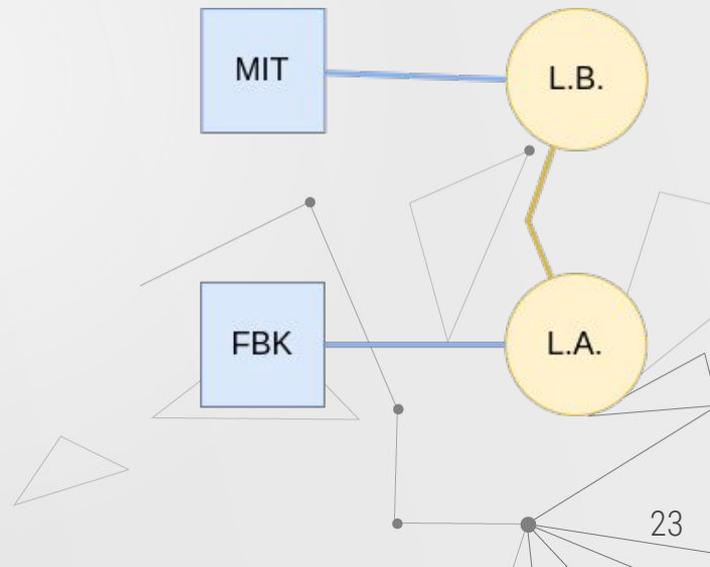
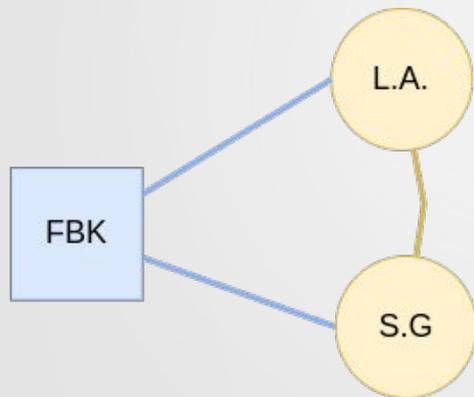
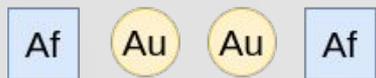
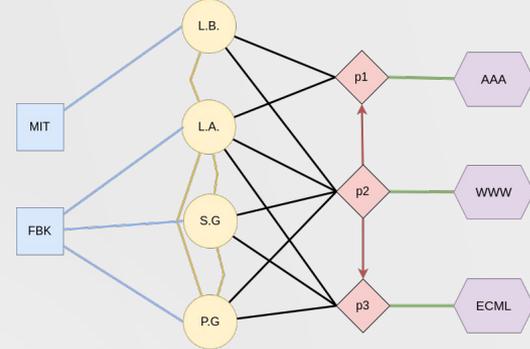
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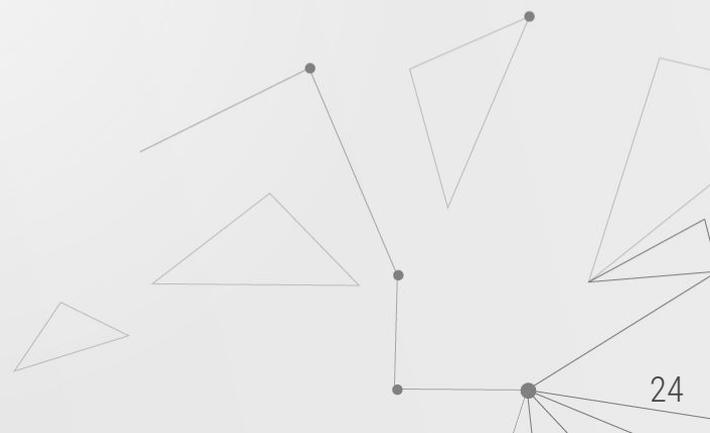
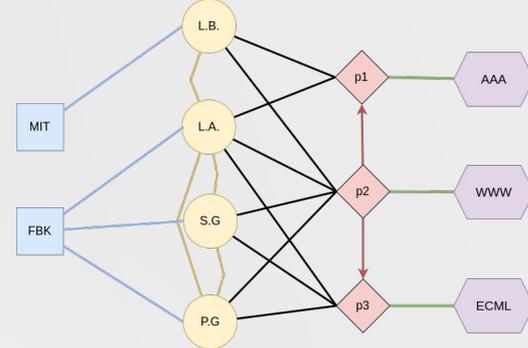


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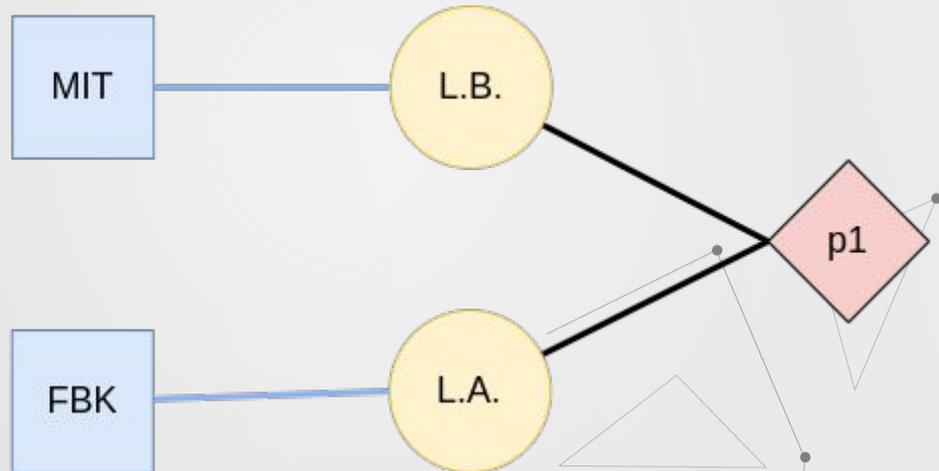
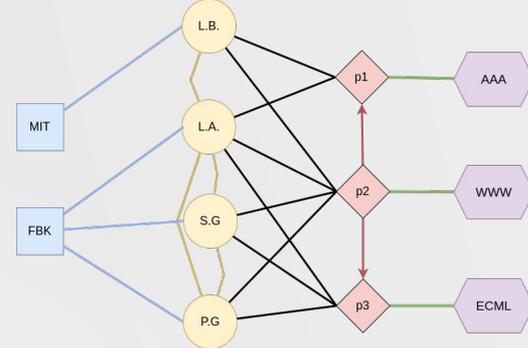
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02 Metapath random walks

Def:

Given an heterogeneous network $G = (V, E, T)$ and a meta path scheme P .

The transition probability at step i is defined as follow:

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Given an heterogeneous network $G = (V, E, T)$ and a meta path scheme \mathcal{P} .

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

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Scheme

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Function that compute the
type of a node

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Node at time $i+1$

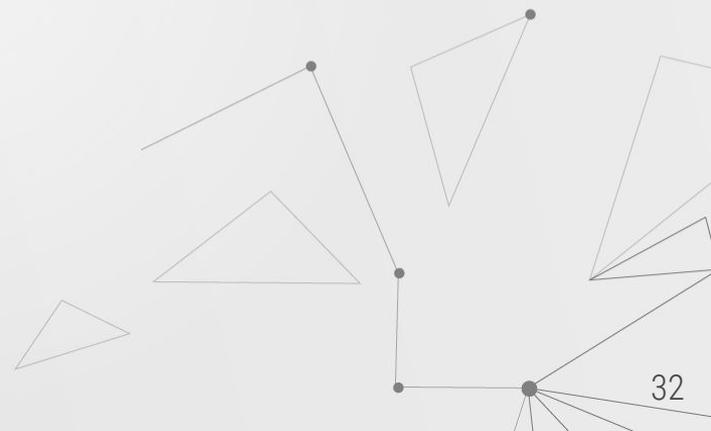
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Scheme

03 The model

Metapath2vec

- Given a specific Scheme P



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Metapath2vec

- Given a specific Scheme P
- Extract random meta path from the input graph

03 The model

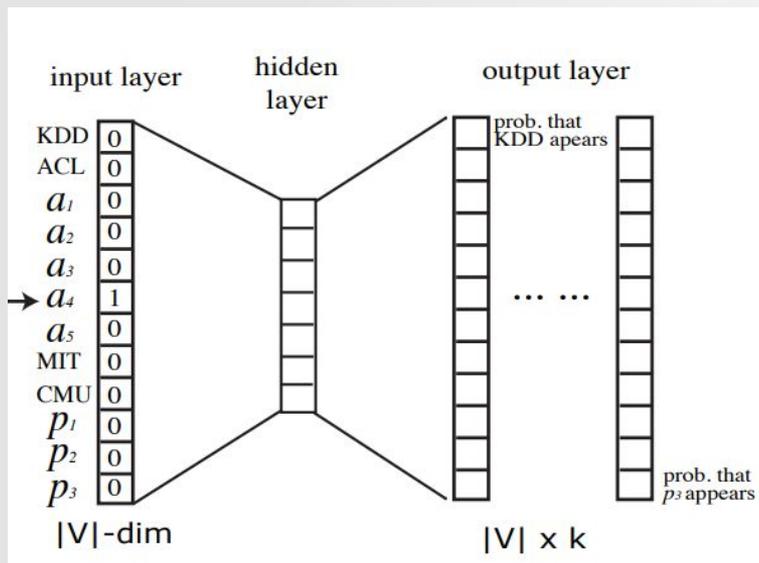
Metapath2vec

- Given a specific Scheme P
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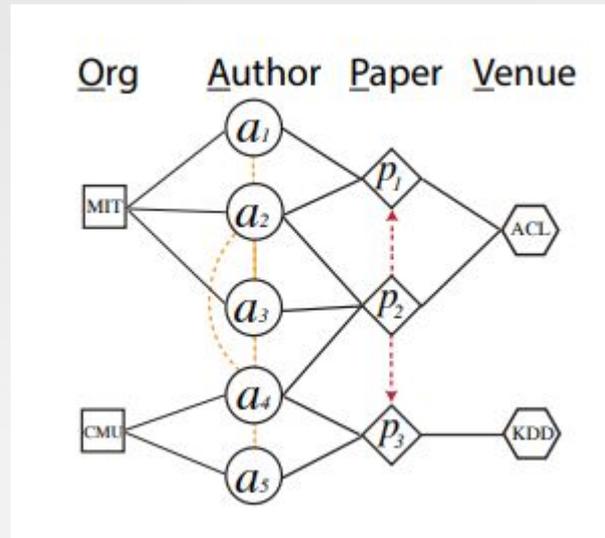
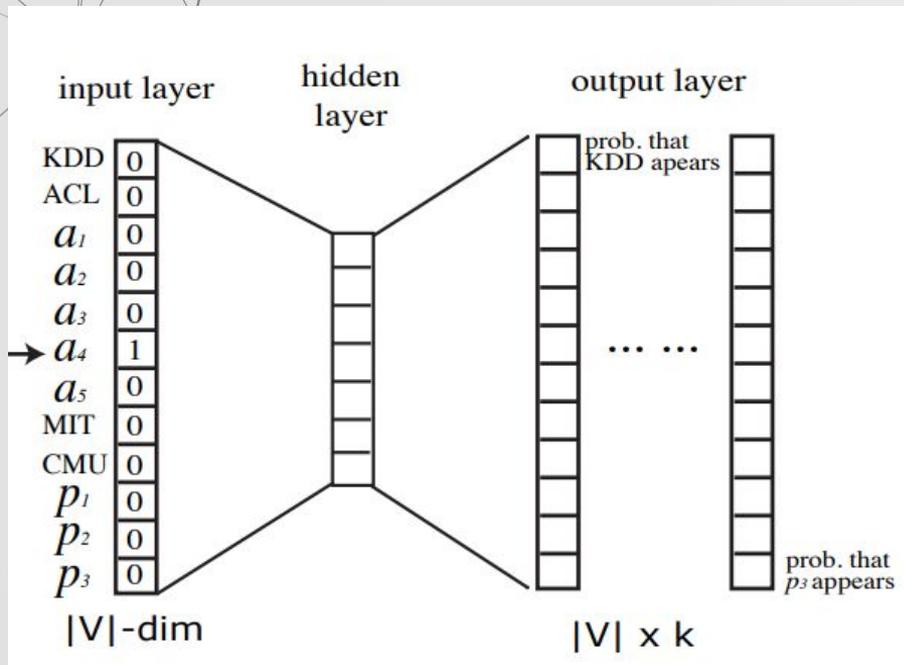
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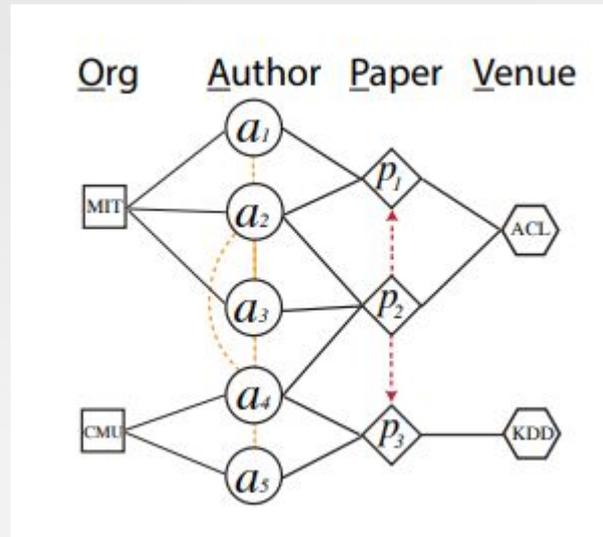
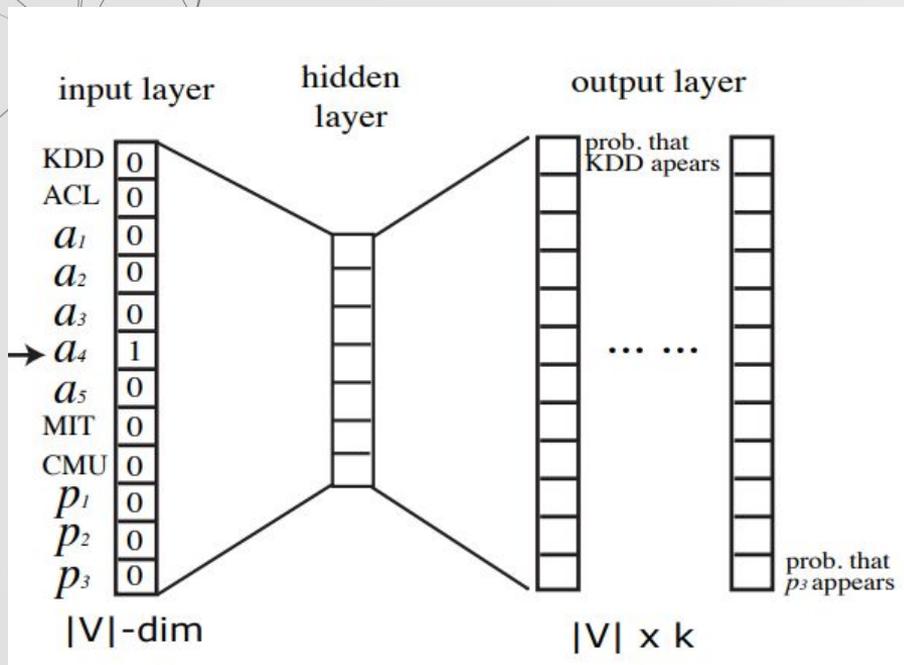
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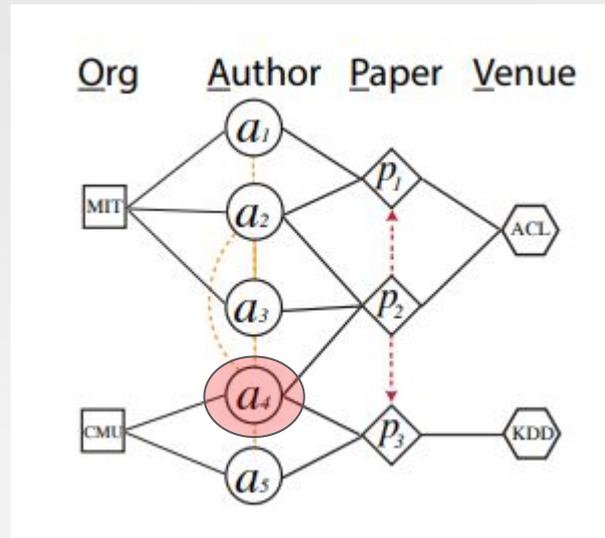
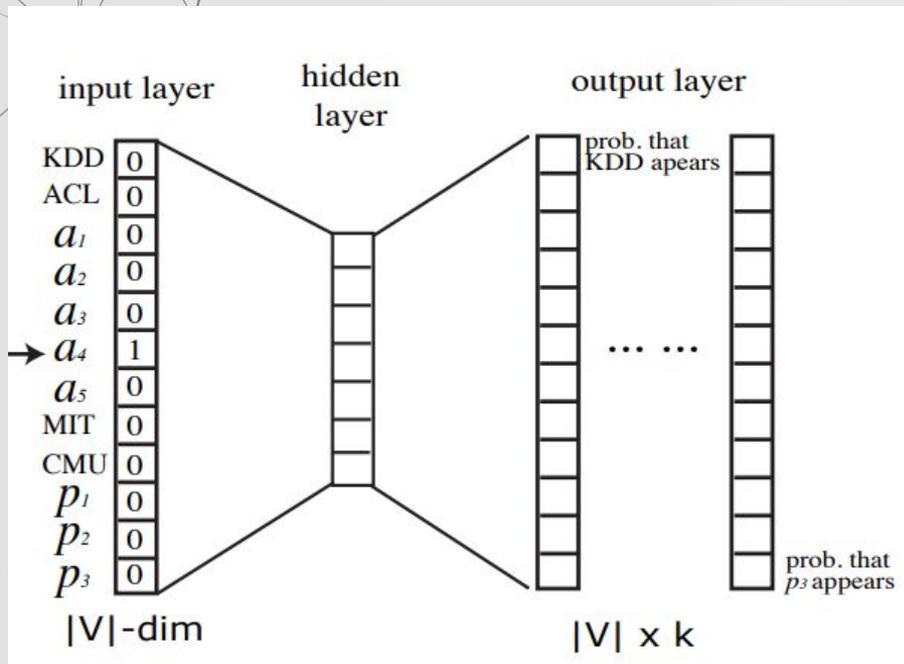
Metapath2vec



In the case of a_4 , the output layer is a **12x8**, because...

03 The model

Metapath2vec

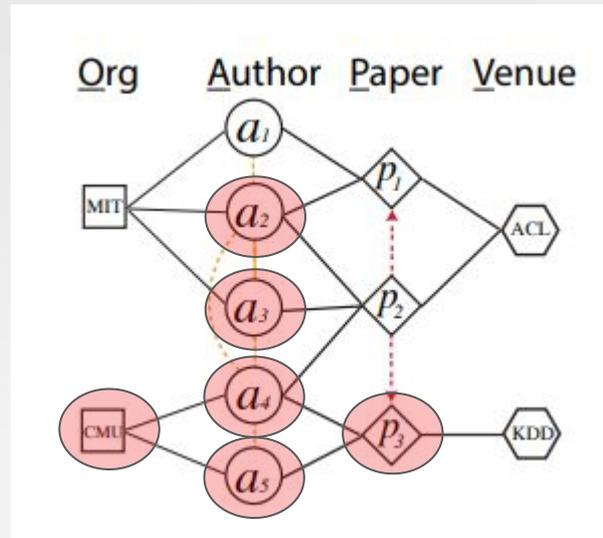
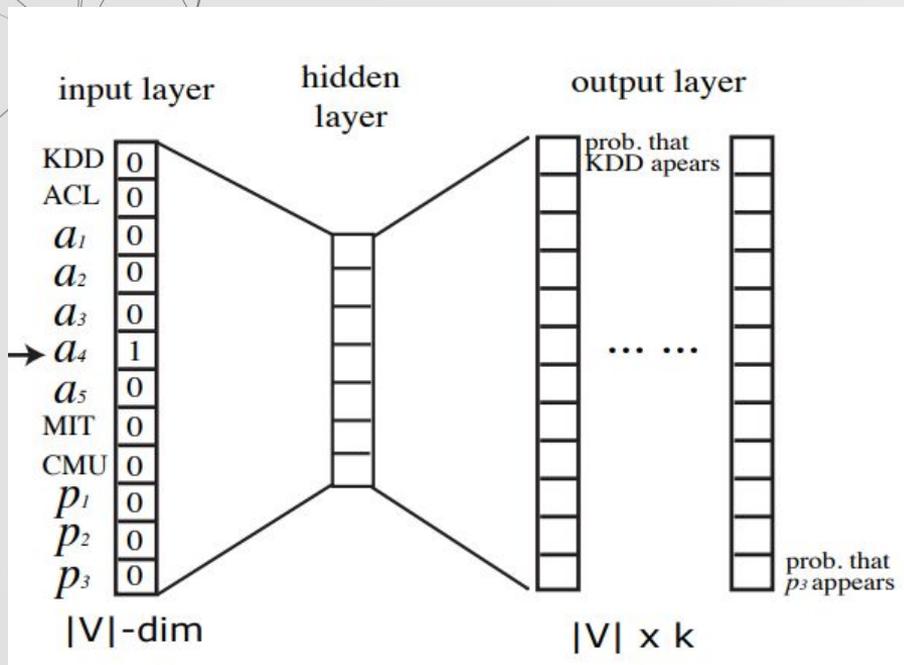


12x0

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03 The model

Metapath2vec

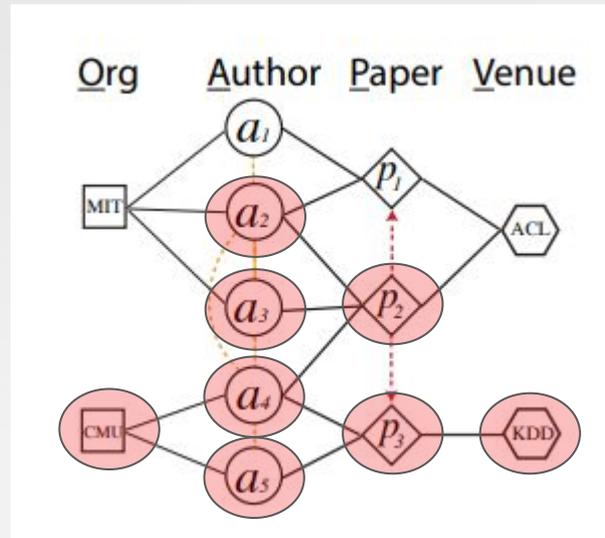
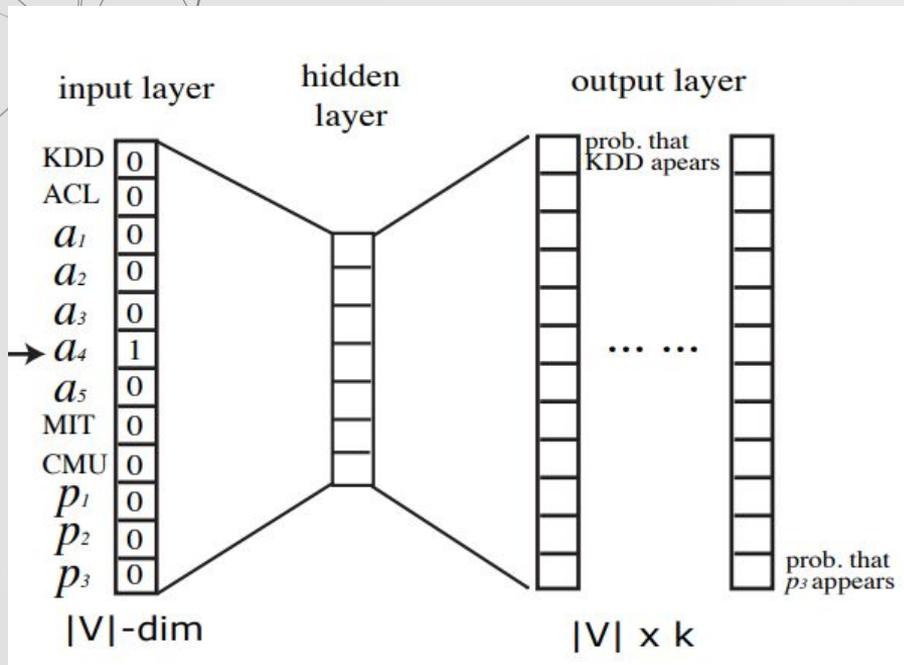


12x5

In the case of a_4 , the output layer is a **12x8**, because...

03 The model

Metapath2vec

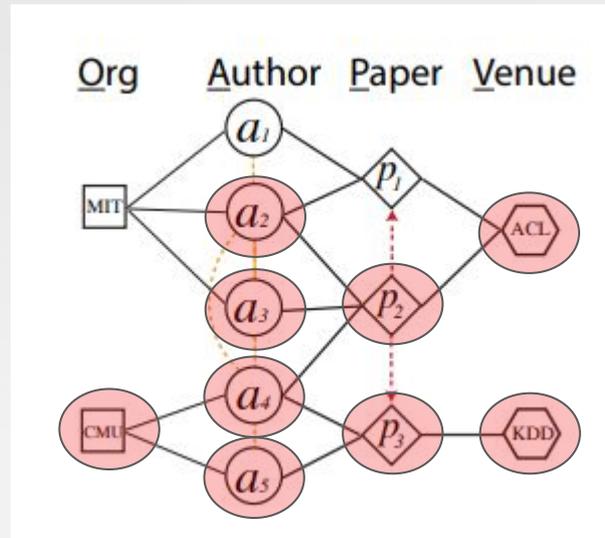
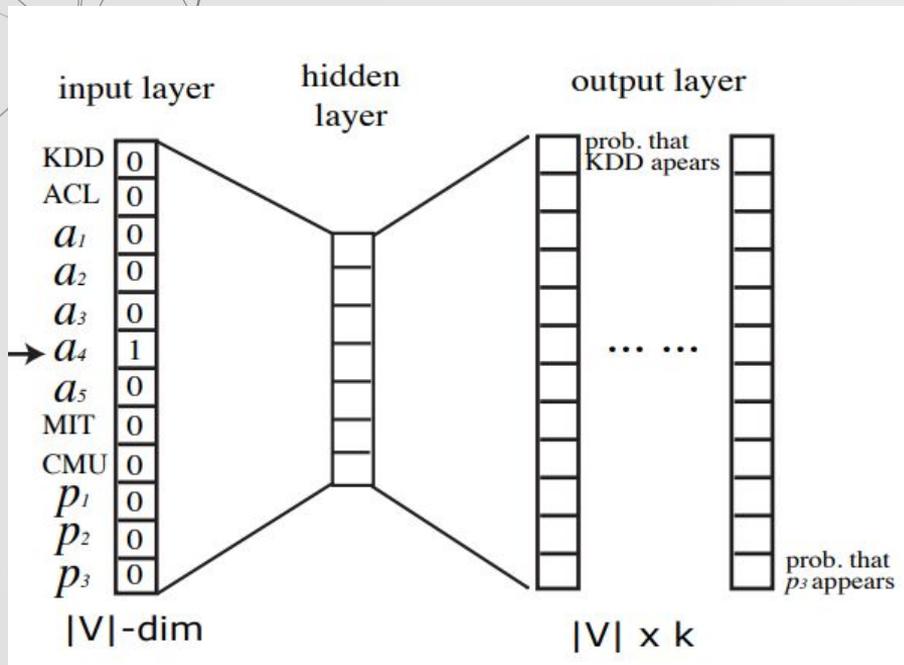


12x7

In the case of a_4 , the output layer is a **12x8**, because...

03 The model

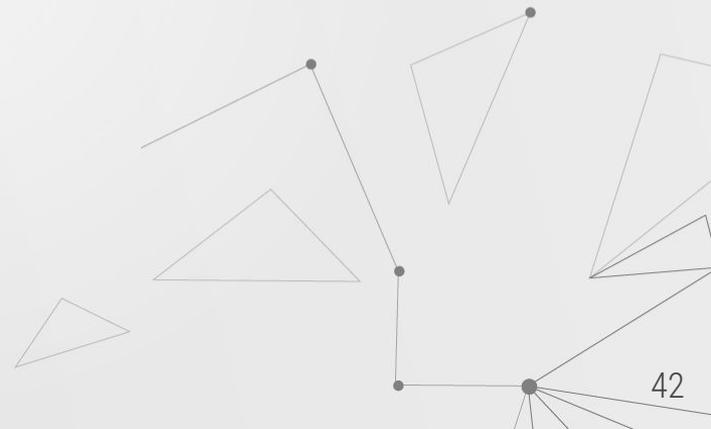
Metapath2vec



12x8

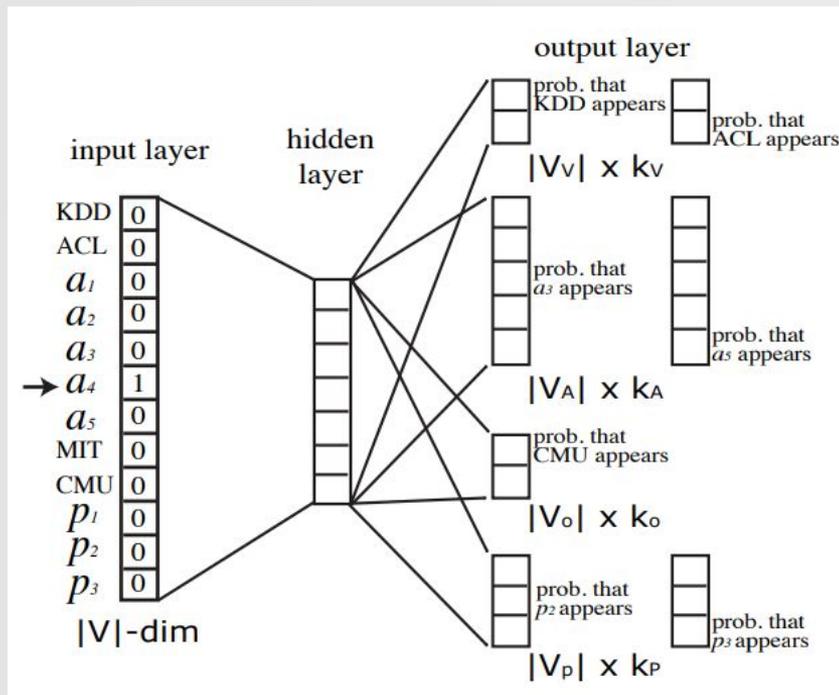
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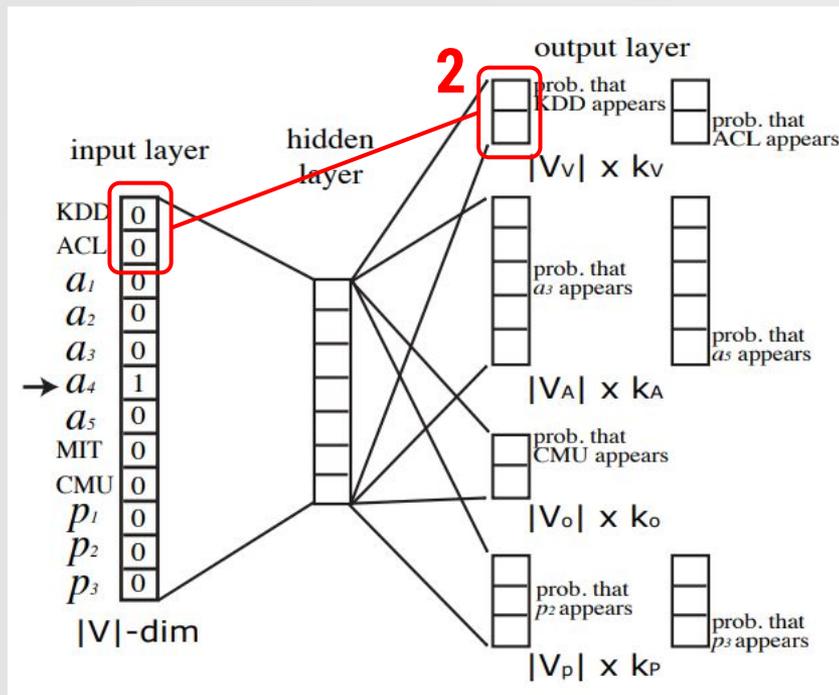
Metapath2vec++



In the case of a_4 , there are 4 output layers, each of them with different size

03 The model

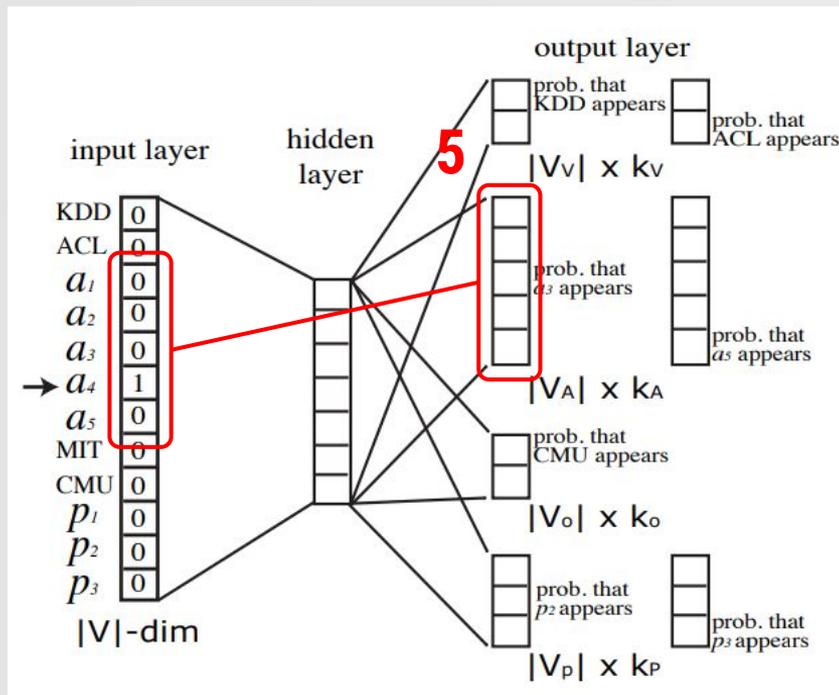
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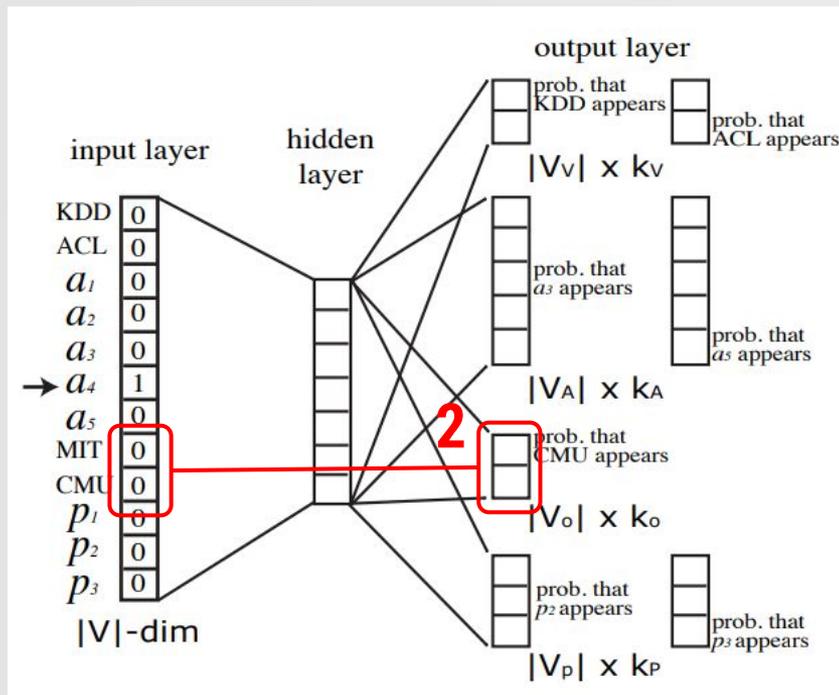
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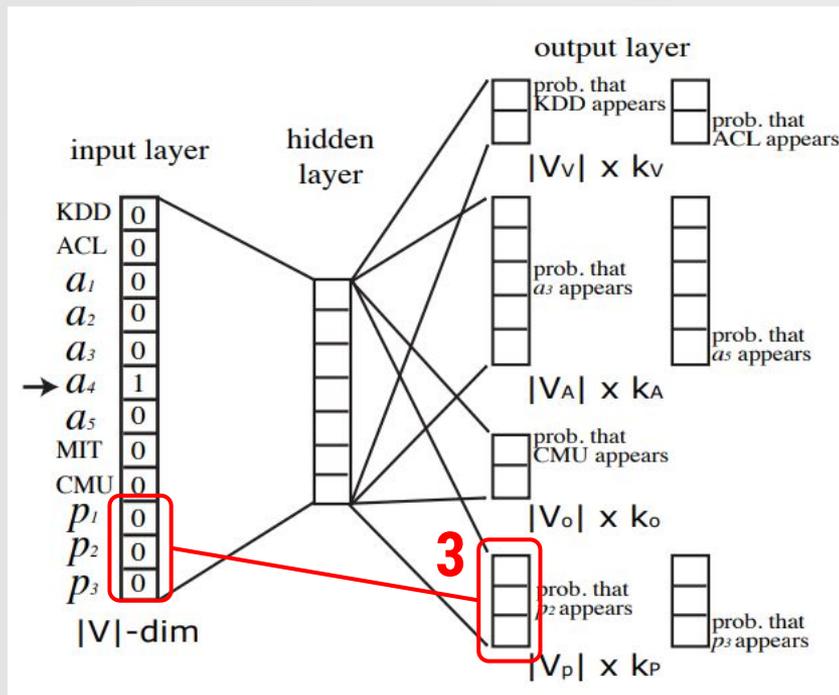
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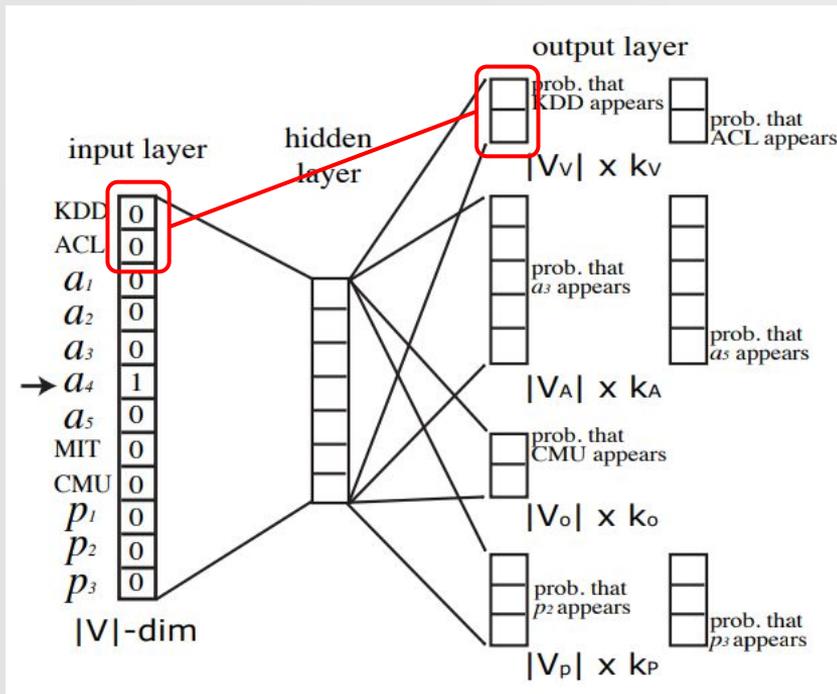
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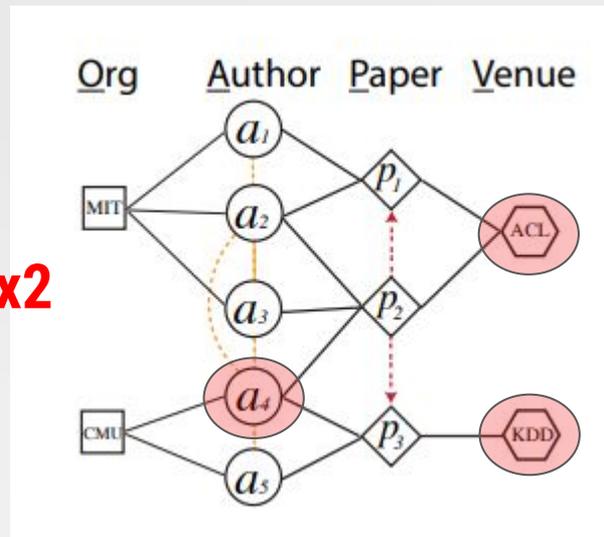
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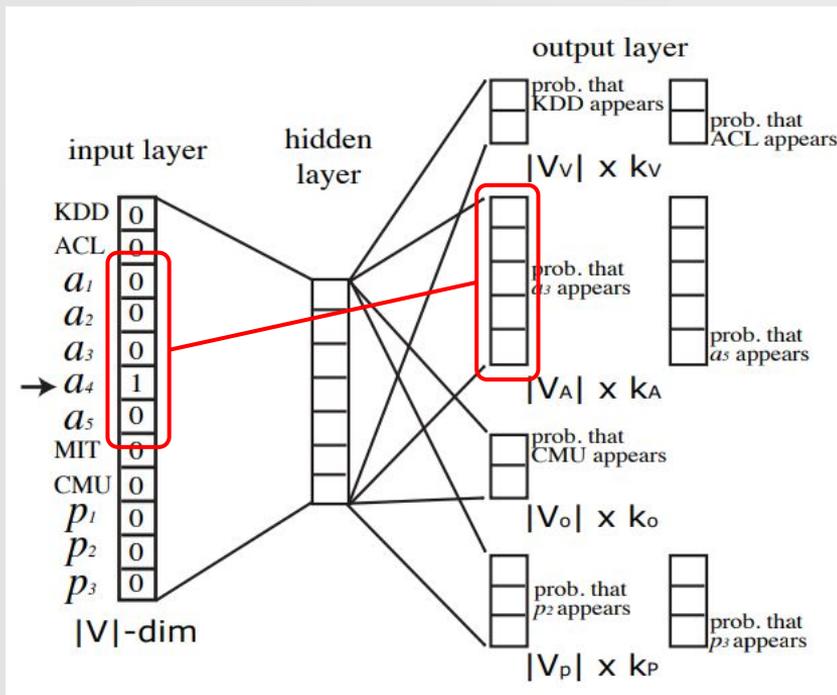
2x2



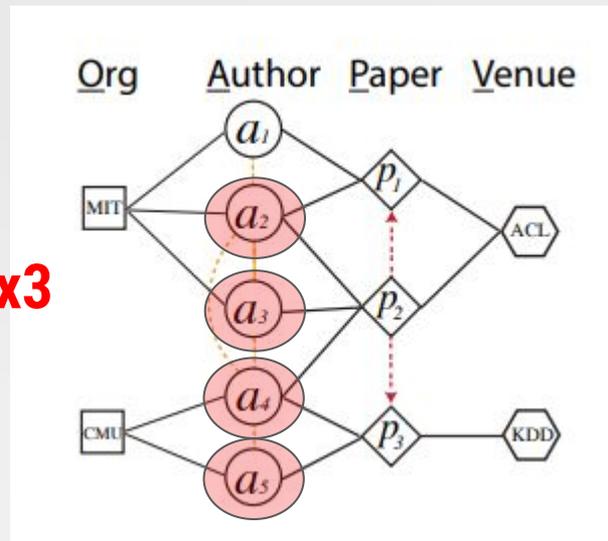
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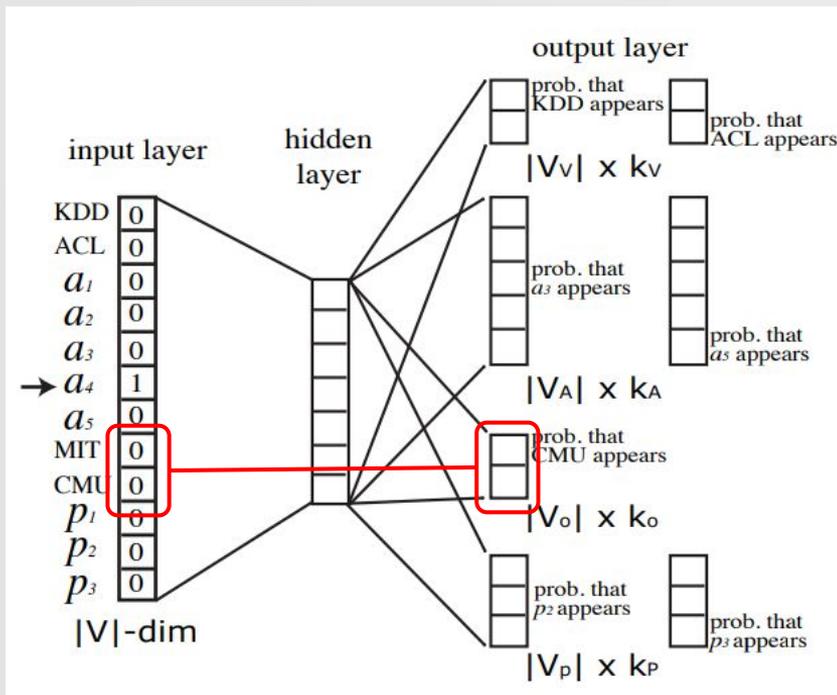
4x3



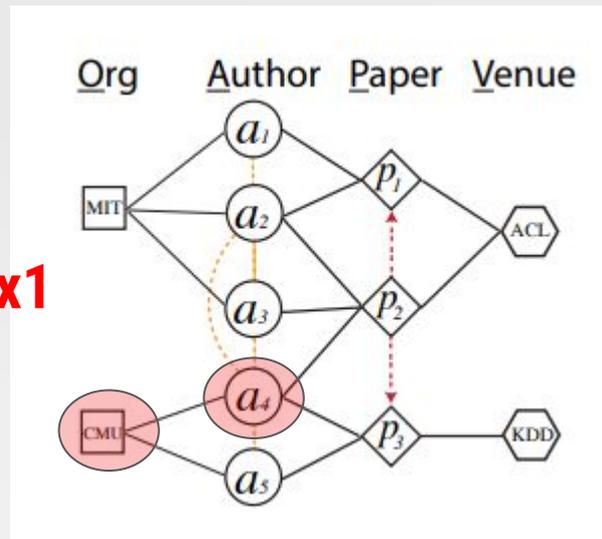
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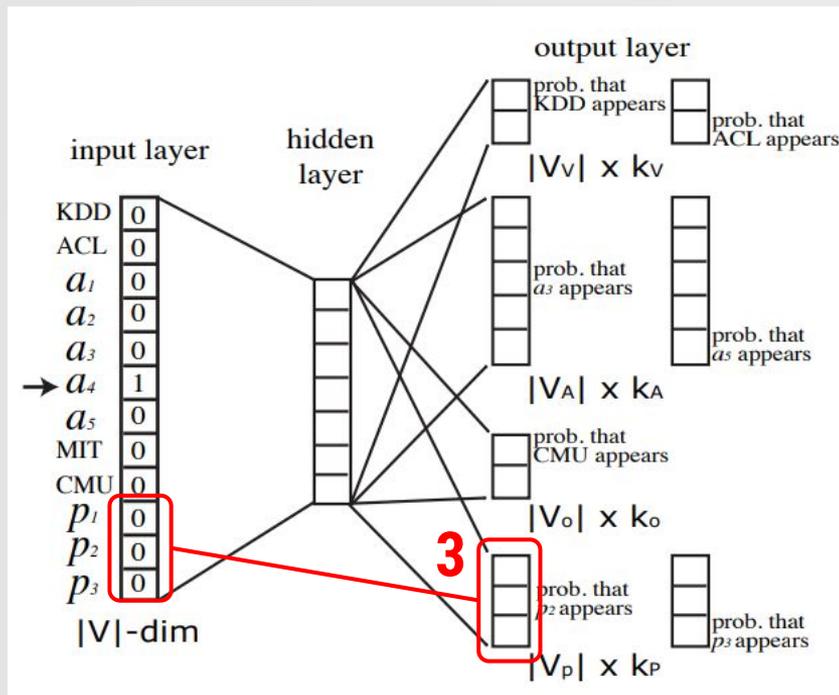
2x1



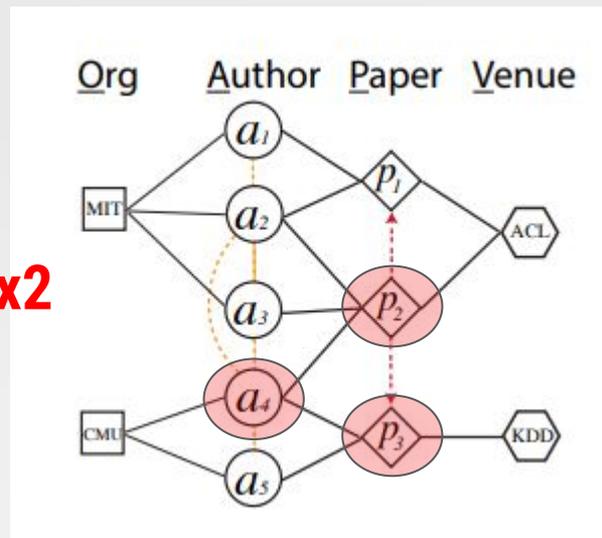
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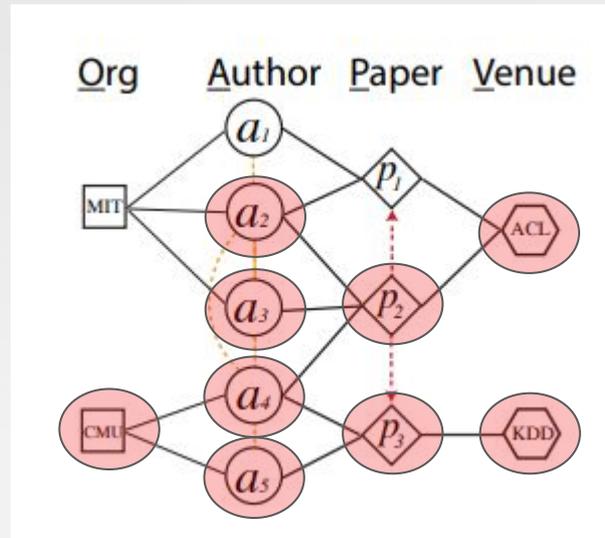
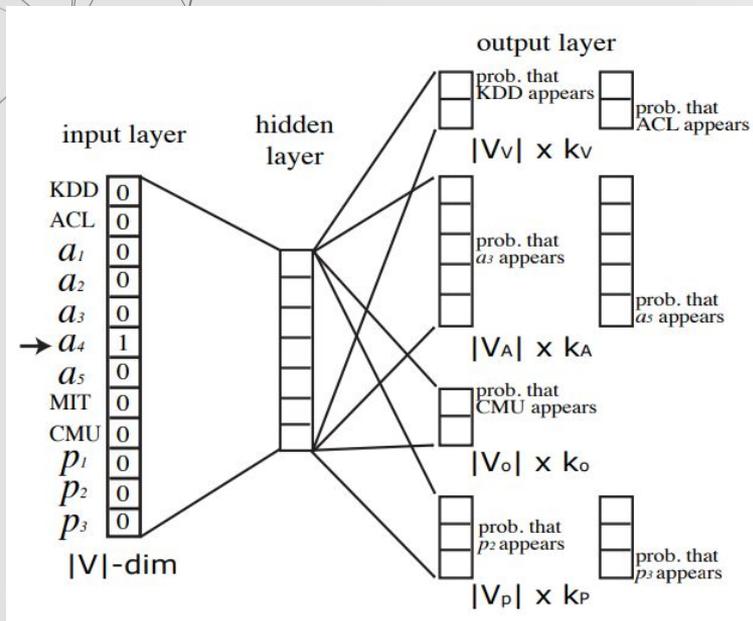
3x2



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04 Training



```
CLASS MetaPath2Vec ( edge_index_dict, embedding_dim, metapath, walk_length, context_size,  
walks_per_node=1, num_negative_samples=1, num_nodes_dict=None, sparse=False ) \[source\]
```

04 Training

```
{'paper',  
  'written by',  
  'author': tensor([[ 0, 1,  
                    [ 0, 1, 2, ...  
( 'author',  
  'wrote',  
  'paper'): tensor([[ 0, 0,  
                    [ 0, 45988, 124807, ...  
( 'paper',  
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  'venue'): tensor([[ 0, 1,  
                    [ 2190, 2190, 2190, ...  
( 'venue',  
  'published',  
  'paper'): tensor([[ 0, 0,  
                    [2203069, 2203070, 2203071, ...
```



CLASS `MetaPath2Vec` (`edge_index_dict`, `embedding_dim`, `metapath`, `walk_length`, `context_size`,
`walks_per_node=1`, `num_negative_samples=1`, `num_nodes_dict=None`, `sparse=False`) [\[source\]](#)

04 Training

```
{'paper',  
 'written by',  
 'author'): tensor([[ 0, 1,  
 [ 0, 1, 2, ...  
{'author',  
 'wrote',  
 'paper'): tensor([[ 0, 0,  
 [ 0, 45988, 124807, ...  
{'paper',  
 'published in',  
 'venue'): tensor([[ 0, 1,  
 [ 2190, 2190, 2190, ...  
{'venue',  
 'published',  
 'paper'): tensor([[ 0, 0,  
 [2203069, 2203070, 2203071, ...
```

Size of the output
embedding

CLASS `MetaPath2Vec` (`edge_index_dict`, `embedding_dim`, `metapath`, `walk_length`, `context_size`,
`walks_per_node=1`, `num_negative_samples=1`, `num_nodes_dict=None`, `sparse=False`) [\[source\]](#)

04 Training

```
{('paper',  
  'written by',  
  'author'): tensor([[ 0, 1,  
    [ 0, 1, 2, ...  
('author',  
  'wrote',  
  'paper'): tensor([[ 0, 0,  
    [ 0, 45988, 124807, ...  
('paper',  
  'published in',  
  'venue'): tensor([[ 0, 1,  
    [ 2190, 2190, 2190, ...  
('venue',  
  'published',  
  'paper'): tensor([[ 0, 0,  
    [2203069, 2203070, 2203071, ...
```

```
[('author', 'wrote', 'paper'),  
 ('paper', 'published in', 'venue'),  
 ('venue', 'published', 'paper'),  
 ('paper', 'written by', 'author')]
```

Size of the output
embedding

```
CLASS MetaPath2Vec ( edge_index_dict, embedding_dim, metapath, walk_length, context_size,  
walks_per_node=1, num_negative_samples=1, num_nodes_dict=None, sparse=False ) \[source\]
```

04 Training

```
{('paper',  
  'written by',  
  'author'): tensor([[ 0, 1,  
    [ 0, 1, 2, ...  
('author',  
  'wrote',  
  'paper'): tensor([[ 0, 0,  
    [ 0, 45988, 124807, ...  
('paper',  
  'published in',  
  'venue'): tensor([[ 0, 1,  
    [ 2190, 2190, 2190, ...  
('venue',  
  'published',  
  'paper'): tensor([[ 0, 0,  
    [2203069, 2203070, 2203071, ...
```

```
[('author', 'wrote', 'paper'),  
 ('paper', 'published in', 'venue'),  
 ('venue', 'published', 'paper'),  
 ('paper', 'written by', 'author')]
```

Size of the output
embedding

Equal to
Node2Vec

```
CLASS MetaPath2Vec ( edge_index_dict, embedding_dim, metapath, walk_length, context_size,  
walks_per_node=1, num_negative_samples=1, num_nodes_dict=None, sparse=False ) \[source\]
```

Equal to
Node2Vec

04 Training

Jupyter notebook

05 Load a pre trained model

Jupyter notebook