Link Prediction

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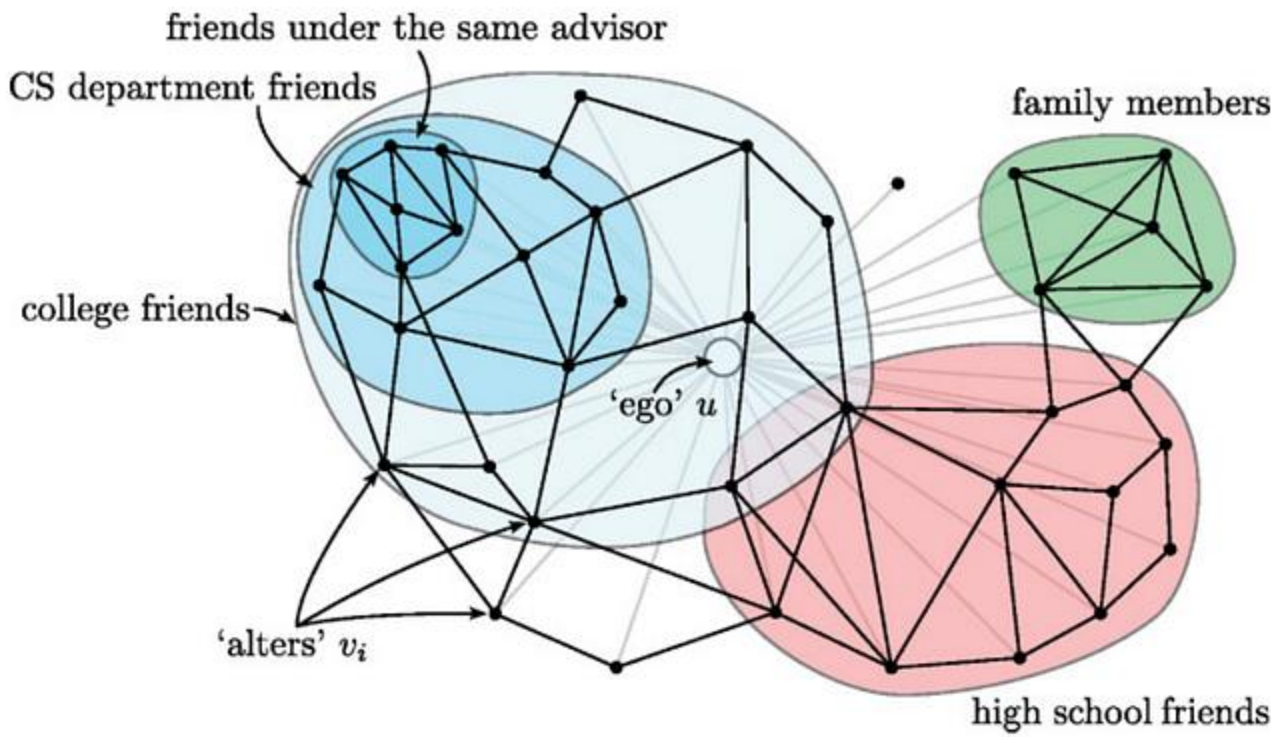
- Challenges in Link prediction
- Common methods
  - Common neighbours
  - Jaccard coefficient
  - Adamic-Adar
  - Preferential attachment
  - Path based
  - SimRank
- Tools for link prediction

Link Prediction in Social Networks

- What we can do in social network prediction:
  - Friend Suggestions
    - Forecast likelihood of connection formation
    - Utilize network structure and historical interactions
  - Community Detection
    - Identify cohesive groups within the network
    - Employ clustering algorithms and network analysis
  - User Behavior Prediction
    - Predict user engagement, churn, or sentiment
    - Inform marketing and product strategies

➢ Friend Suggestions task



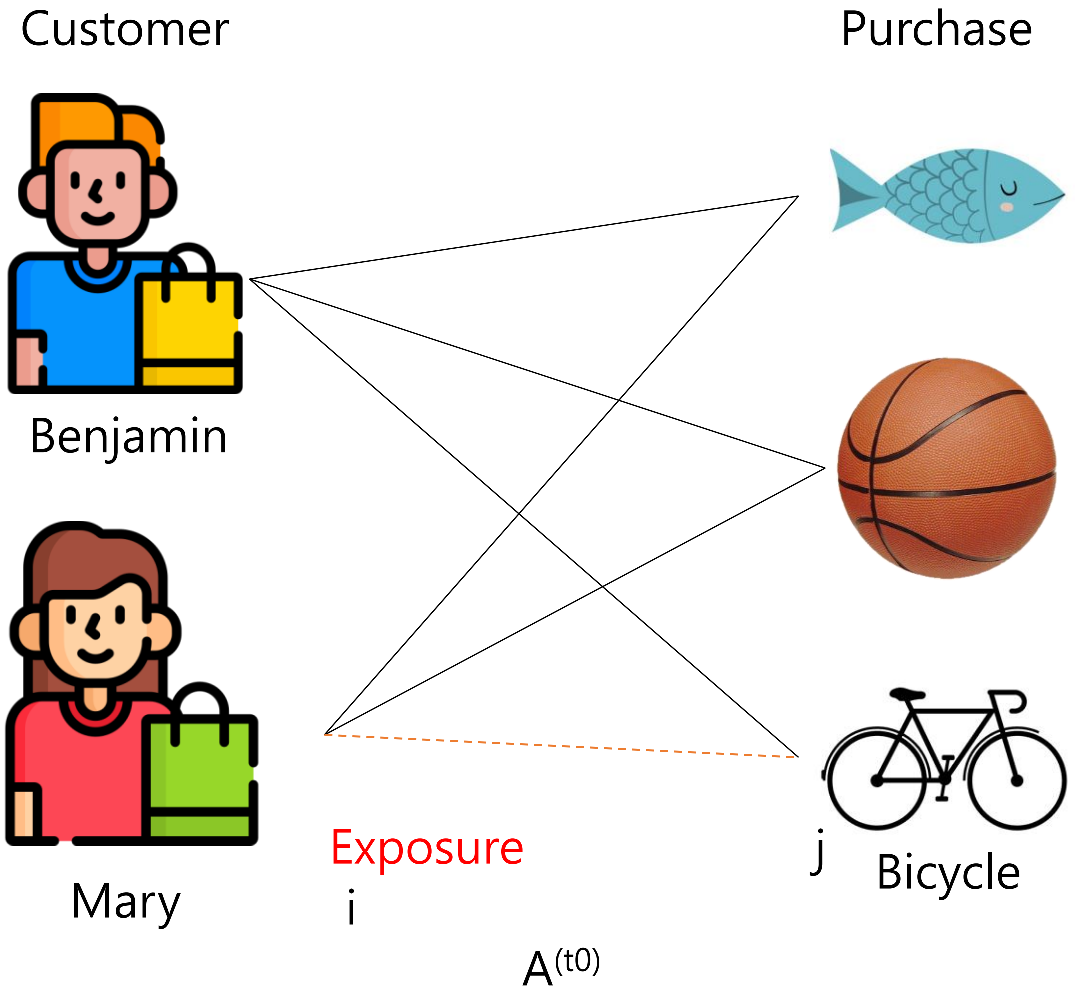
Facebook social circles where 'ego' is owner

Link Prediction in Recommendation Systems

- What we can do in recommendation systems prediction:
  - Rating Prediction
    - Predict user-item ratings
  - Cold-Start Recommendation
    - Address cold-start problem for new users or items
    - Utilize content-based information or hybrid approaches
  - Implicit Feedback Prediction
    - Predict user interaction likelihood from implicit feedback

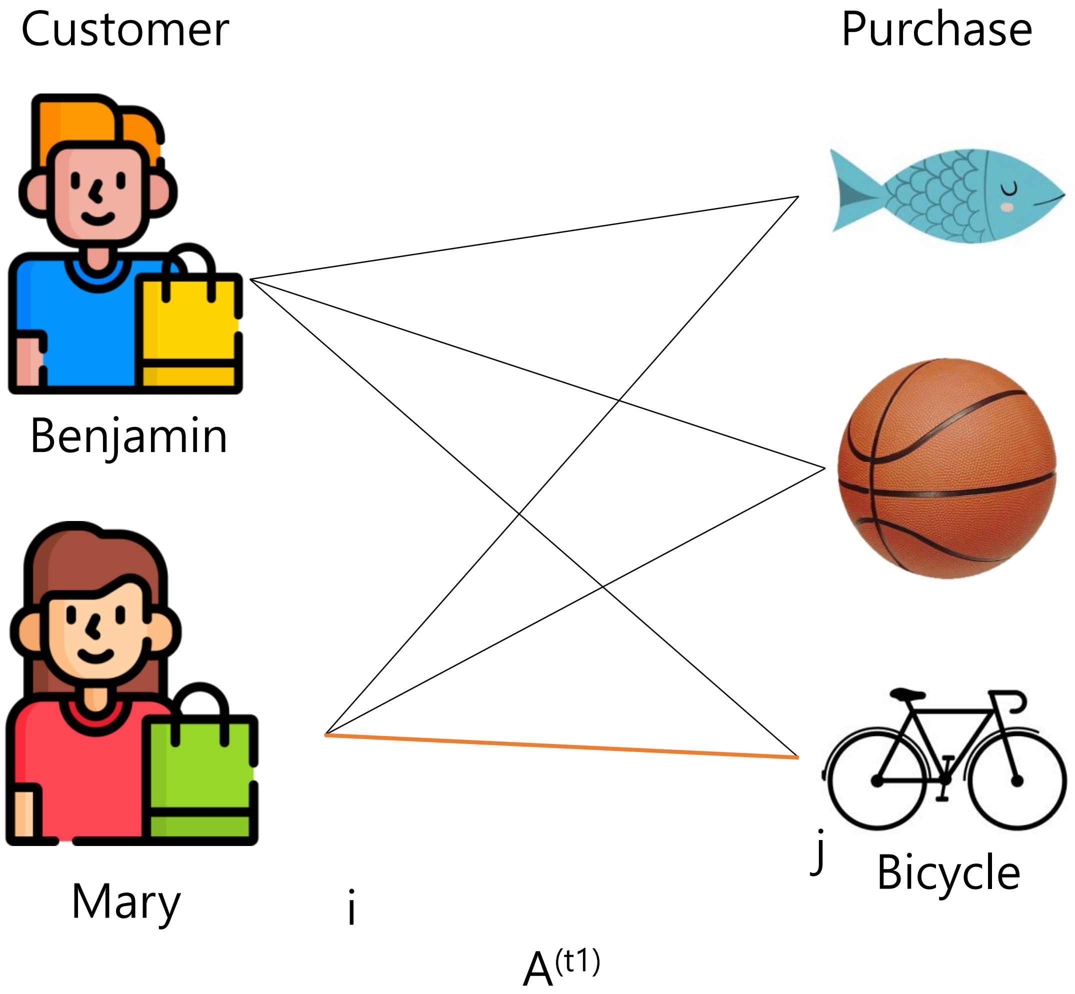
Link prediction as an exposure

- At time t_0 we expose Mary to Bicycle
- We will define this intervention exposure as
  - $E^{(t0)}$ = (Mary, Bicycle)



Link prediction as an exposure

- At time t_1 we see if Lincoln bought Bicycle
- The outcome of the exposure at t_1
  - $A^{(t_1)}_{Mary,Bicycle} \in \{0,1\}$



Link Prediction in Chemistry

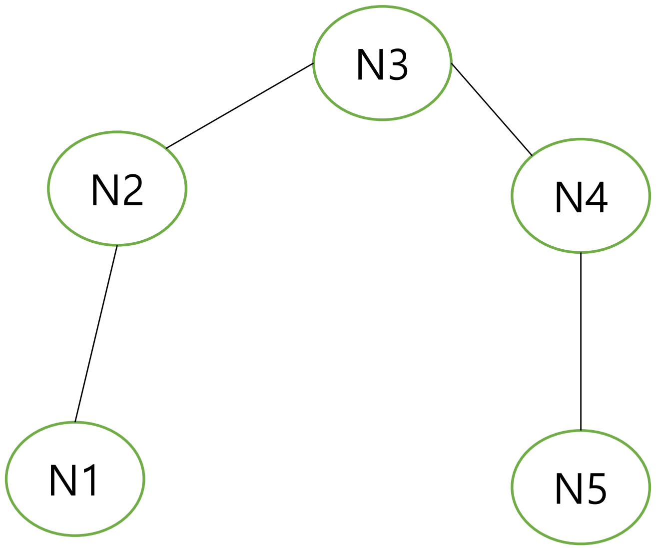
- What we can do in recommendation systems prediction:
  - Chemical Property Prediction
    - Forecast physicochemical properties (e.g., solubility, toxicity)
  - Drug Discovery and Design
    - Identify drug candidates and optimize molecules
  - Reaction Prediction
    - Predict chemical reaction outcomes and pathways

Link Prediction in Transportation Systems

- What we can do in recommendation systems prediction:
  - Traffic Flow Prediction
    - Forecast traffic congestion, flow rates, and travel times
  - Demand Forecasting
    - Predict future demand for transportation services
  - Route Optimization
    - Optimize routes for vehicles, passengers, or freight
  - Accident Prediction
    - Predict the likelihood of traffic accidents and identify high-risk areas
  - Travel Time Estimation
    - Estimate travel times for different transportation modes and routes

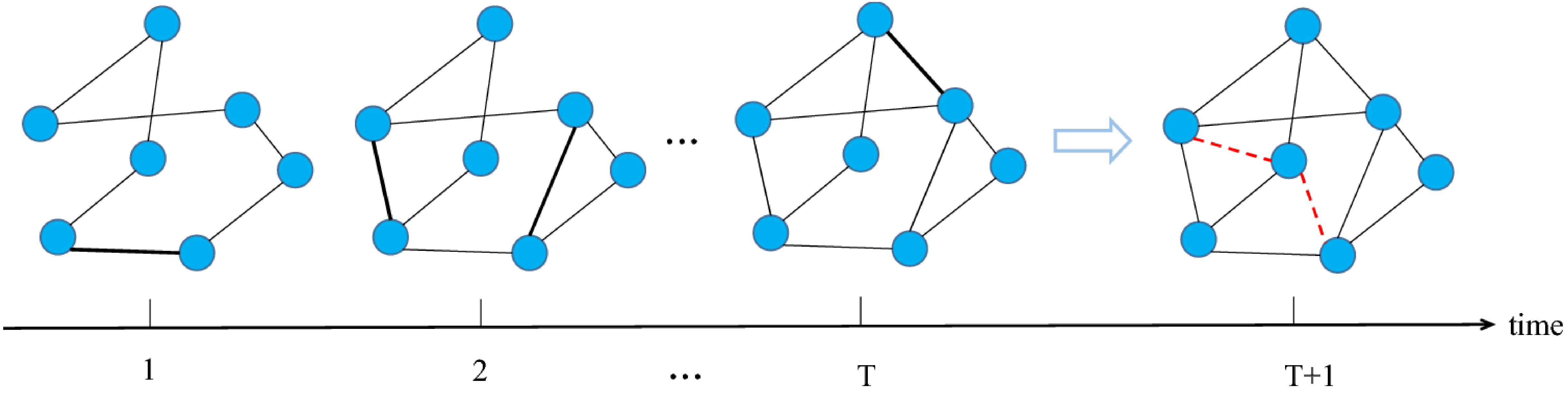
Challenges in Link predictions: Graph sparsity

- Networks often exhibit sparsity, where the number of observed connections is much smaller than the total number of possible connections.
- This makes it challenging to infer missing links accurately, especially in large-scale networks
- A sparse graph has a number of edges closer to the minimal number of edges
- Eg: A graph has 5 nodes and only 4 edges



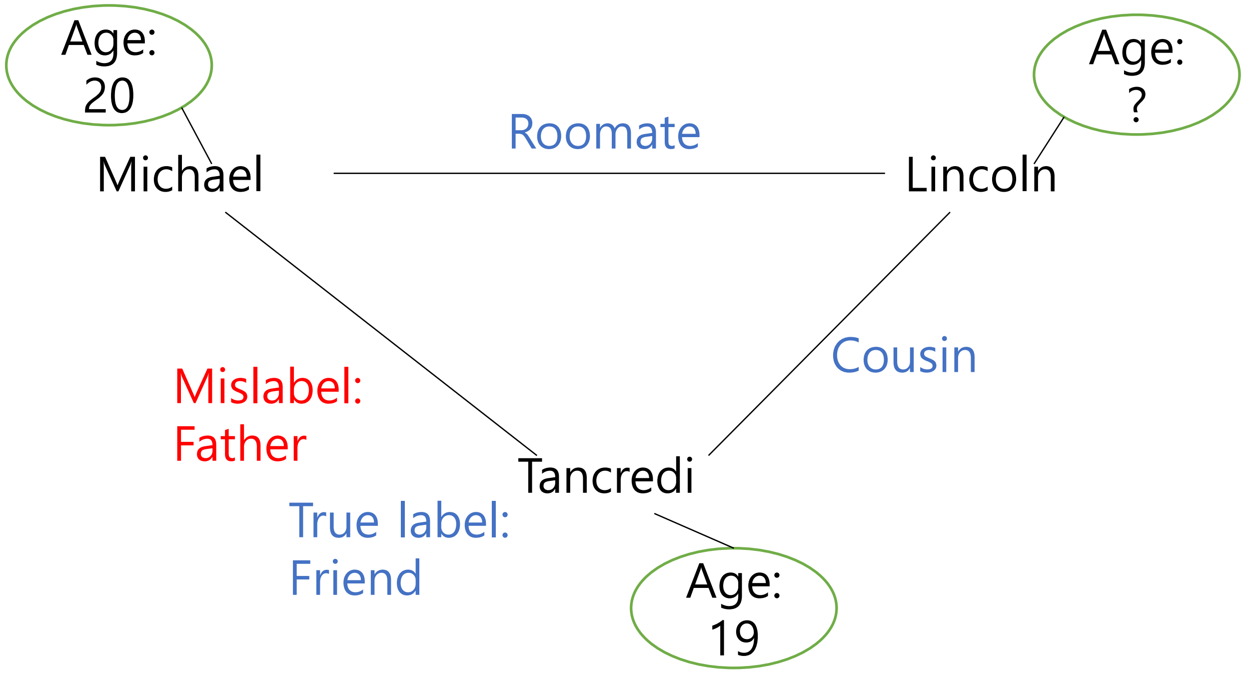
Challenges in Link predictions: Temporal dynamic

- Networks evolve over time, with new connections forming and existing connections breaking.
- Link prediction models must be able to capture and adapt to temporal dynamics, predicting future links based on past network states.



Challenges in Link predictions: Noisy data and missing attributes

- Link prediction models often rely on node and edge attributes to infer connections
- However, real-world data may be incomplete or noisy, leading to challenges in feature selection and model training

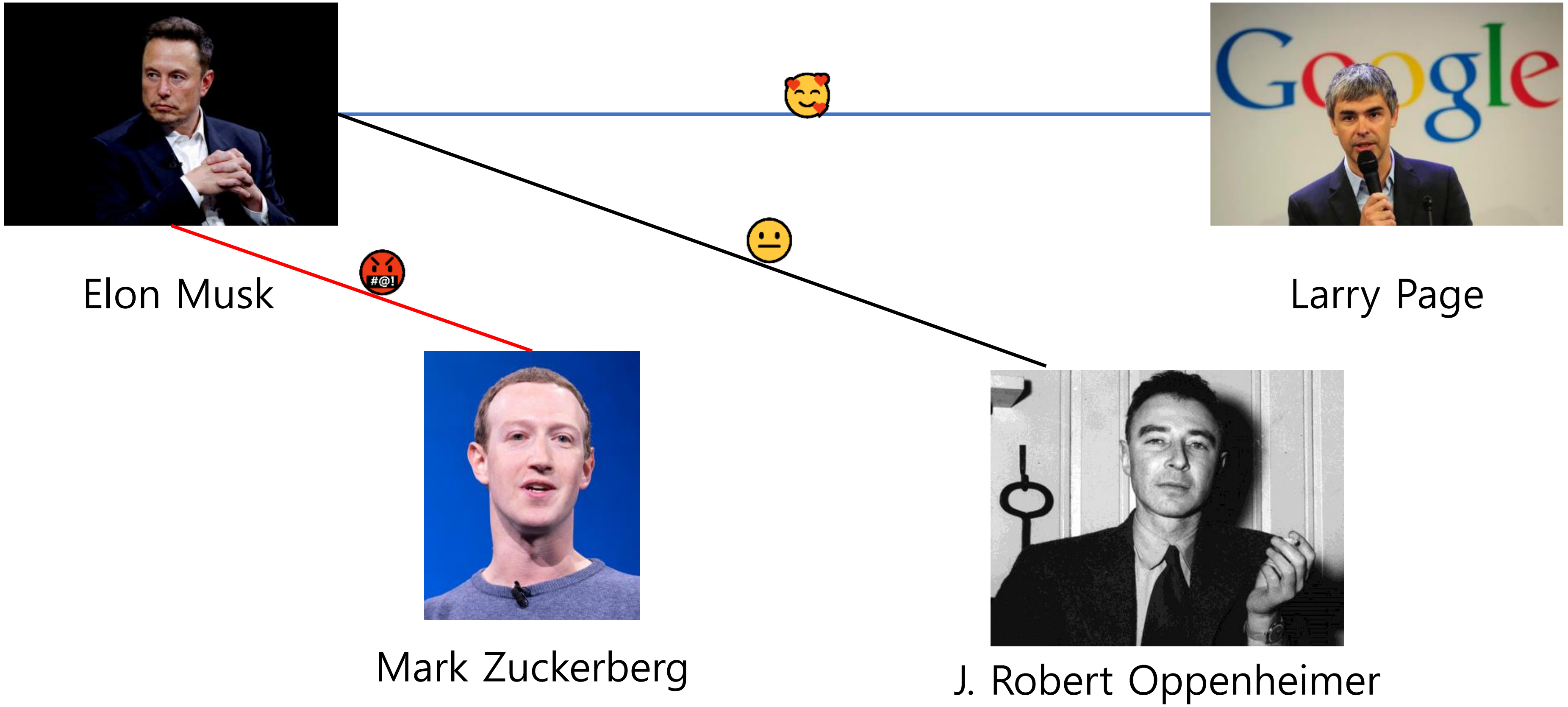


Types of Link Prediction

- There are 3 types of Link Prediction
  - Positive Link
    - Positive links refer to connections or relationships that are expected or desirable in a network
    - These connections typically represent friendships, collaborations, interactions, or any other positive associations between nodes
  - Negative Link
    - Negative links represent relationships or connections that are undesirable or unlikely in a network
    - These connections might indicate conflicts, disagreements, competition, or any other negative associations between nodes
  - Neutral Link
    - Neutral links refer to connections that neither positively nor negatively affect the network
    - These connections are typically neither desirable nor undesirable; they might represent indifference or lack of significant interaction between nodes

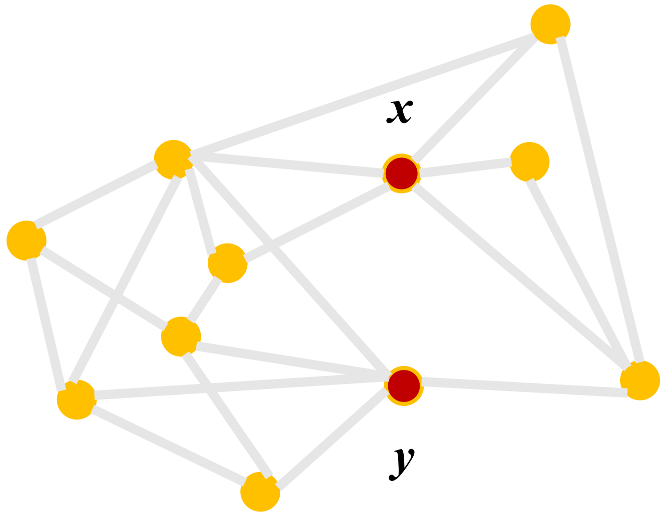
Types of Link Prediction

- There are 3 types of Link Prediction
  - Positive Link
  - Negative Link
  - Neutral Link

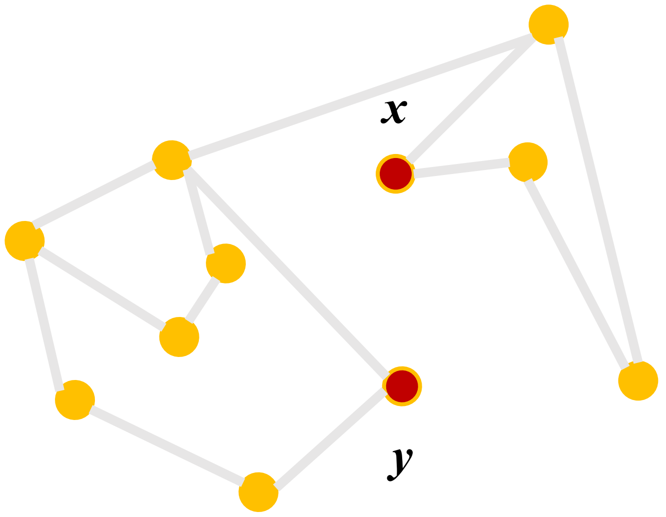


The intuition

- Link prediction also equals to “Relation prediction” or “Graph completion” or “Relational inference” depending on the specific application domain
- In many networks, people who are “close” belong to the same social circles and will inevitably encounter one another and become linked themselves.
- Link prediction heuristics measure how “close” people are

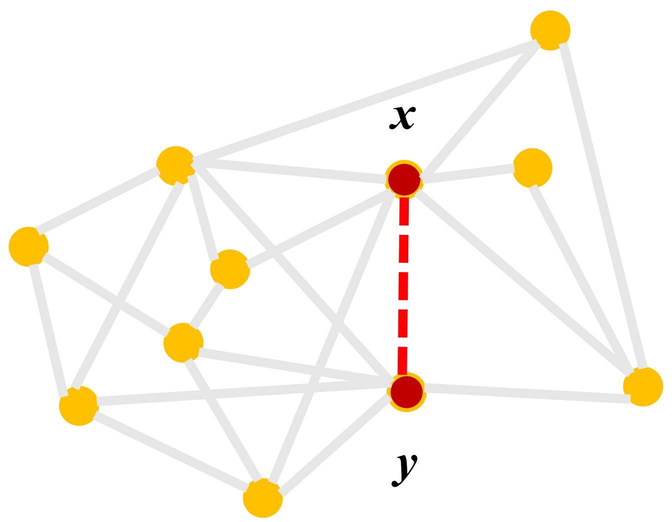


Red nodes are close to each other



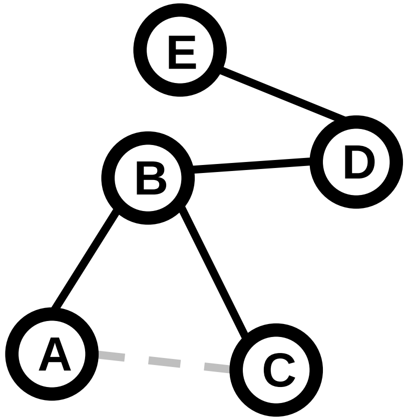
Red nodes are more distant

- Local
  - Common Neighbours (CN)
  - Jaccard’s Coefficient (JC)
  - Adamic-Adar (AA)
  - Preferential attachment (PA)
  - Other:
    - Salton index
    - Sorensen index
    - Hub Promoted index
    - Hub Depressed Index
- Global
  - Path based
  - Path based Hitting time
  - SimRank



Graph Distance

- Graph distance: Length of shortest path between two nodes in the graphs
- E.g., the distance between nodes in graphs:



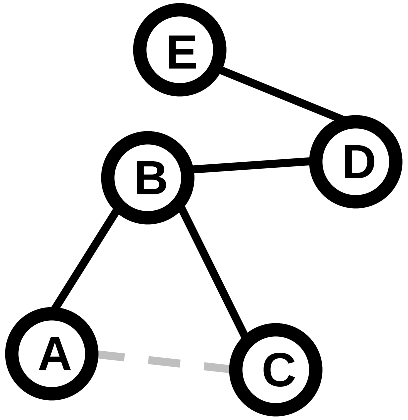
(A, C)	?
(C, D)	?
(A, E)	?

Graph Distance


```python
# Calculate graph distance
def calculate_graph_distance(G, source, target):
    return nx.shortest_path_length(G, source=source, target=target)

# Instantiate the graph
G = nx.Graph()

edges = [("A", "B"), ("B", "C"), ("B", "D"), ("D", "E")]
# add node/edge pairs
G.add_edges_from(edges)

# Use spring layout for better visualization
pos = nx.spring_layout(G)
nx.draw(G, pos, with_labels=True)

# Calculate distances
distances = {
    ("A", "C"): calculate_graph_distance(G, 'A', 'C'),
    ("C", "D"): calculate_graph_distance(G, 'C', 'D'),
    ("A", "E"): calculate_graph_distance(G, 'A', 'E'),
}

print("Graph distances:")
for nodes, distance in distances.items():
    print(f"{nodes} | {distance}")
```

✓ 0.0s

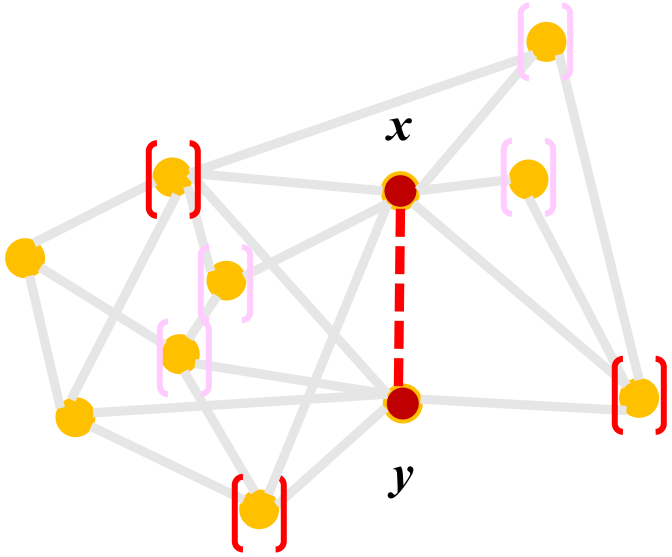
```
Graph distances:
('A', 'C') | 2
('C', 'D') | 2
('A', 'E') | 3
```



(A, C)	2
(C, D)	2
(A, E)	3

Common Neighbors

- How many neighbours are in common between x and y
- X and Y have 3 common neighbours, more likely to collaborate
- Let N(x) denote the set of nodes adjacent to x, N(x)= {m| (x , m) ∈ E}



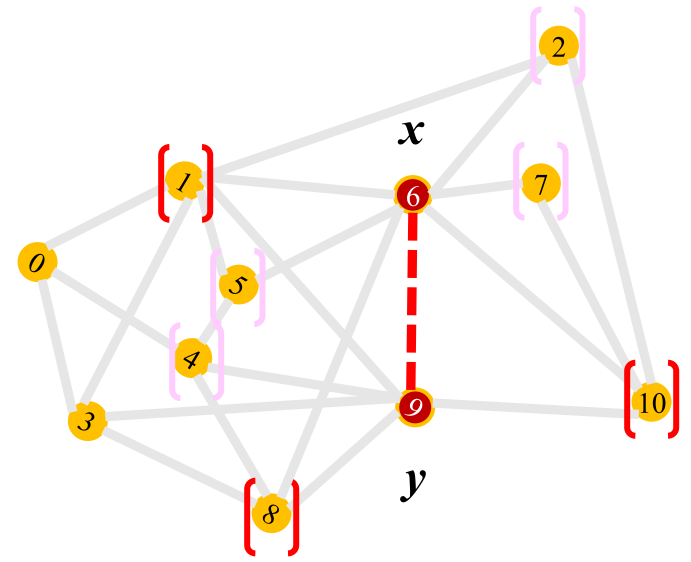
$$CN = |N(x)| \cap |N(y)| = 3$$

Common Neighbours: Sample code

```python
# Instantiate the graph
G = nx.Graph()

# Define edges
edges = [(0, 1), (1, 2), (0, 3), (1, 3), (0, 4), (1, 5), (4, 5), (1, 6),
         (2, 6), (5, 6), (6, 7), (3, 8), (4, 8), (6, 8), (3, 9), (4, 9),
         (1, 9), (8, 9), (2, 10), (6, 10), (7, 10), (9, 10)]

# Add edges to the graph
G.add_edges_from(edges)

# Use spring layout for better visualization
pos = nx.spring_layout(G)
nx.draw(G, pos, with_labels=True)

# Calculate common neighbors of nodes 6 and 9
cn_list = sorted(nx.common_neighbors(G, 6, 9))

# Print common neighbors
print(f"The common neighbors of nodes 6 and 9 are: {cn_list}")
```

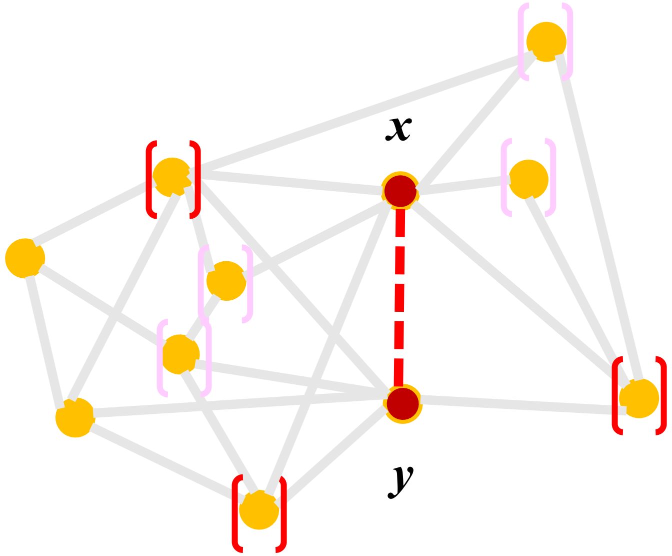
✓ 0.0s

```
The common neighbors of nodes 6 and 9 are: [1, 8, 10]
```



Jaccard's coefficient

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



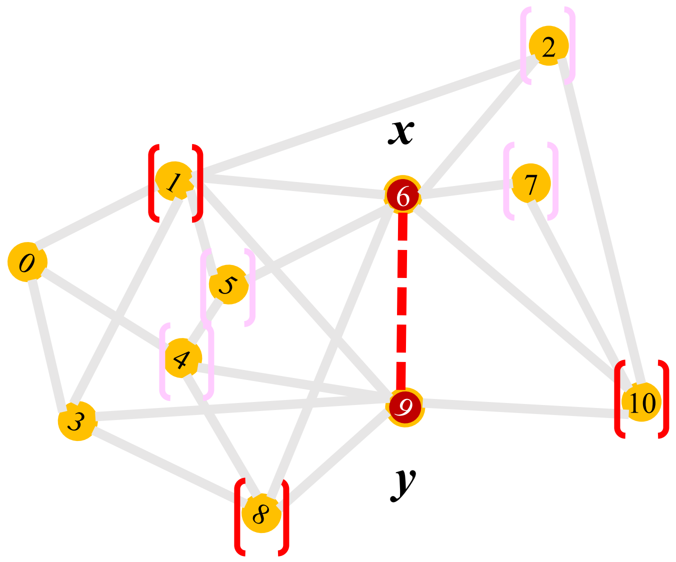
$$JC = \frac{|N(x) \cap N(\mathrm{y})|}{|N(x) \cup N(\mathrm{y})|} = \frac{CN}{d_x + d_y - CN}$$

Jaccard's coefficient: sample code

```python
# Define list of node pairs
node_list = [(6, 9), (1, 3), (3, 9)]

# Calculate Jaccard coefficients for each pair
coefficients = {}
preds = nx.jaccard_coefficient(G, node_list)
for u, v, p in preds:
    coefficients[(u, v)] = p

# Print Jaccard coefficients
for nodes, coeff in coefficients.items():
    print(f"The Jaccard coefficient of nodes {nodes} is: {coeff:.8f}")
```

✓ 0.0s

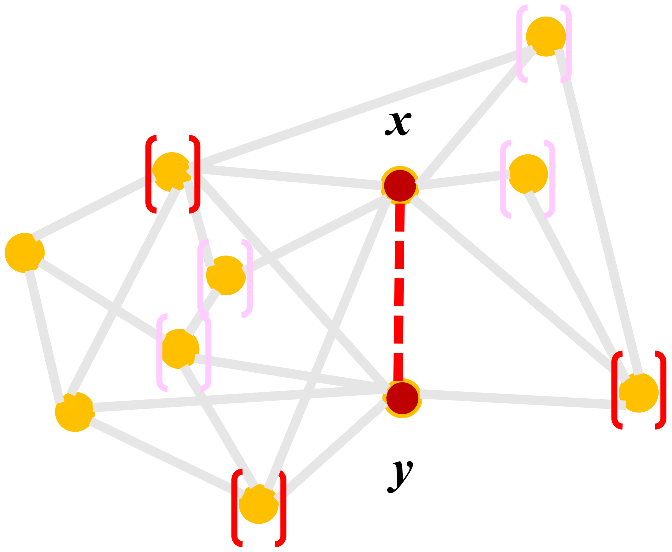
```
The Jaccard coefficient of nodes (6, 9) is: 0.37500000
The Jaccard coefficient of nodes (1, 3) is: 0.25000000
The Jaccard coefficient of nodes (3, 9) is: 0.28571429
```

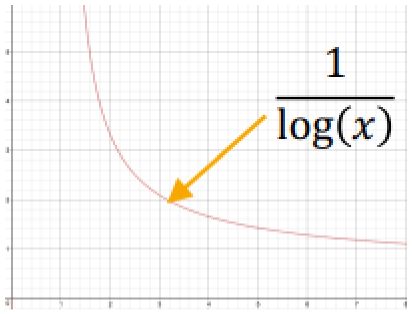


Adamic-Adar (AA)

- Large weight to common neighbours with low degree (the lower the degree the higher the relevance)
- E.g., Neighbours who are linked with 2 nodes are assigned weight = 1/log(2) = 1.4
  - Neighbours who are linked with 5 nodes are assigned weight = 1/log(5) = 0.62

$$AA = \sum_{z \in CN} \frac{1}{\log d_z}$$



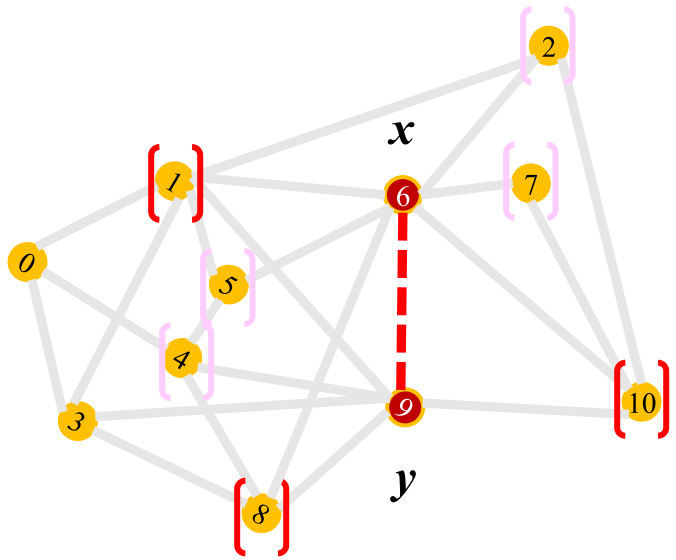


Adamic-Adar (AA): sample code


```python
# Define list of node pairs
node_list = [(6, 9), (1, 3), (3, 9)]

# Calculate Adamic-Adar indices for each pair
indices = {}
preds = nx.adamic_adar_index(G, node_list)
for u, v, p in preds:
    indices[(u, v)] = p

# Print Adamic-Adar indices
for nodes, index in indices.items():
    print(f"The Adamic-Adar index of nodes {nodes} is: {index:.8f}")
```

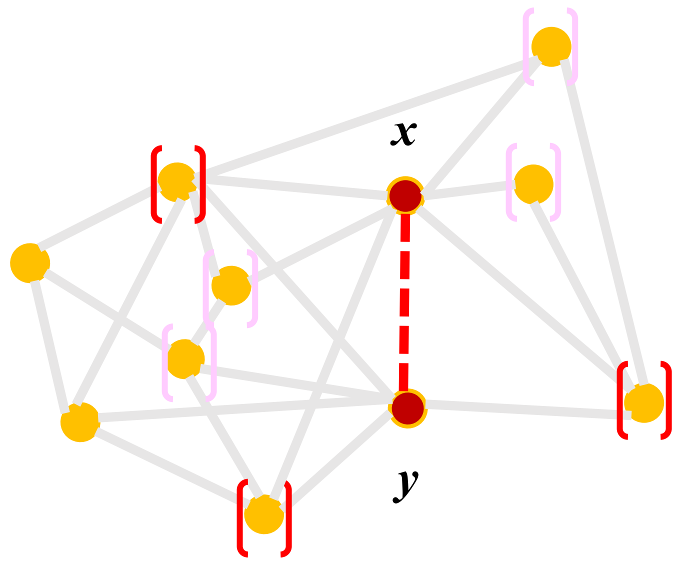
✓ 0.0s

```
The Adamic-Adar index of nodes (6, 9) is: 2.00080567
The Adamic-Adar index of nodes (1, 3) is: 1.53157416
The Adamic-Adar index of nodes (3, 9) is: 1.27945815
```



Preferential attachment (PA)

- Better connected nodes are more likely to form more links.
- The more popular a node is the more probable it will form a link with popular nodes.
- This depends on the degrees of the nodes not on their neighbourhoods



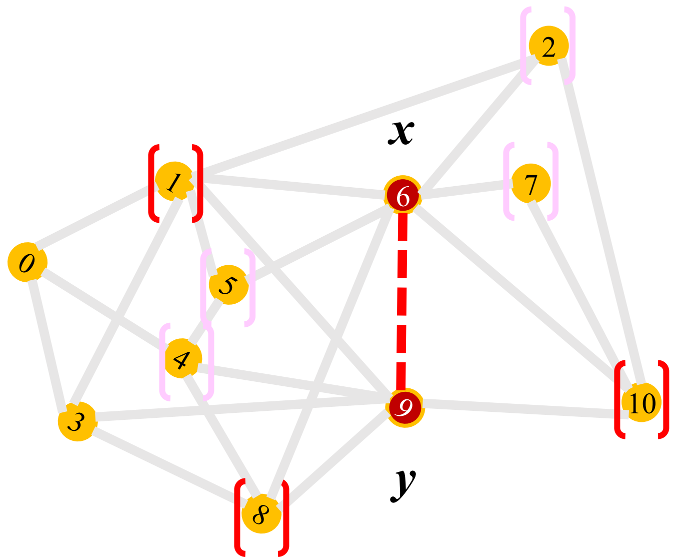
$$PA = |N(x)|.|N(y)| = d_x.d_y$$

Preferential attachment (PA): sample code

```python
# Define list of node pairs
node_list = [(6, 9), (1, 3), (3, 9)]

# Calculate Preferential Attachment scores for each pair
scores = {}
preds = nx.preferential_attachment(G, node_list)
for u, v, p in preds:
    scores[(u, v)] = p

# Print Preferential Attachment scores
for nodes, score in scores.items():
    print(f"The Preferential Attachment score of nodes {nodes} is: {score:.8f}")
```

✓ 0.0s

```
The Preferential Attachment score of nodes (6, 9) is: 30.00000000
The Preferential Attachment score of nodes (1, 3) is: 24.00000000
The Preferential Attachment score of nodes (3, 9) is: 20.00000000
```



Other neighbourhood-based methods

- Salton index

$$score(x,y)=\frac{|N(x)\cap N(y)|}{\sqrt{|N(x)||N(y)|}}$$

- Sorensen index

$$score(x,y)=\frac{2|N(x)\cap N(y)|}{|N(x)|+|N(y)|}$$

- Hub Promoted index

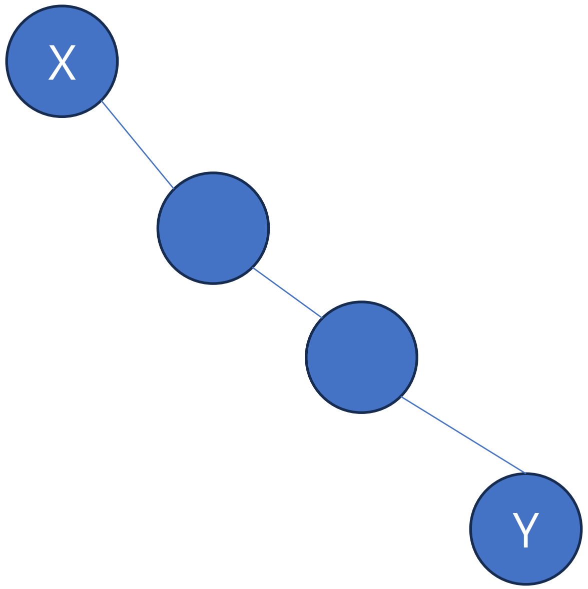
$$score(x,y)=\frac{|N(x)\cap N(y)|}{\min\{|N(x)|,|N(y)|\}}$$

- Hub Depressed Index

$$score(x,y)=\frac{|N(x)\cap N(y)|}{\max\{|N(x)|,|N(y)|\}}$$

Methods for Link Prediction: Path based

- Use the (shortest) distance between two nodes as a link prediction measure
- Score(x,y) = length of shortest path between x and y.
- Very basic approach, it does not consider connections among (x,y) but only the distance



Score(X,Y) = 3

Methods for Link Prediction: Path based

- 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

Link Prediction Methods: Path based Hitting time

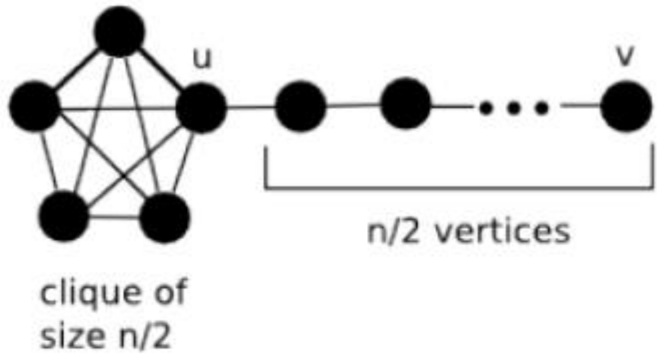
- Consider a random walk on graph G that starts at x and iteratively moves to a neighbour of x chosen uniformly random from N(x)
- **Hitting time (Hxy)** from x to y is the expected number of steps it takes for the random walk starting at x to reach y.

$$score(x,y) = -H_{x,y} = -\frac{1}{|N(\mathrm{x})|}\sum_k (1 + H_{\mathrm{k},y})$$

$$H(i,j) = 1 + \sum_{k \sim i} p_{ik} H(k,j),\ j \neq i, \quad H(i,i) = 0.$$

- Is Hitting Time Symmetric?
  - NOT symmetric
  - E.g., path from u to v is different

  From v to u



Link Prediction Methods: SimRank

- Intuition: Two objects are similar, if they are related to similar objects
- Two objects x and y are similar, if they are related to objects a and b respectively and a and b are themselves similar

$$similarity\ (x, y) = \frac{\sum_{a \in N(x)} \sum_{b \in N(y)} similarity(a, b)}{|N(x)|.\,|N(y)|}$$

- Expresses the average similarity between neighbours of x and neighbours of y:

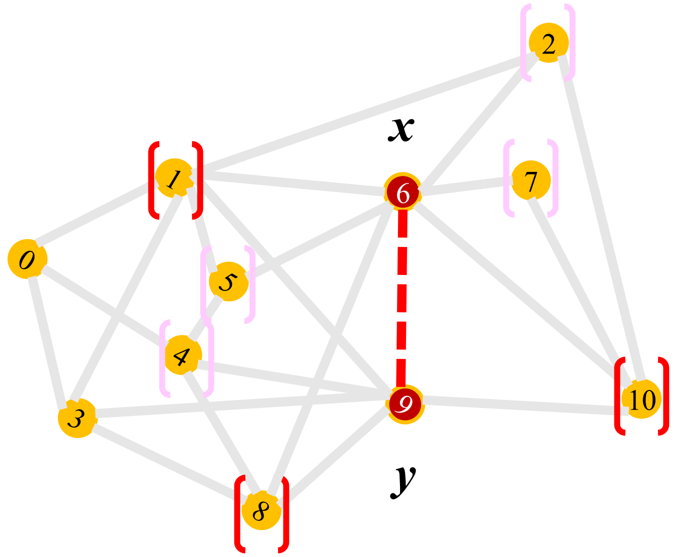
score(x, y) = similarity(x, y)

SimRank: sample code


```python
# Define source and target nodes
source = 6
target = 9

# Calculate SimRank similarity between source and target
similarity = nx.simrank_similarity(G, source, target)

# Print SimRank similarity
print(f"The SimRank similarity between nodes {source} and {target} is: {similarity}")
```

✓ 0.0s

```
The SimRank similarity between nodes 6 and 9 is: 0.4283123305678891
```



Software Tools

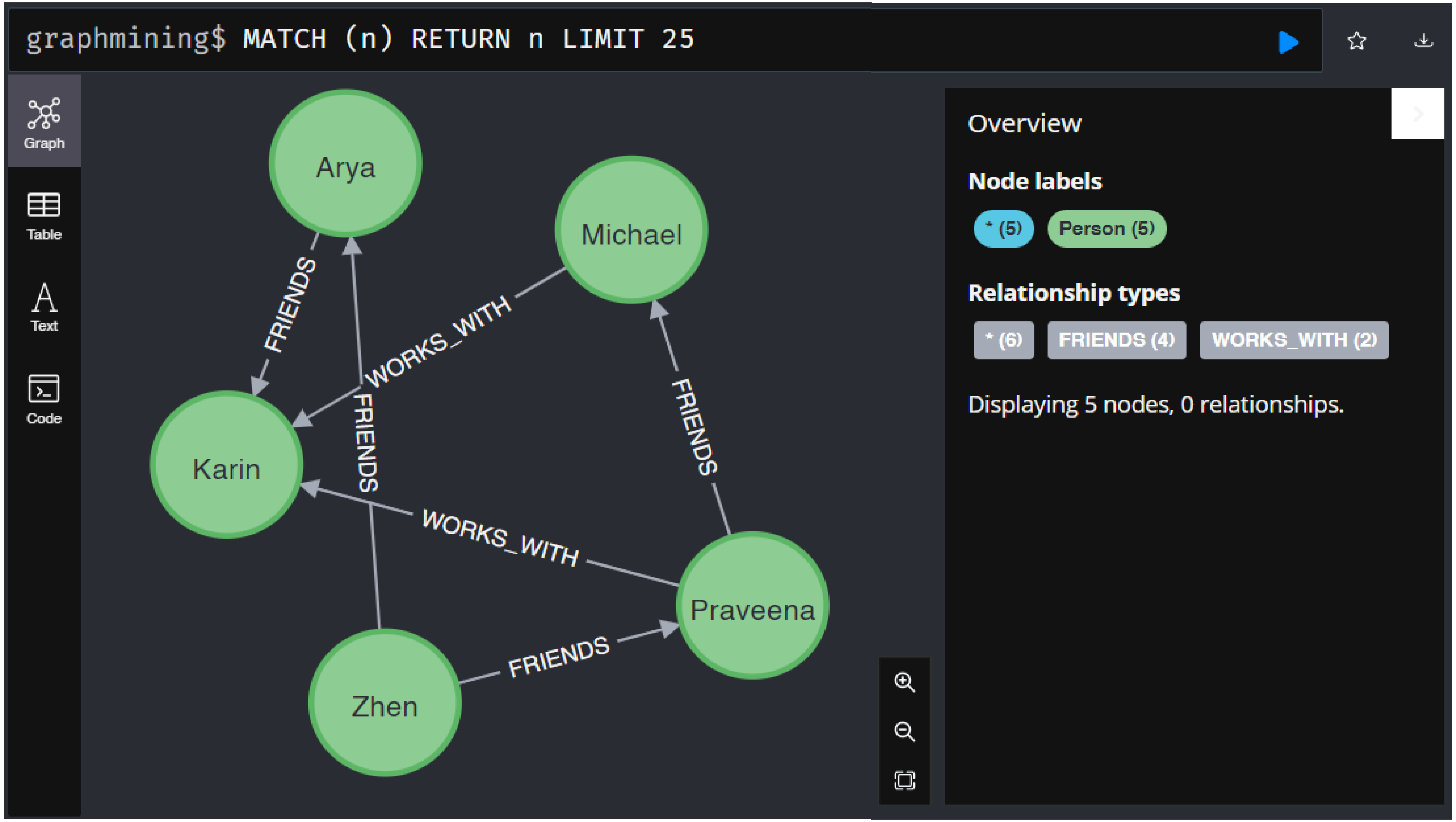
- NodeXL
  - Integrates network analysis into Microsoft Office and Excel
  - No programming skills required
  - Utilizes SNAP library
- InfoVis Cyberinfrastructure
  - Software framework for information visualization
  - Supports Linux, MacOSX, and Windows
  - Enables creation of interactive visualizations
- Analytic Technologies
  - Specialized software for social network analysis
  - Windows-based platform
  - Facilitates data preprocessing and advanced analysis

Software Tools

- Neo4j
  - Graph visualization software
  - Scalable and performance-oriented
  - Ideal for modeling and querying large-scale graph data
- NetworkX
  - Python package for complex network analysis
  - Comprehensive suite of algorithms
  - Widely used by researchers and data scientists

Software Tools: sample code

- Show database



Software Tools: sample code

```
CREATE
 (zhen:Person {name: 'Zhen'}),
 (praveena:Person {name: 'Praveena'}),
 (michael:Person {name: 'Michael'}),
 (arya:Person {name: 'Arya'}),
 (karin:Person {name: 'Karin'}),

 (zhen)-[:FRIENDS]->(arya),
 (zhen)-[:FRIENDS]->(praveena),
 (praveena)-[:WORKS_WITH]->(karin),
 (praveena)-[:FRIENDS]->(michael),
 (michael)-[:WORKS_WITH]->(karin),
 (arya)-[:FRIENDS]->(karin)
```

Table

Code

Added 5 labels, created 5 nodes, set 5 properties, created 6 relationships, completed after 21 ms.

Use this:

CREATE (zhen:Person {name: 'Zhen'}), (praveena:Person {name: 'Praveena'}), (michael:Person {name: 'Michael'}), (arya:Person {name: 'Arya'}), (karin:Person {name: 'Karin'}), (zhen)-[:FRIENDS]->(arya), (zhen)-[:FRIENDS]->(praveena), (praveena)-[:WORKS_WITH]->(karin), (praveena)-[:FRIENDS]->(michael), (michael)-[:WORKS_WITH]->(karin), (arya)-[:FRIENDS]->(karin)

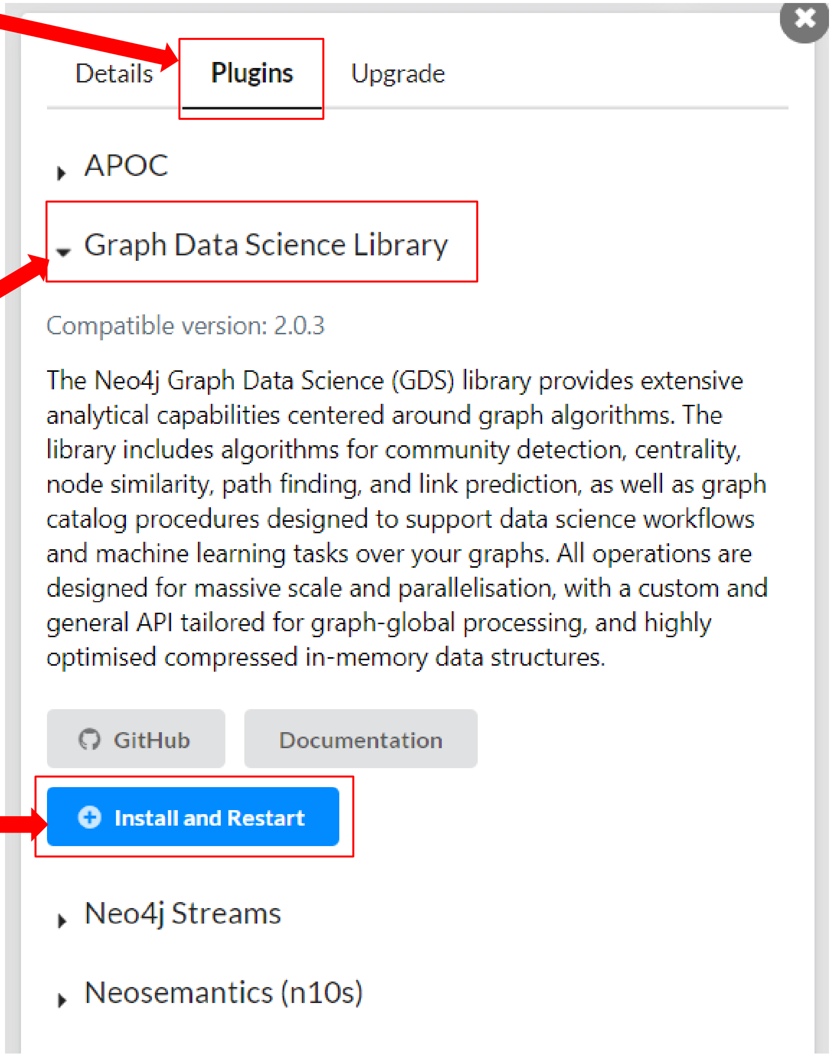
Software Tools: sample code

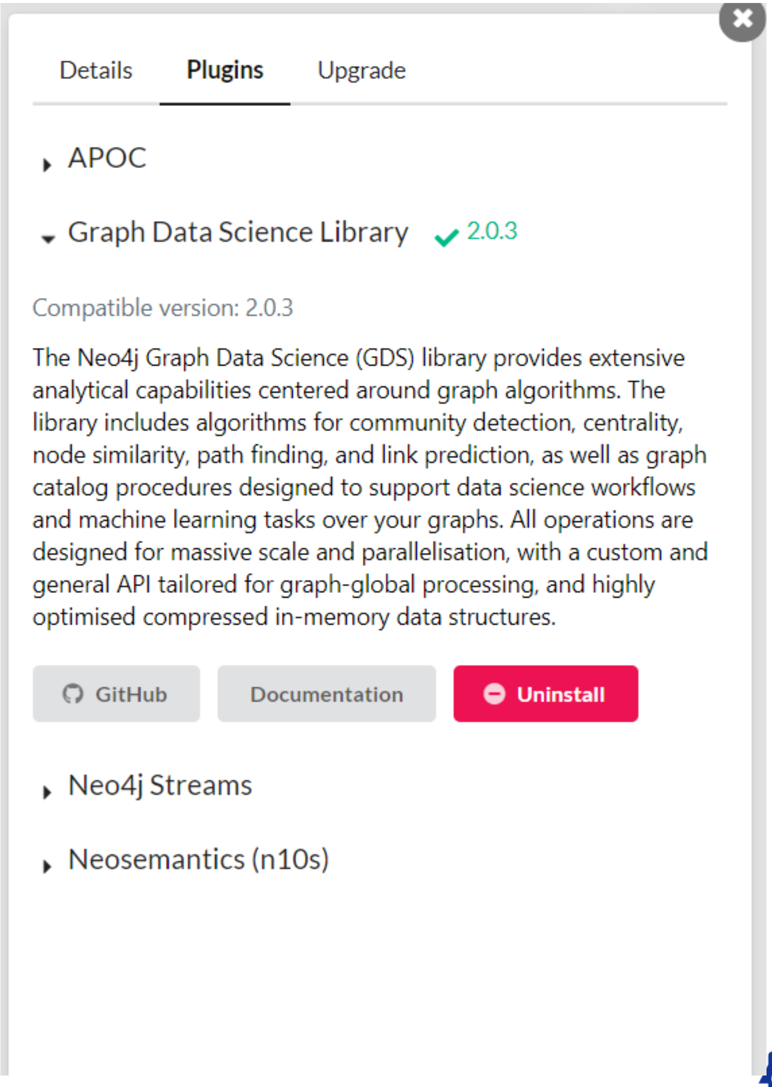
➢ Install the plugin to use graph algorithms

1. Click "Plugins" tab in the pane on the right.

2. Click on "Graph Data Science Library".

3. Install plugin.

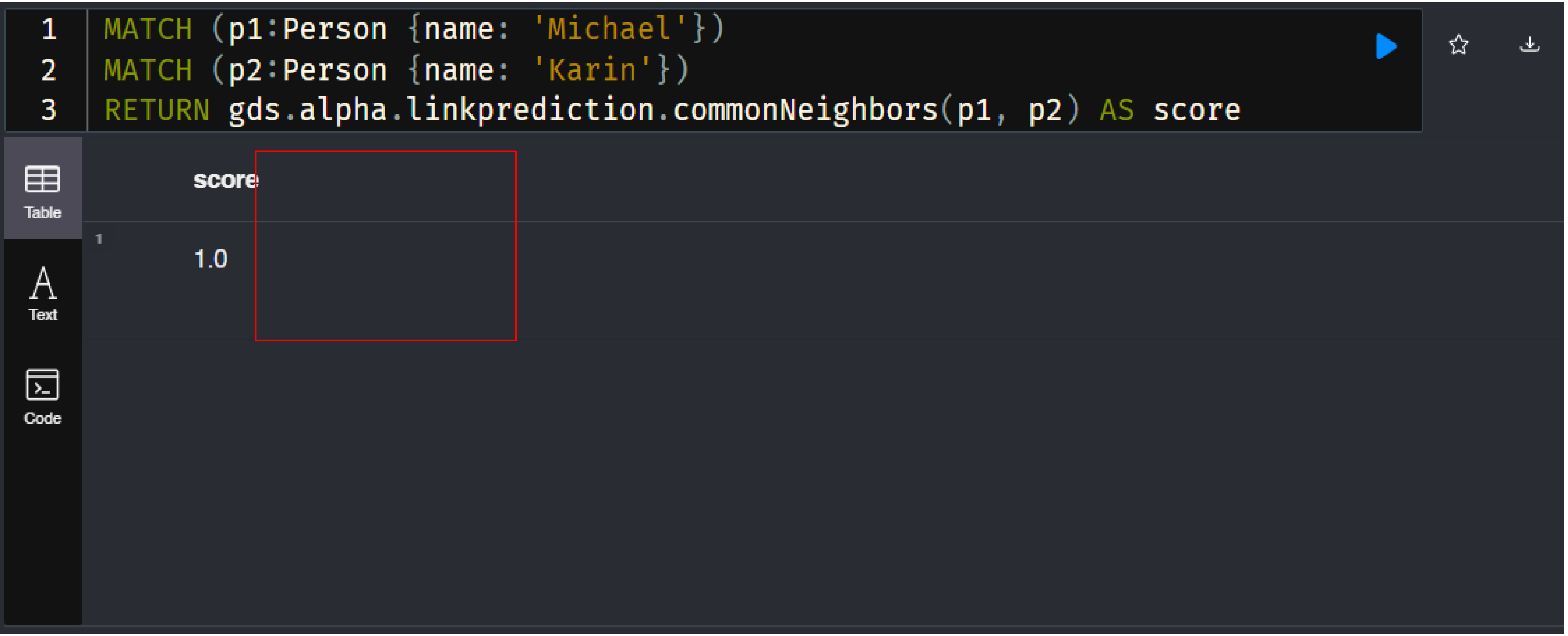




Restart Neo4j to apply graph Data Science Library

Software Tools: sample code

- Calculate the number of common neighbors without considering relation type



Use this:
MATCH (p1:Person {name: 'Michael'}) MATCH (p2:Person {name: 'Karin'}) RETURN gds.alpha.linkprediction.commonNeighbors(p1, p2) AS score

Software Tools: sample code

- Calculate the number of common neighbors with considering relation type

```
MATCH (p1:Person {name: 'Michael'})
MATCH (p2:Person {name: 'Karin'})
RETURN gds.alpha.linkprediction.commonNeighbors(p1, p2, {relationshipQuery: "FRIENDS"})
AS score
```

Table | Text | Code

	score
1	0.0

Use this:
MATCH (p1:Person {name: 'Michael'}) MATCH (p2:Person {name: 'Karin'}) RETURN gds.alpha.linkprediction.commonNeighbors(p1, p2, {relationshipQuery: "FRIENDS"}) AS score

Software Tools: sample code

- Calculate the Adamic Adar without considering relation type

```
MATCH (p1:Person {name: 'Michael'})
MATCH (p2:Person {name: 'Karin'})
RETURN gds.alpha.linkprediction.adamicAdar(p1, p2) AS score
```

Table

Text

Code

"score"
0.9102392266268373

Use this:
MATCH (p1:Person {name: 'Michael'}) MATCH (p2:Person {name: 'Karin'}) RETURN gds.alpha.linkprediction.adamicAdar(p1, p2) AS score

Software Tools: sample code

- Calculate the Adamic Adar without considering relation type

```
MATCH (p1:Person {name: 'Michael'})
MATCH (p2:Person {name: 'Karin'})
RETURN gds.alpha.linkprediction.adamicAdar(p1, p2, {relationshipQuery: 'FRIENDS'})
AS score
```

Table
Text
Code

"score"
0.0

Use this:
MATCH (p1:Person {name: 'Michael'}) MATCH (p2:Person {name: 'Karin'}) RETURN gds.alpha.linkprediction.adamicAdar(p1, p2, {relationshipQuery: 'FRIENDS'}) AS score

Software Tools: sample code

- Calculate the Preferential Attachment without considering the relation type

```
MATCH (p1:Person {name: 'Michael'})
MATCH (p2:Person {name: 'Karin'})
RETURN gds.alpha.linkprediction.preferentialAttachment(p1, p2) AS score
```

Table

Text

Code

```
╒═══════╕
│"score"│
╞═══════╡
│6.0    │
└───────┘
```

Use this:
MATCH (p1:Person {name: 'Michael'}) MATCH (p2:Person {name: 'Karin'}) RETURN gds.alpha.linkprediction.preferentialAttachment(p1, p2) AS score

Software Tools: sample code

- Calculate the Preferential Attachment with considering the relation type

```
MATCH (p1:Person {name: 'Michael'})
MATCH (p2:Person {name: 'Karin'})
RETURN gds.alpha.linkprediction.preferentialAttachment(p1, p2,
{relationshipQuery: "FRIENDS"}) AS score
```

Table

Text

Code

```
╒═══════╕
│"score"│
╞═══════╡
│1.0    │
└───────┘
```

Use this:
MATCH (p1:Person {name: 'Michael'}) MATCH (p2:Person {name: 'Karin'}) RETURN gds.alpha.linkprediction.preferentialAttachment(p1, p2, {relationshipQuery: "FRIENDS"}) AS score


Q
A