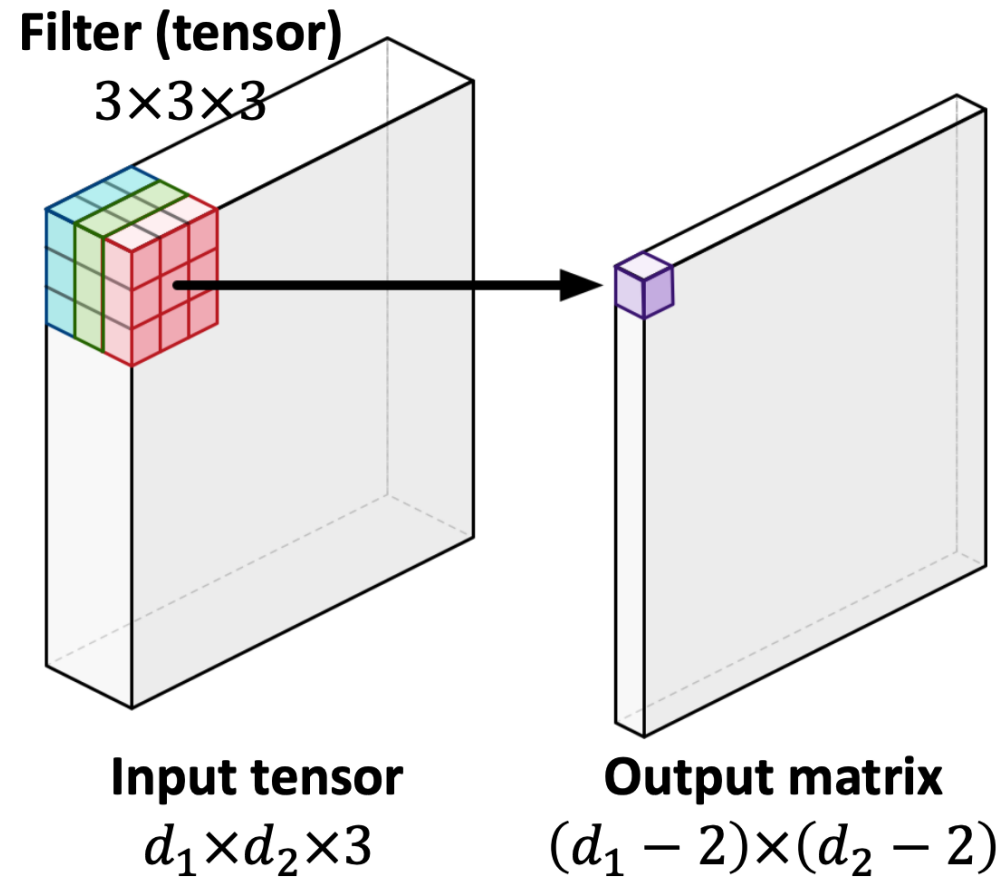


Graph Data and Graph Representation

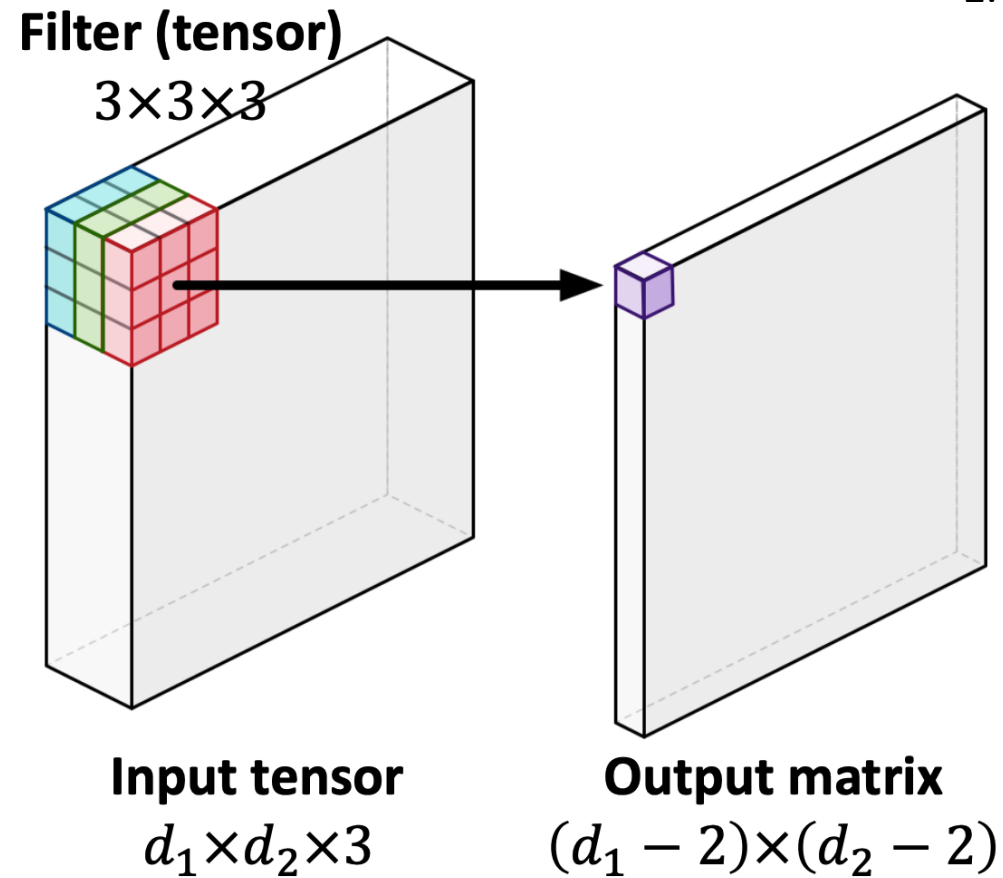
Neural Networks Design And Application

Correlation between data



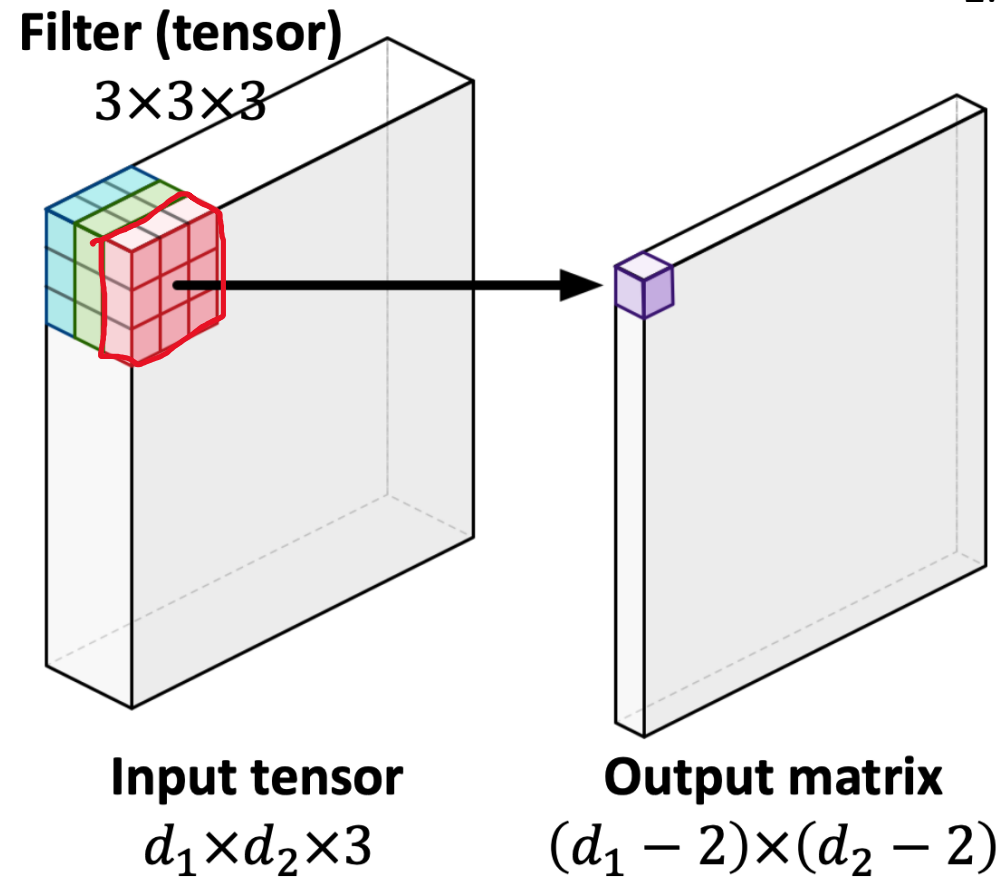
Correlation between data

Q: is there correlation between:
1. locations?



Correlation between data

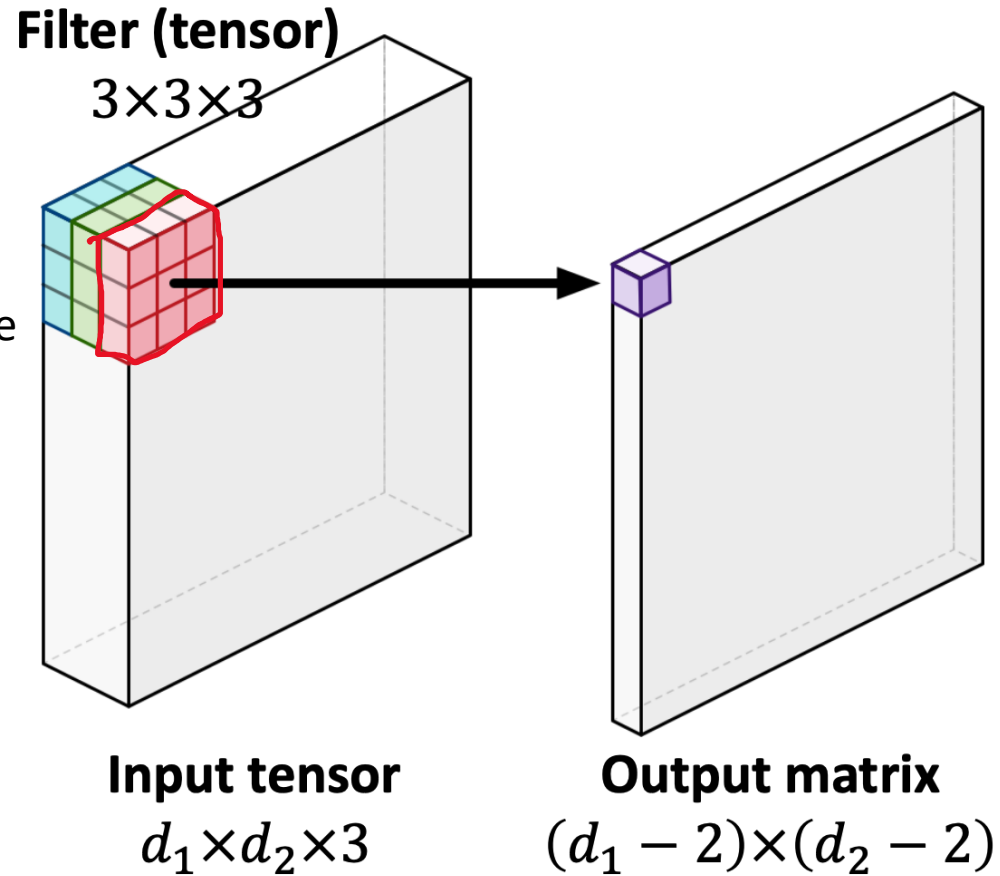
Q: is there correlation between:
1. locations?



Correlation between data

Q: is there correlation between:
1. locations?

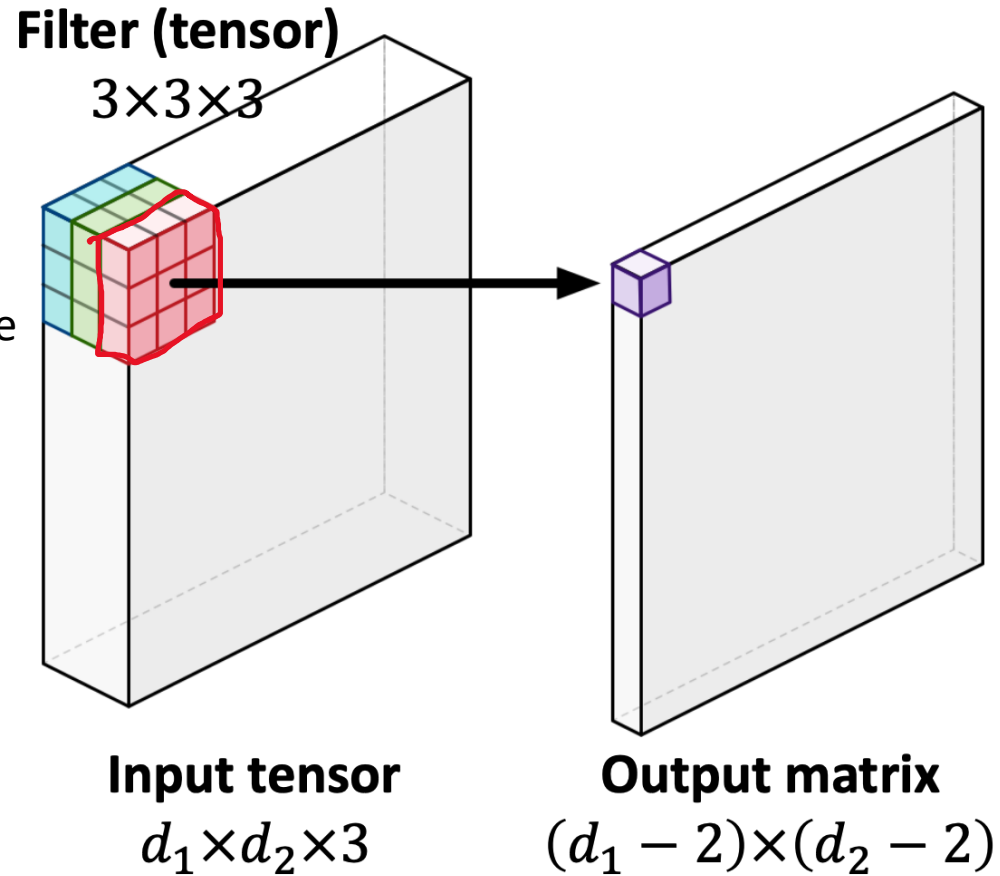
For each channel:
Summarize 9 numbers to one value



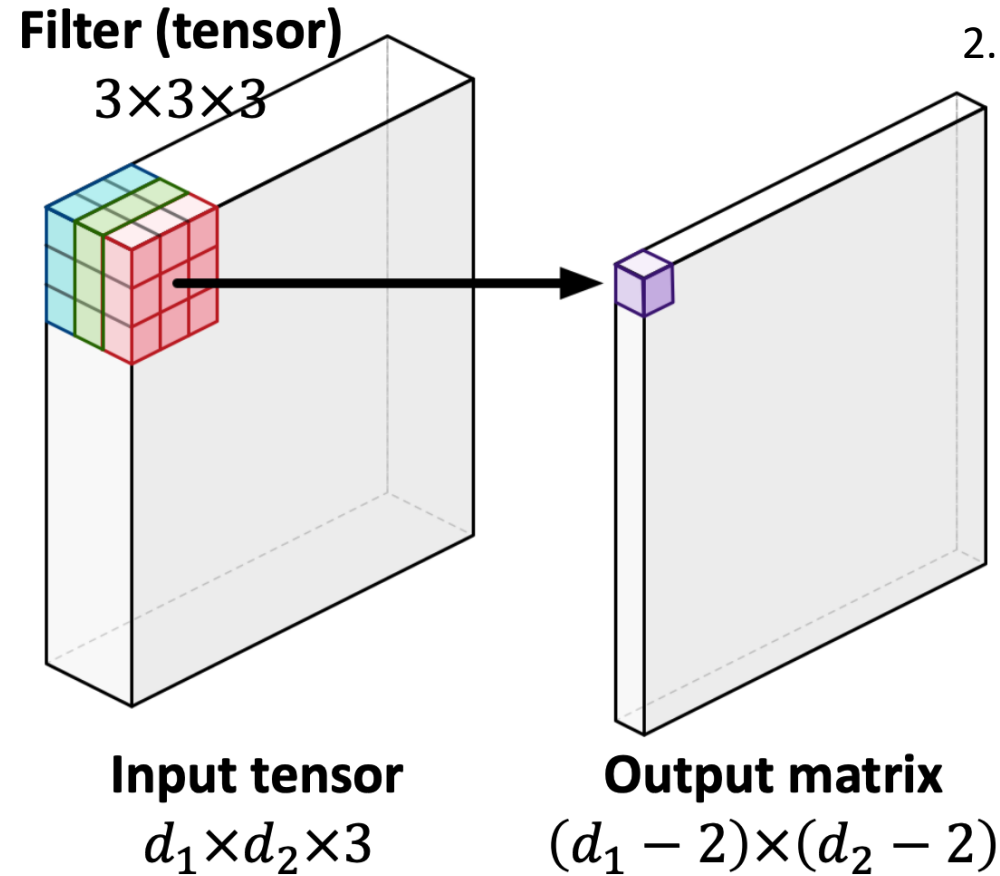
Correlation between data

Q: is there correlation between:
1. locations?

For each channel:
Summarize 9 numbers to one value
(correlation among locations)



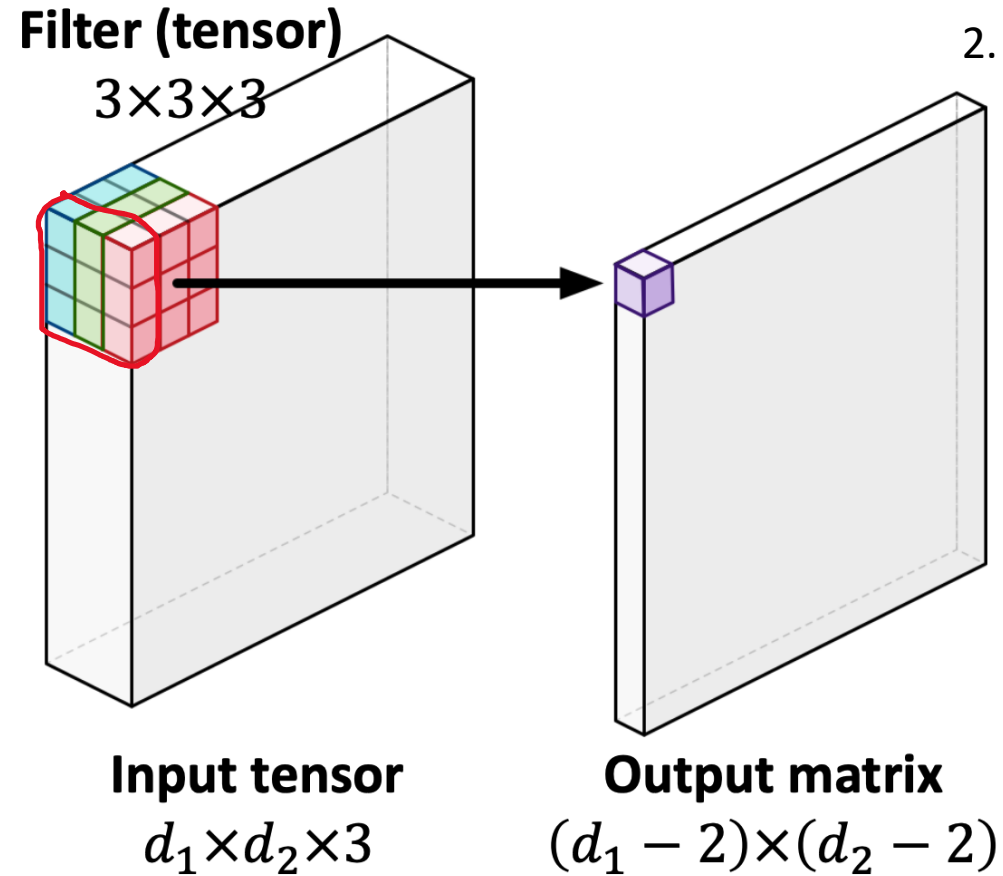
Correlation between data



Q: is there correlation between:

1. locations?
2. channels?

Correlation between data

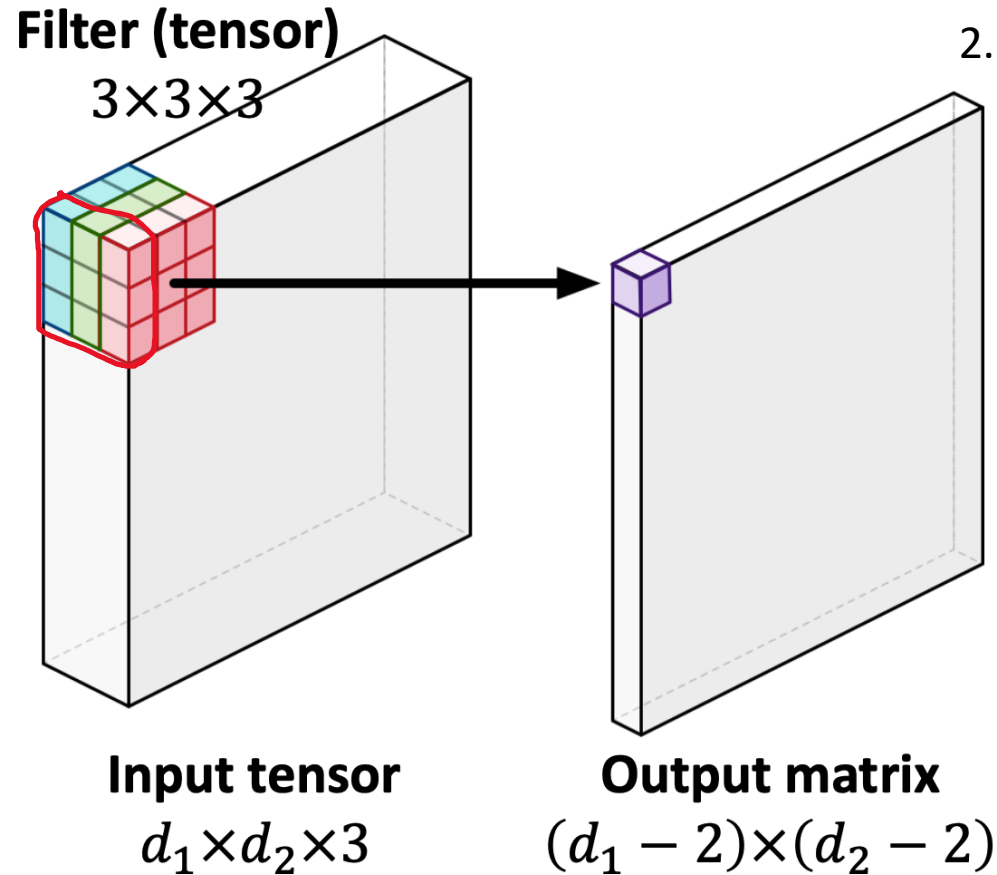


Q: is there correlation between:

1. locations?
2. channels?

Correlation between data

For each location:
Summarize 9 numbers to one value

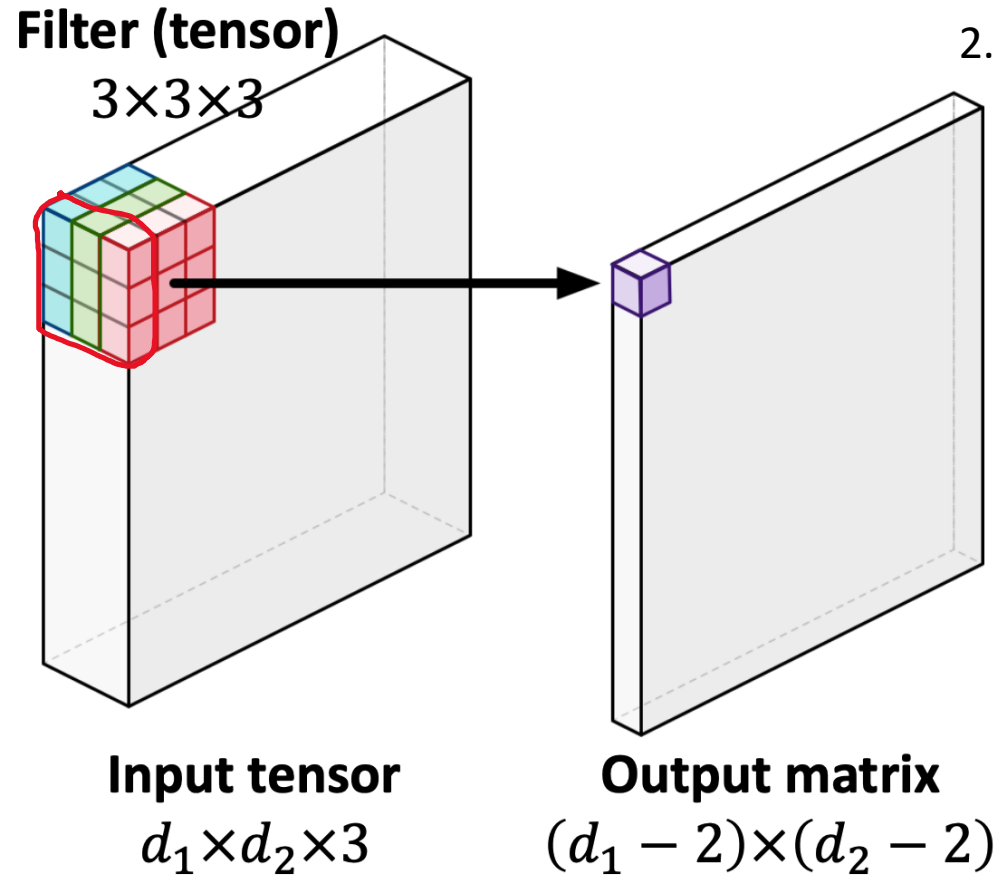


Q: is there correlation between:

1. locations?
2. channels?

Correlation between data

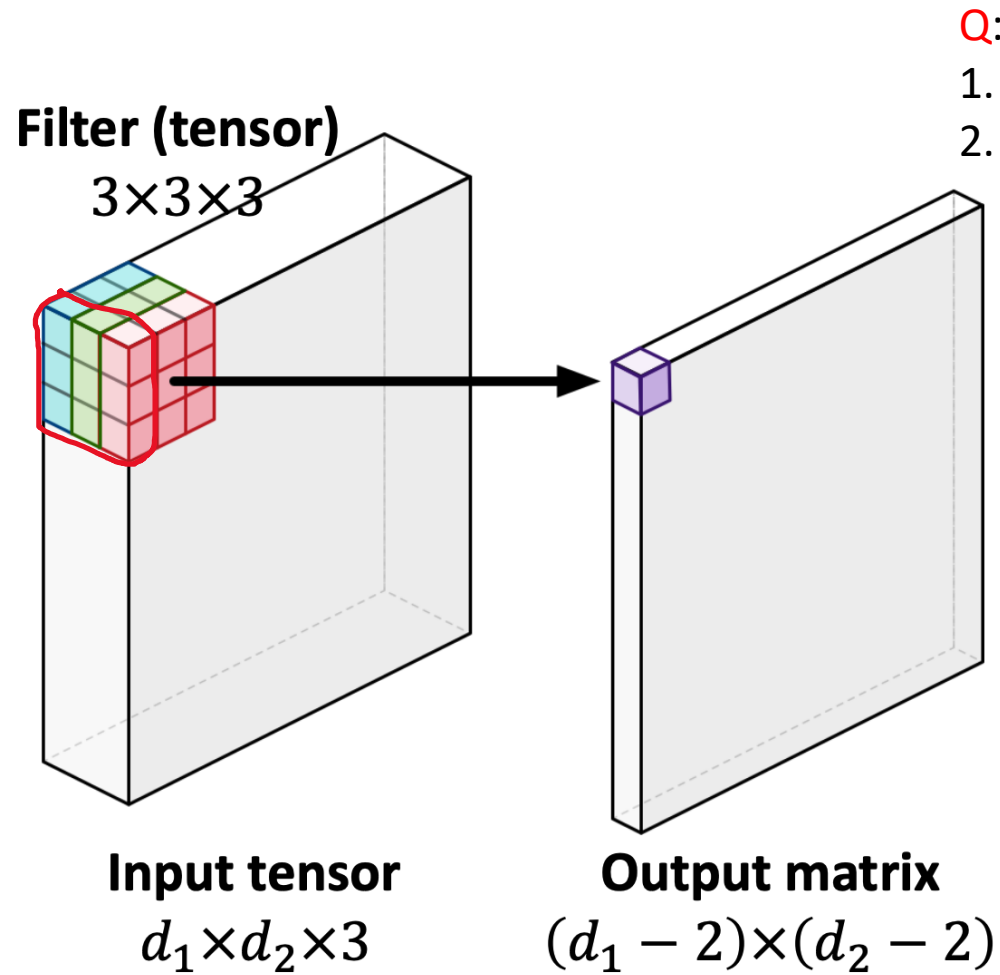
For each location:
Summarize 9 numbers to one value
(correlation among channels)



Q: is there correlation between:

1. locations?
2. channels?

Correlation between data

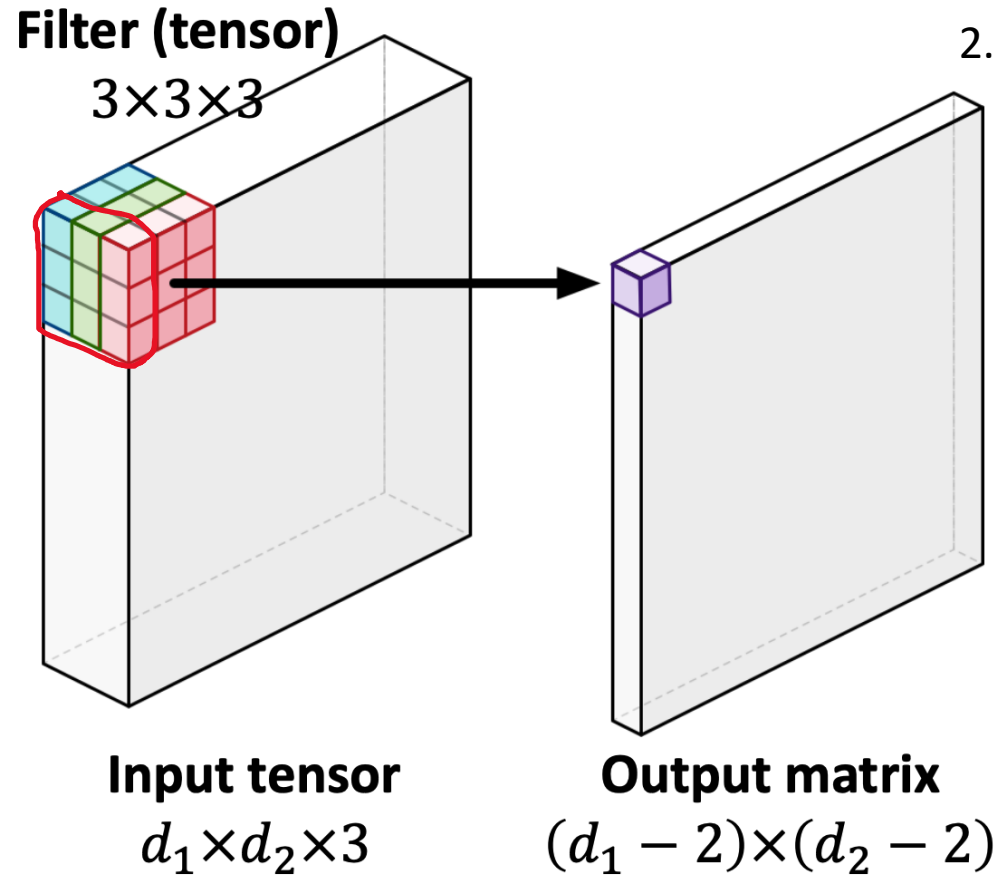


Q: is there correlation between:

1. locations?
2. channels?

Regard feature maps as a grid

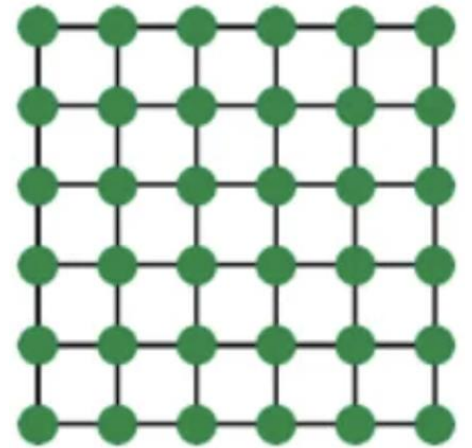
Correlation between data



Q: is there correlation between:

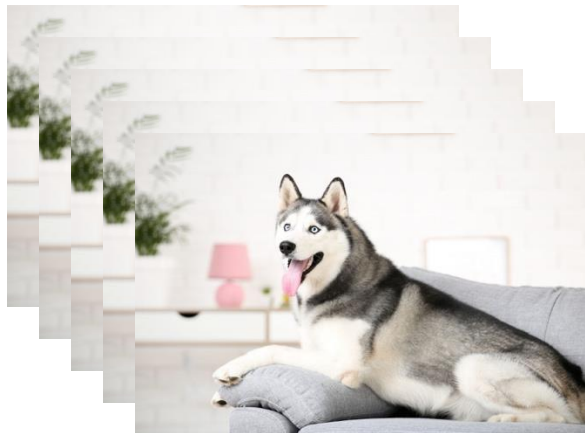
1. locations?
2. channels?

Regard feature maps as a grid



Pixel values or feature values

Correlation between data



Cat or dog?

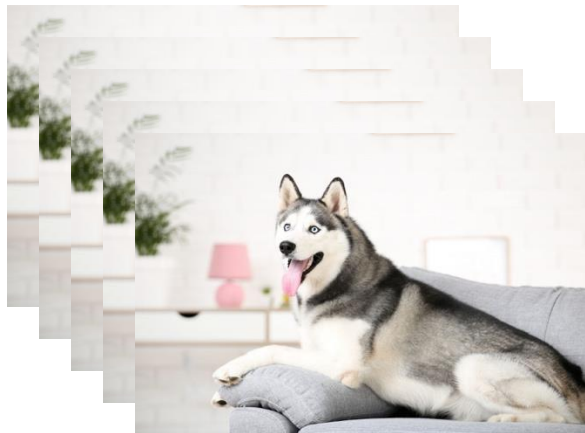
Correlation between data



Cat or dog?

Q: is there correlation **between images**?

Correlation between data

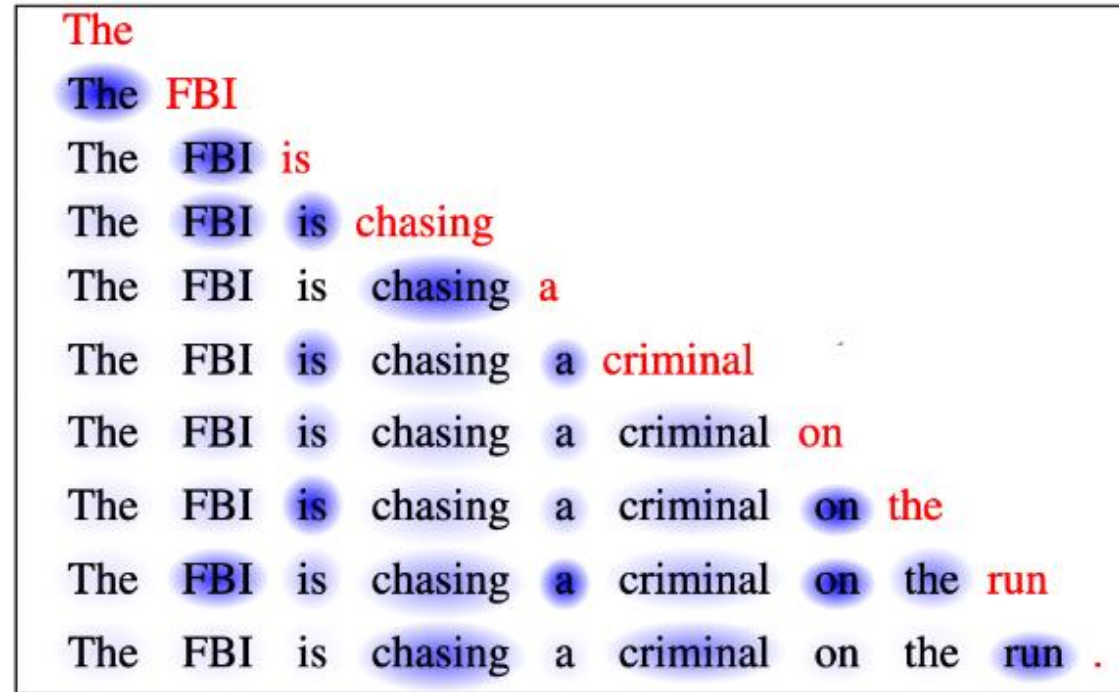


Cat or dog?

Q: is there correlation **between images**?

No

Correlation between data



The
The FBI
The FBI is
The FBI is chasing
The FBI is chasing a
The FBI is chasing a criminal
The FBI is chasing a criminal on
The FBI is chasing a criminal on the
The FBI is chasing a criminal on the run
The FBI is chasing a criminal on the run .

Figure is from the paper "Long Short-Term Memory-Networks for Machine Reading."

Correlation between data

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The FBI is

Correlation between data

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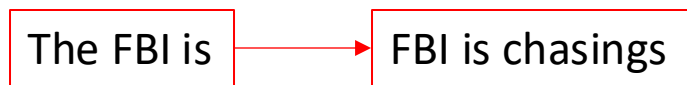
The FBI is

FBI is chasings

Correlation between data

The
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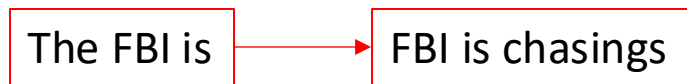
Figure is from the paper "Long Short-Term Memory-Networks for Machine Reading."



Correlation between data

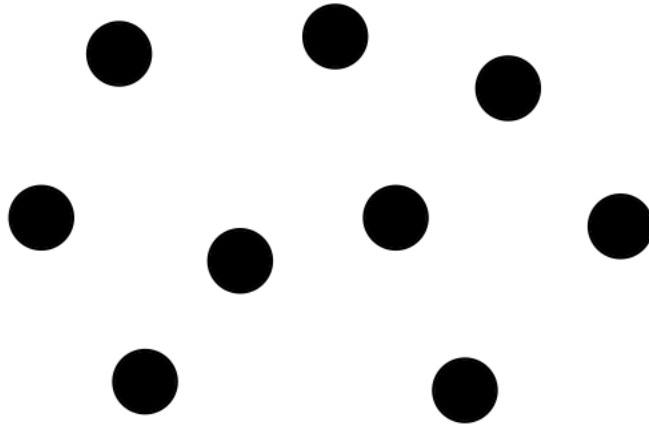
The
The FBI
The FBI is
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The FBI is chasing a criminal
The FBI is chasing a criminal on
The FBI is chasing a criminal on the
The FBI is chasing a criminal on the run
The FBI is chasing a criminal on the run .

Figure is from the paper "Long Short-Term Memory-Networks for Machine Reading."

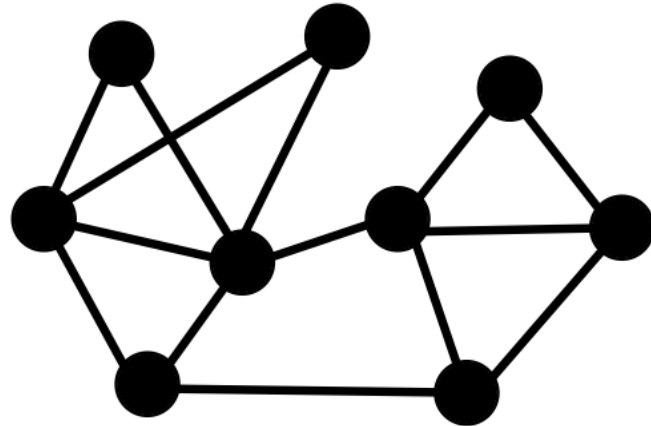


Q: what if we need more complicated correlation?

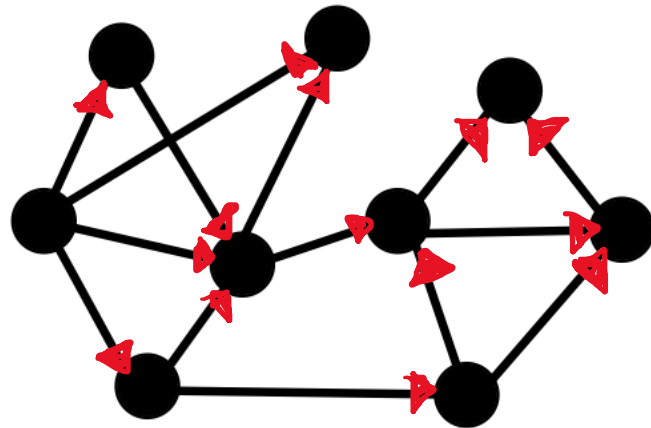
Correlation between data



Correlation between data

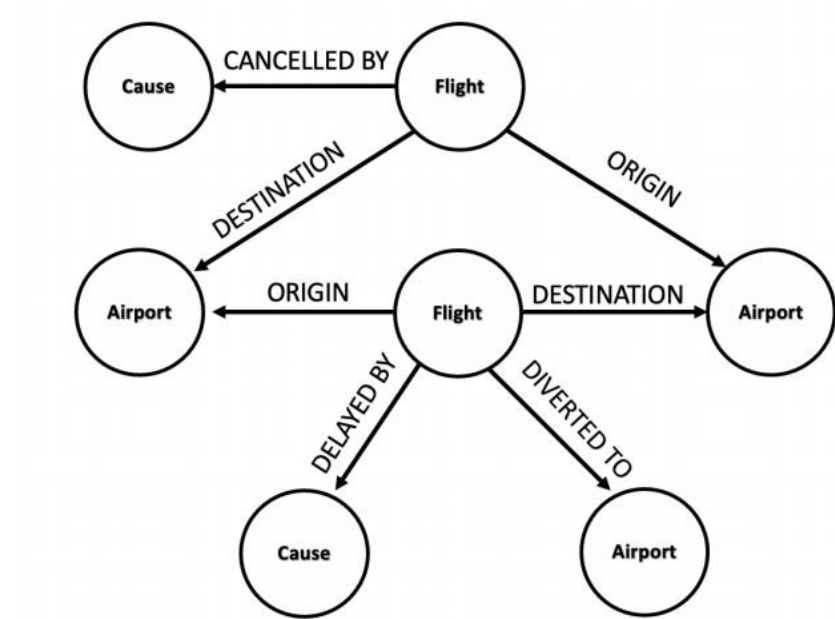


Correlation between data



(with directions)

Correlation between data



Event Graphs

Correlation between data



Image credit: [SalientNetworks](#)

Computer Networks

Correlation between data

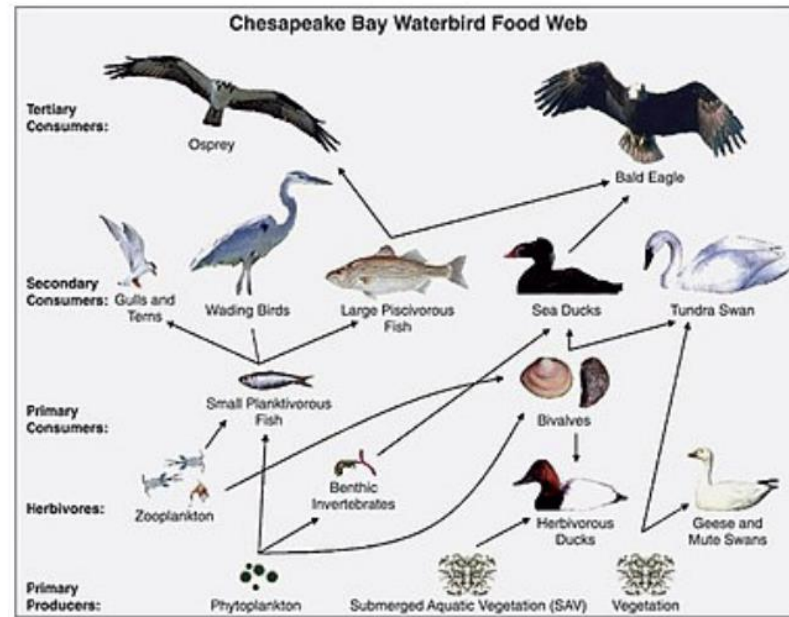


Image credit: [Wikipedia](#)

Food Webs

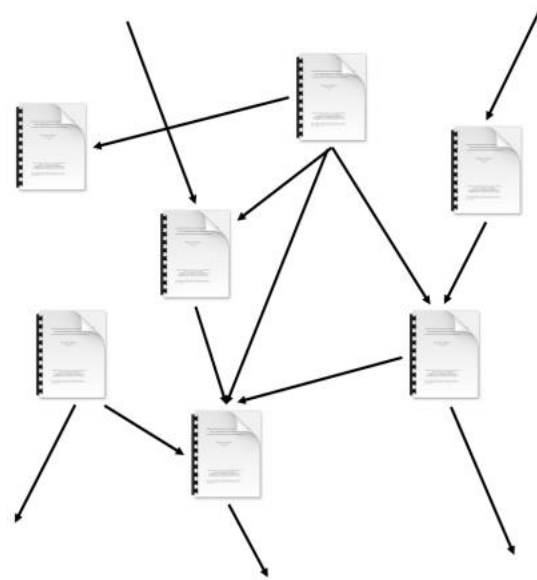
Correlation between data



Image credit: [Medium](#)

Social Networks

Correlation between data



Citation Networks

Correlation between data

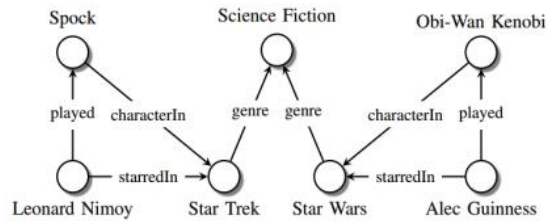


Image credit: [Maximilian Nickel et al](#)

Knowledge Graphs

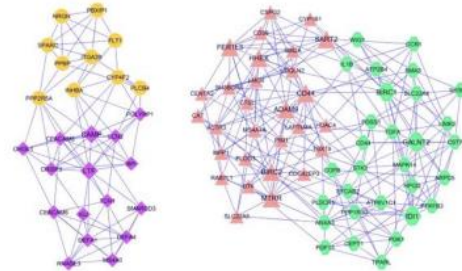


Image credit: [ese.wustl.edu](#)

Regulatory Networks

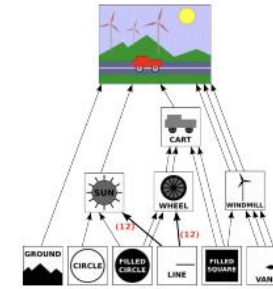


Image credit: [math.hws.edu](#)

Scene Graphs

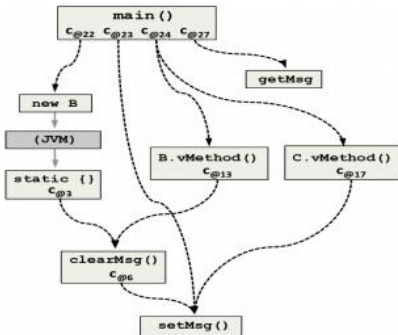


Image credit: [ResearchGate](#)

Code Graphs

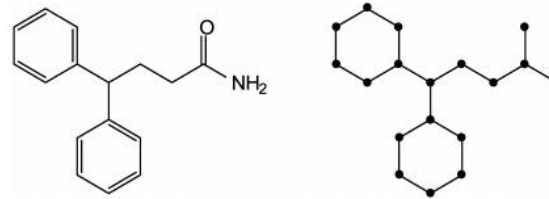


Image credit: [MDPI](#)

Molecules

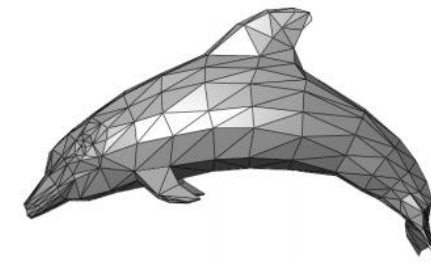
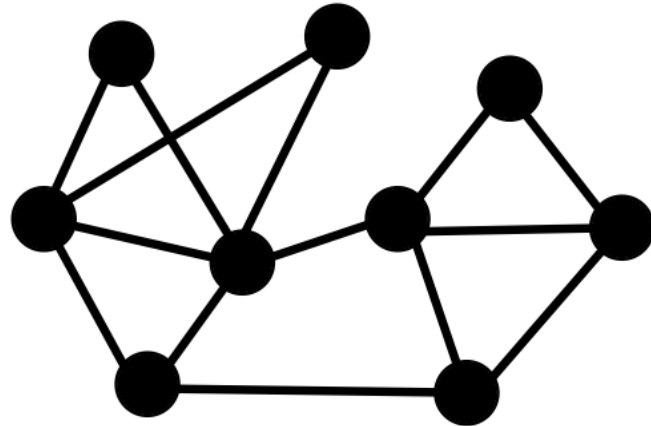


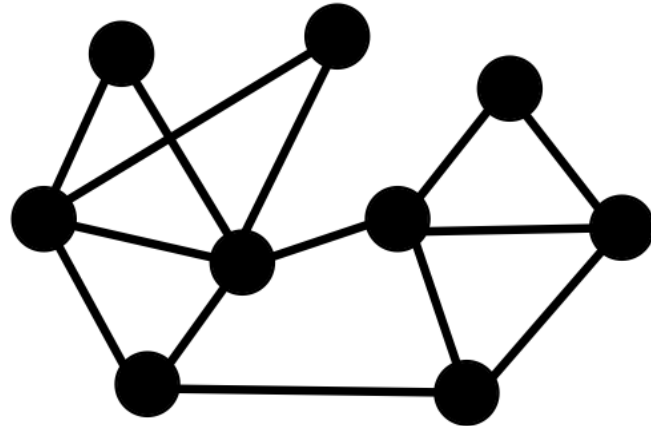
Image credit: [Wikipedia](#)

3D Shapes

Correlation between data

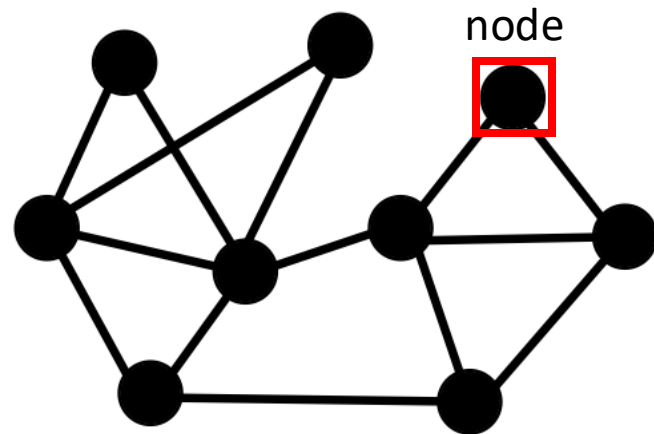


Correlation between data



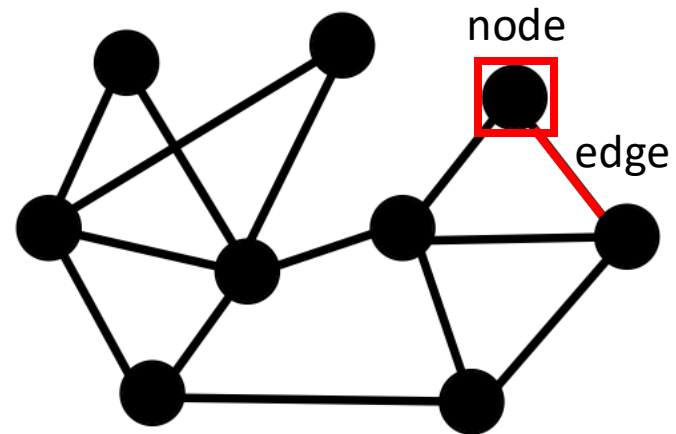
undirected graph

Correlation between data



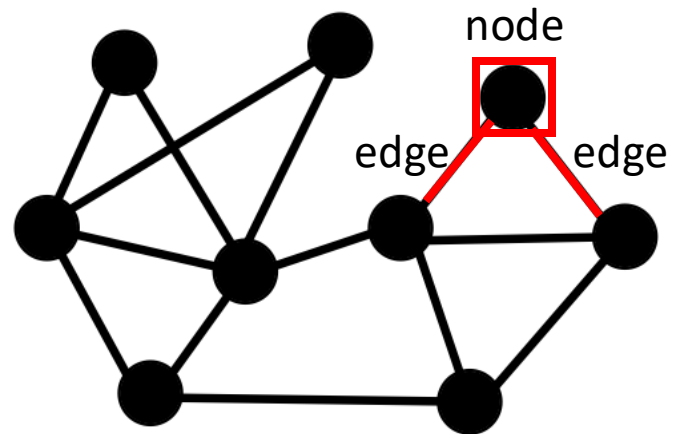
undirected graph

Correlation between data



undirected graph

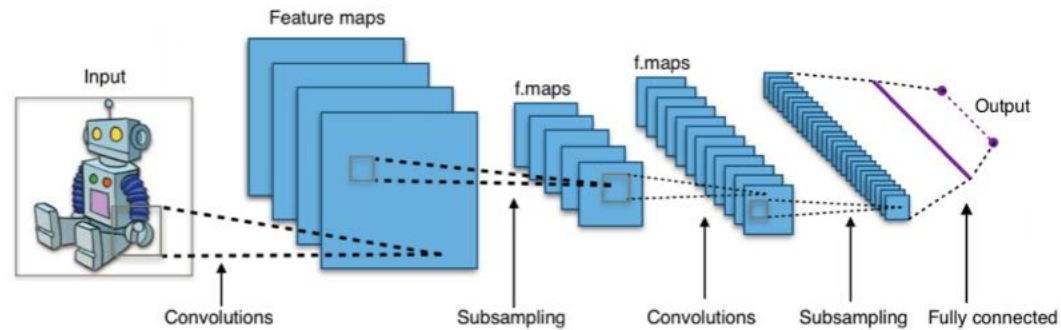
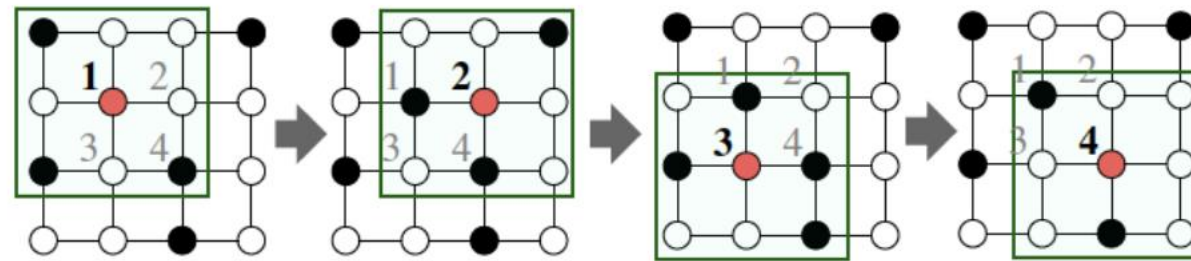
Correlation between data



undirected graph

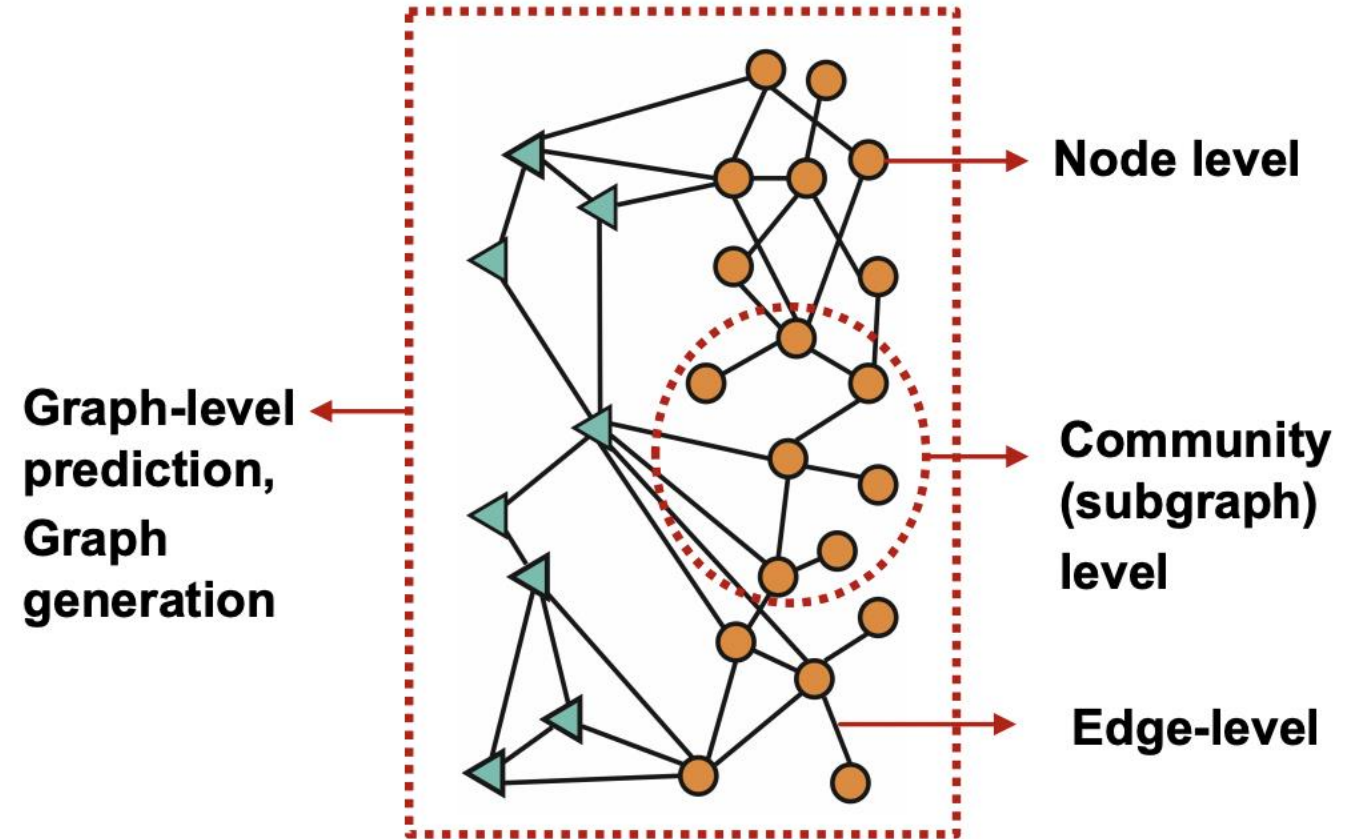
Correlation between data

CNN on an image:



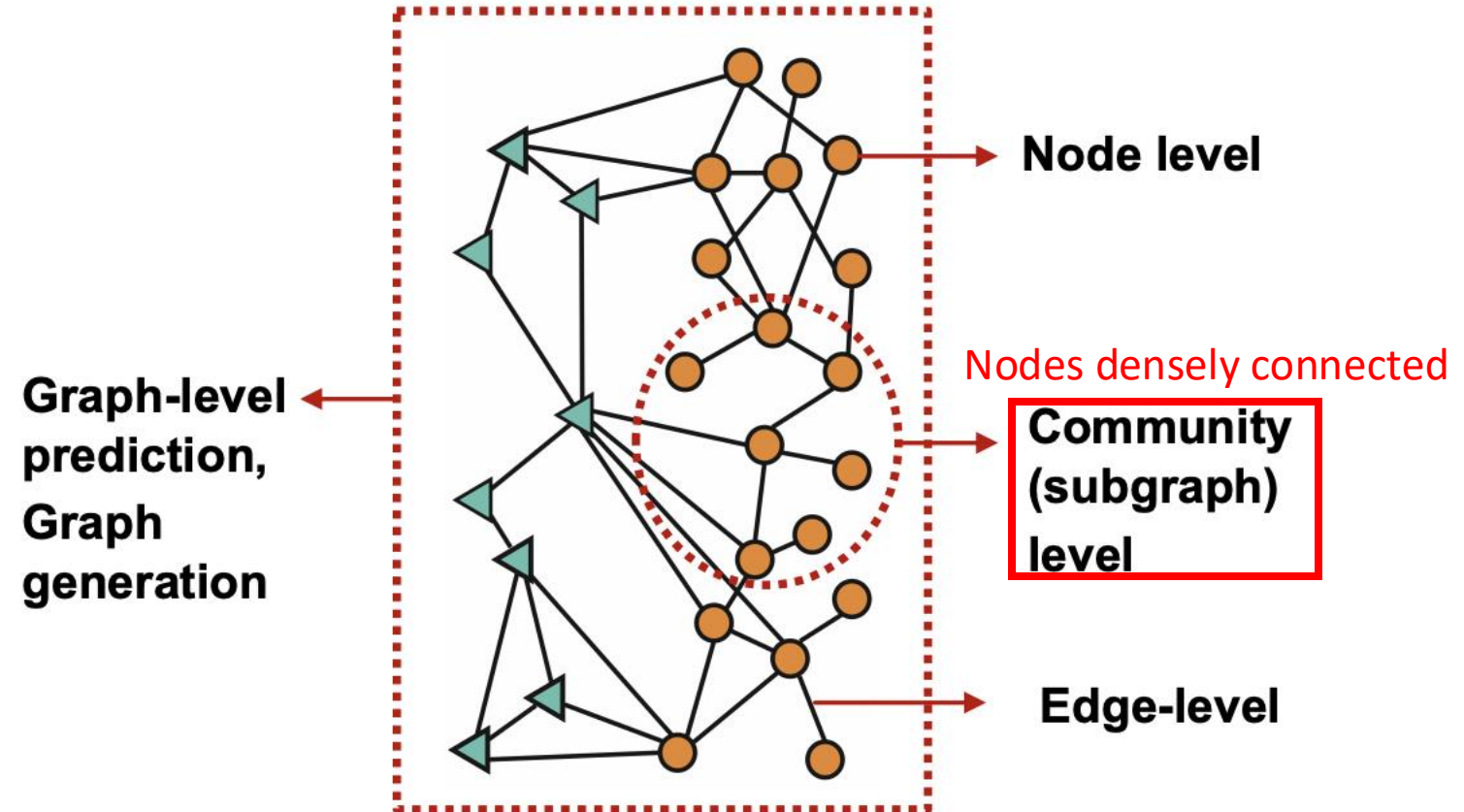
Machine learning tasks for graph data

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



Machine learning tasks for graph data

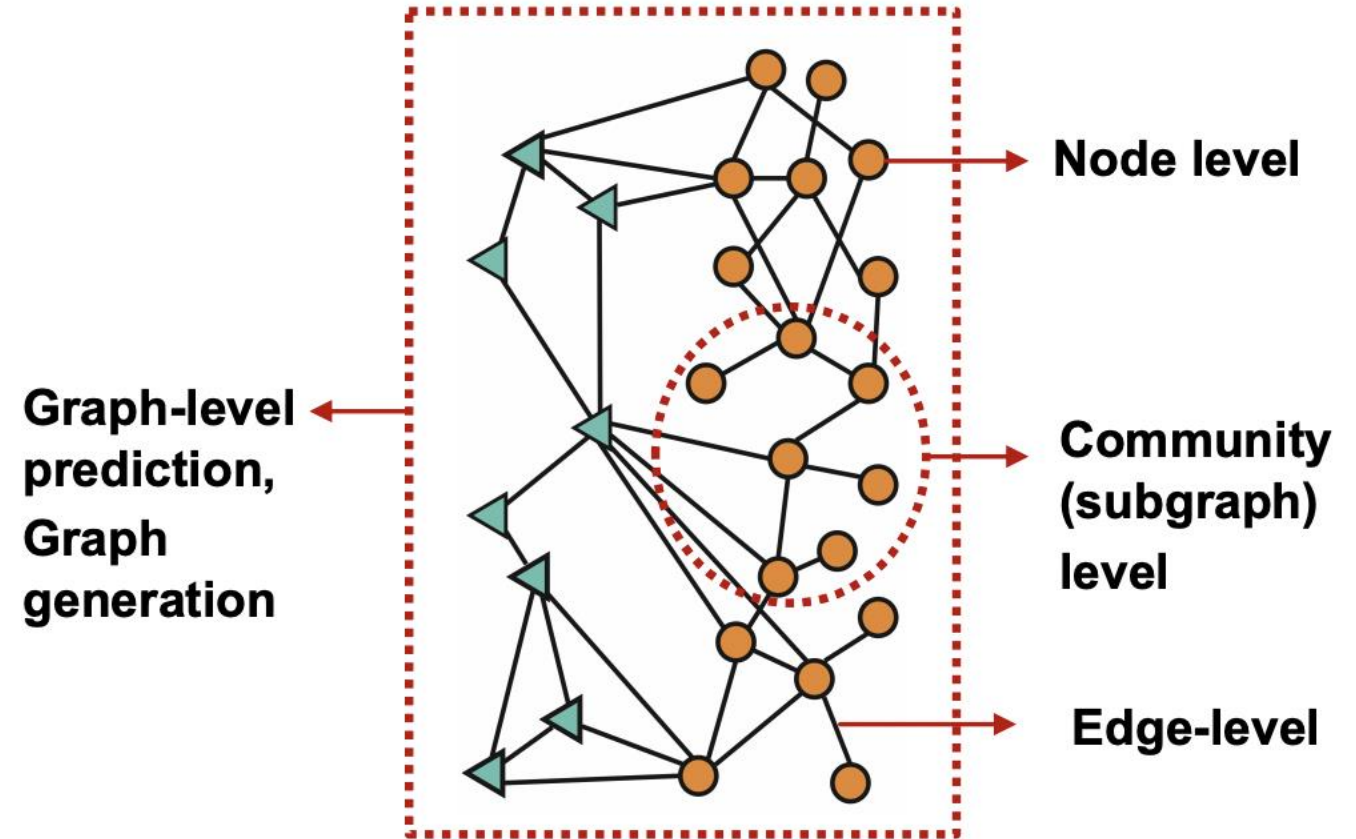
- Node level
- Edge level
- Community level
- Graph level



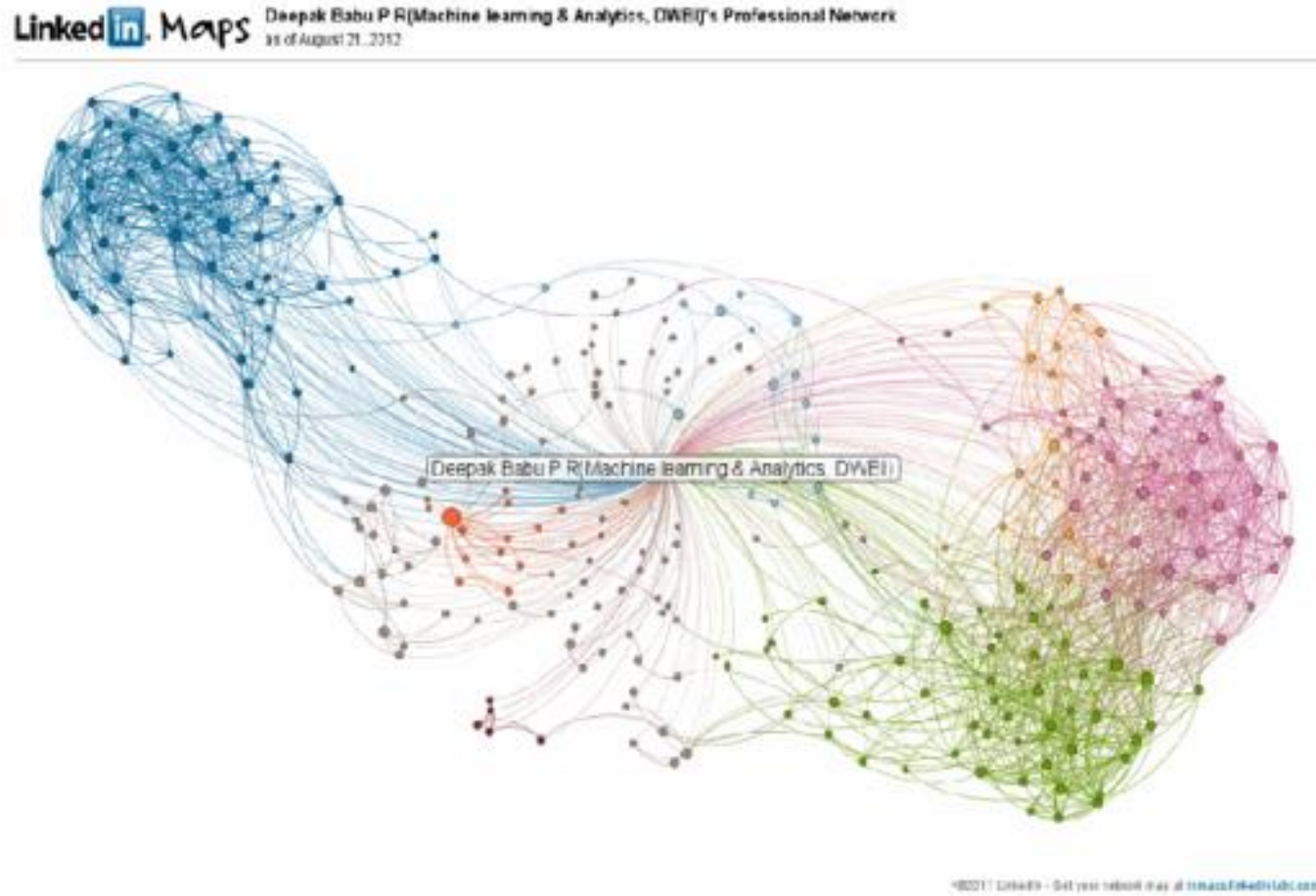
Machine learning tasks for graph data

classification

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

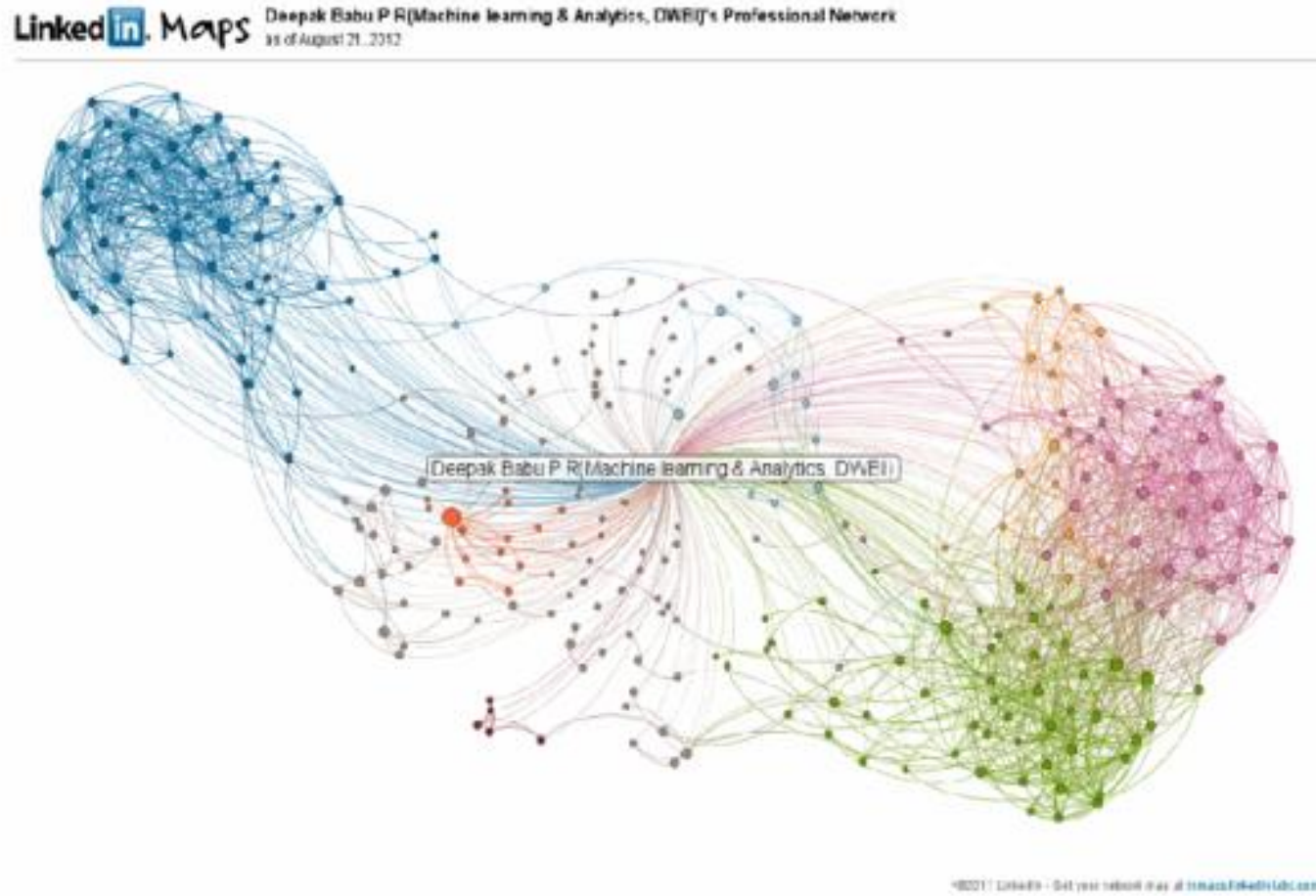


Social network

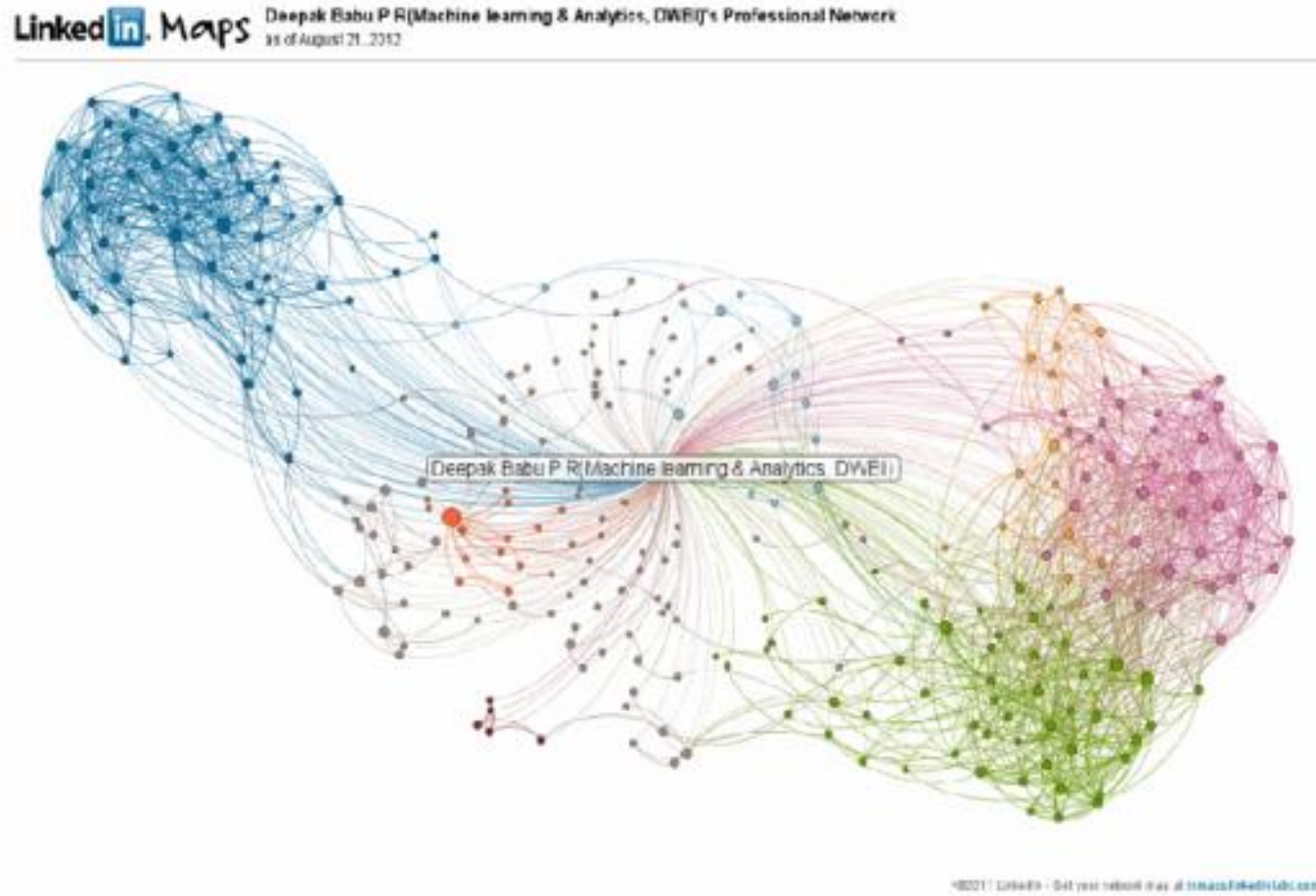


Social network

Nodes: users



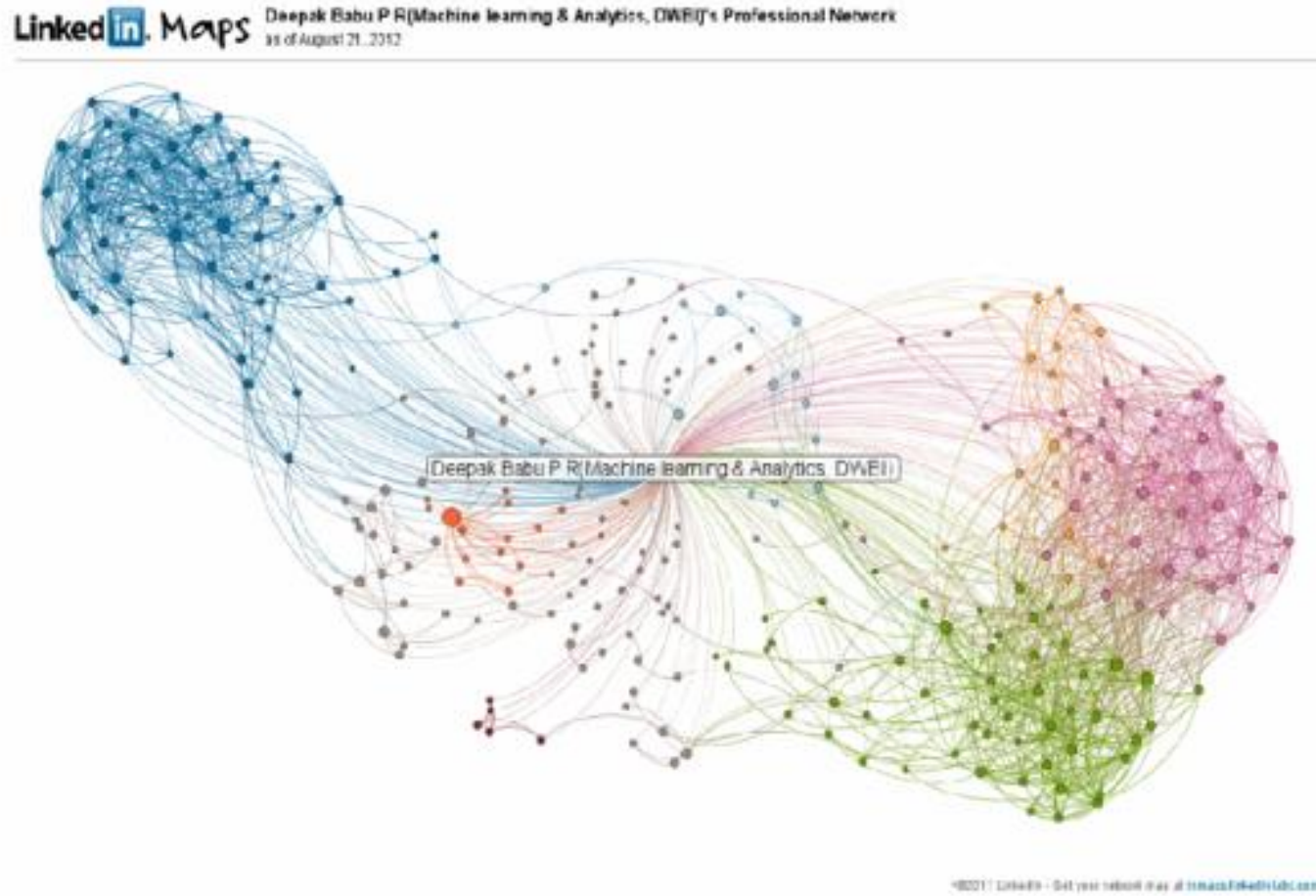
Social network



Nodes: users

Edges: interactions

Social network

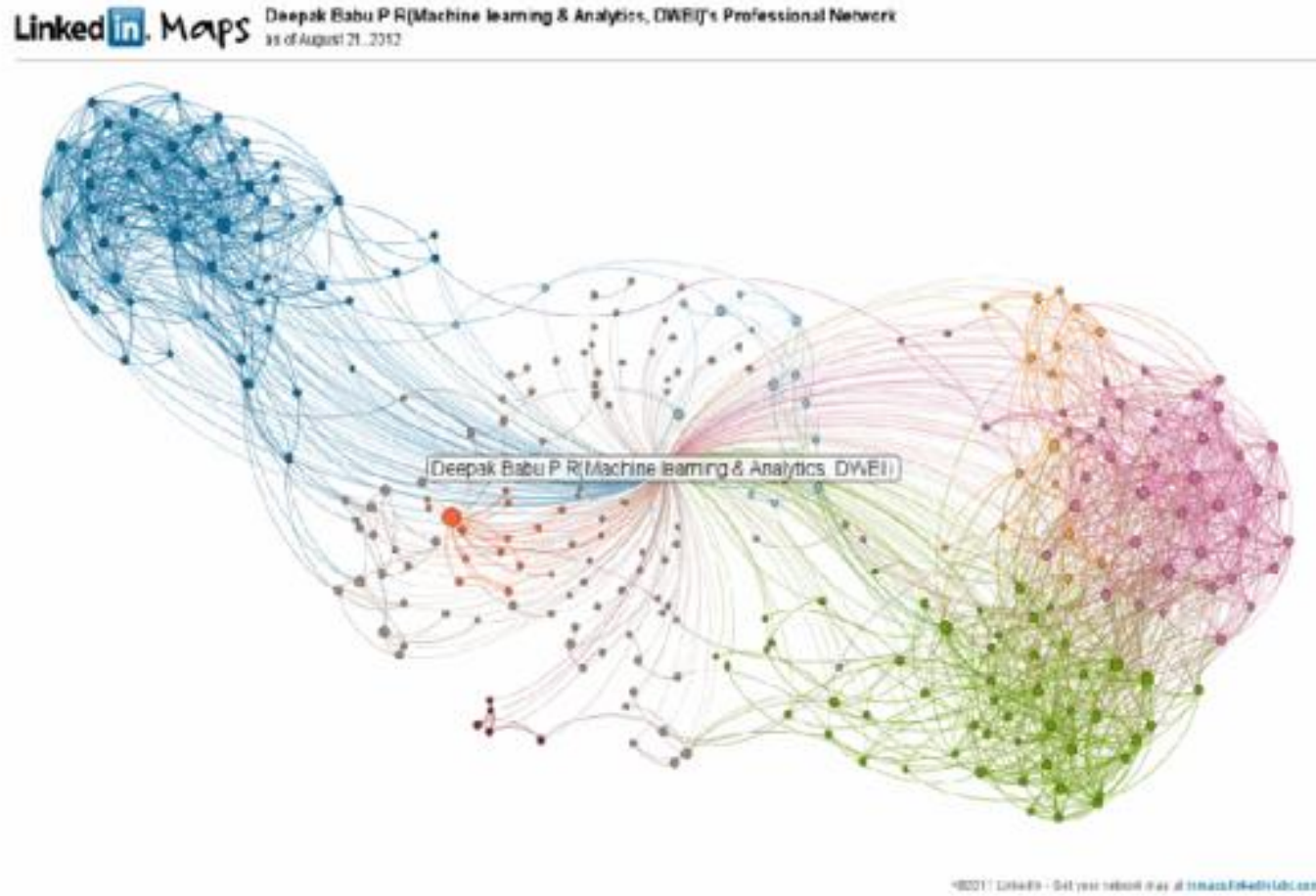


Nodes: users

Edges: interactions

FB: add friend

Social network

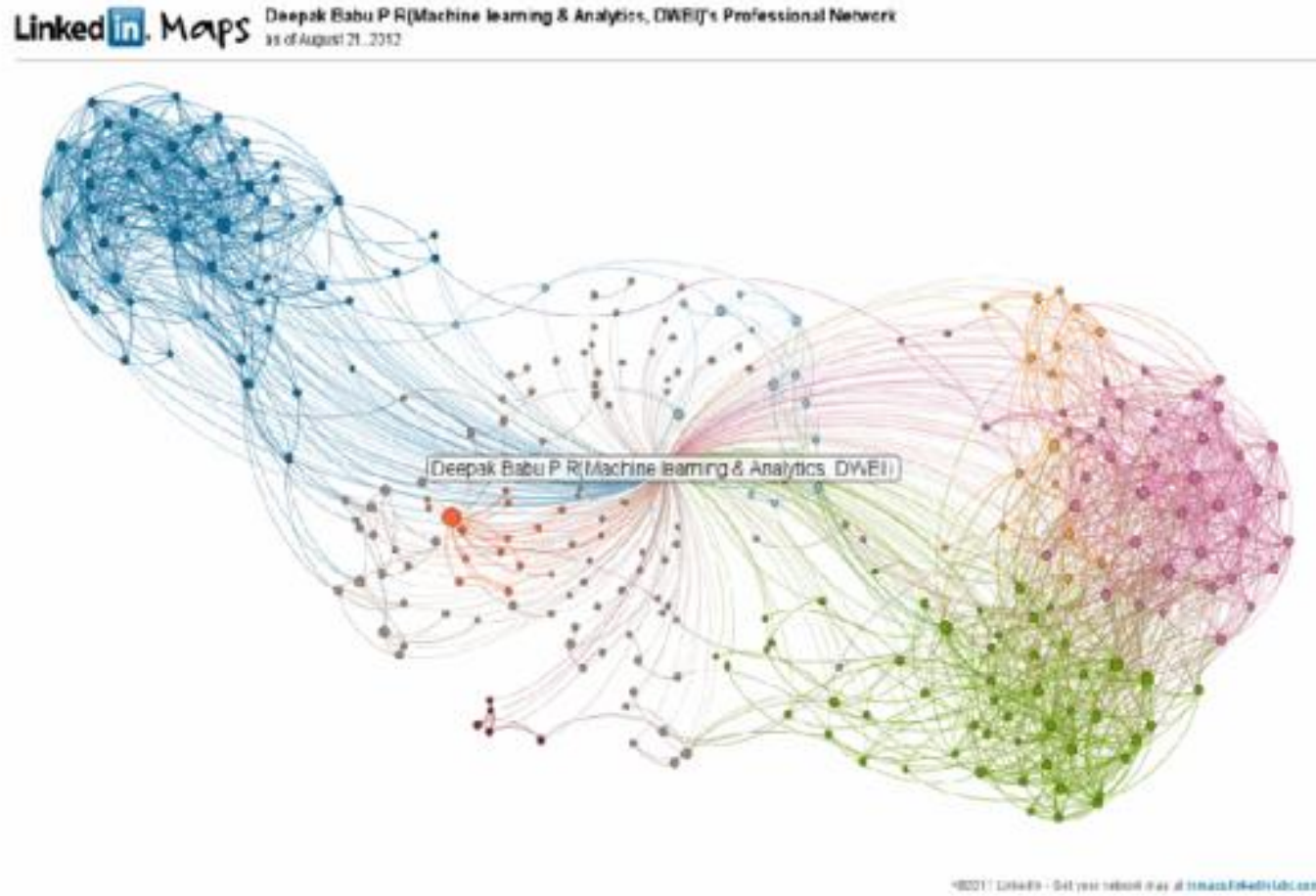


Nodes: users

Edges: interactions

LinkedIn: connect

Social network

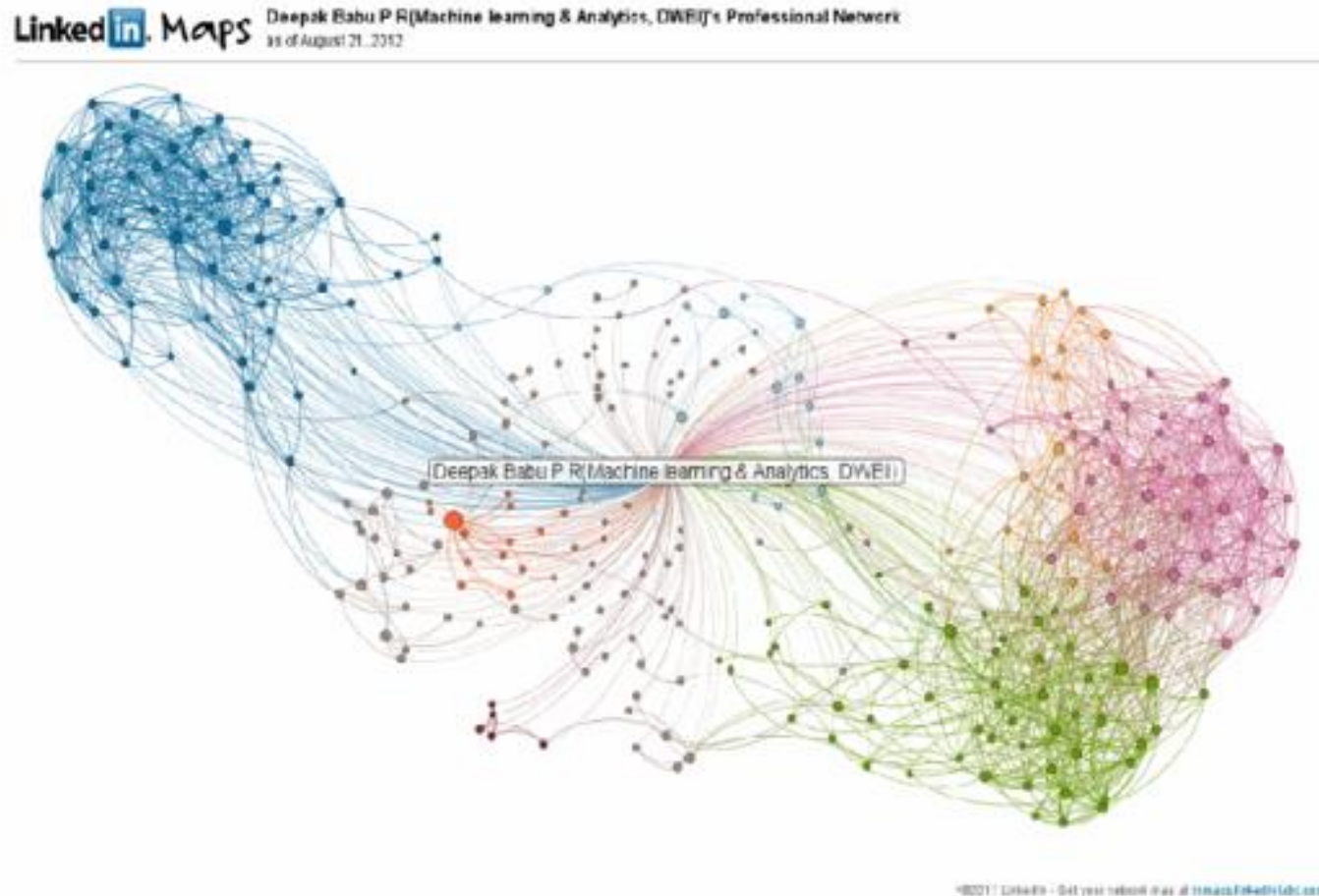


Nodes: users

Edges: interactions

Amazon: same purchase

Social network



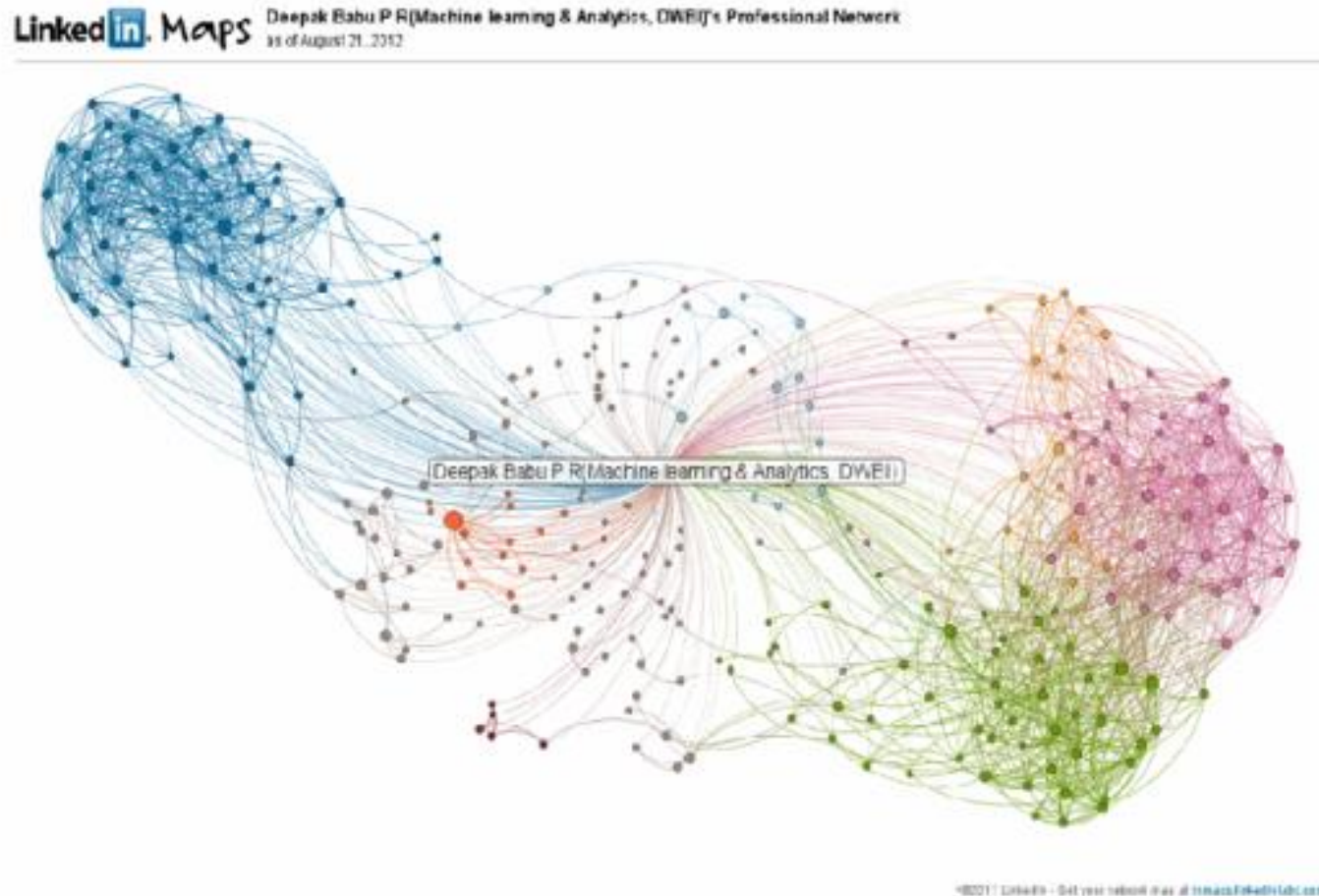
Nodes: users

Edges: interactions

Node classification:

Group nodes by their properties

Social network



Nodes: users

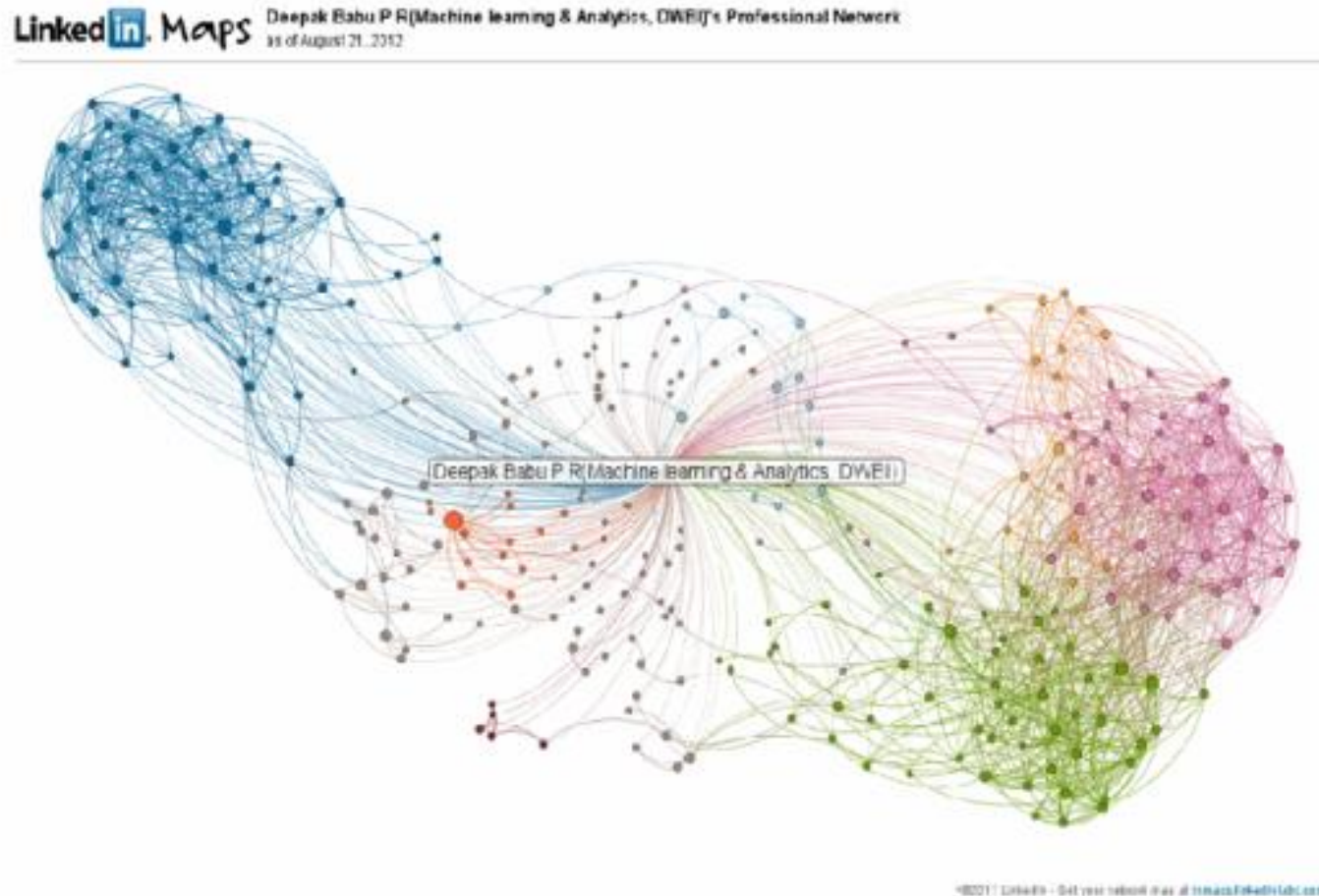
Edges: interactions

Edge classification:

Predict whether there are missing links between two nodes

e.g., friend recommendation

Social network

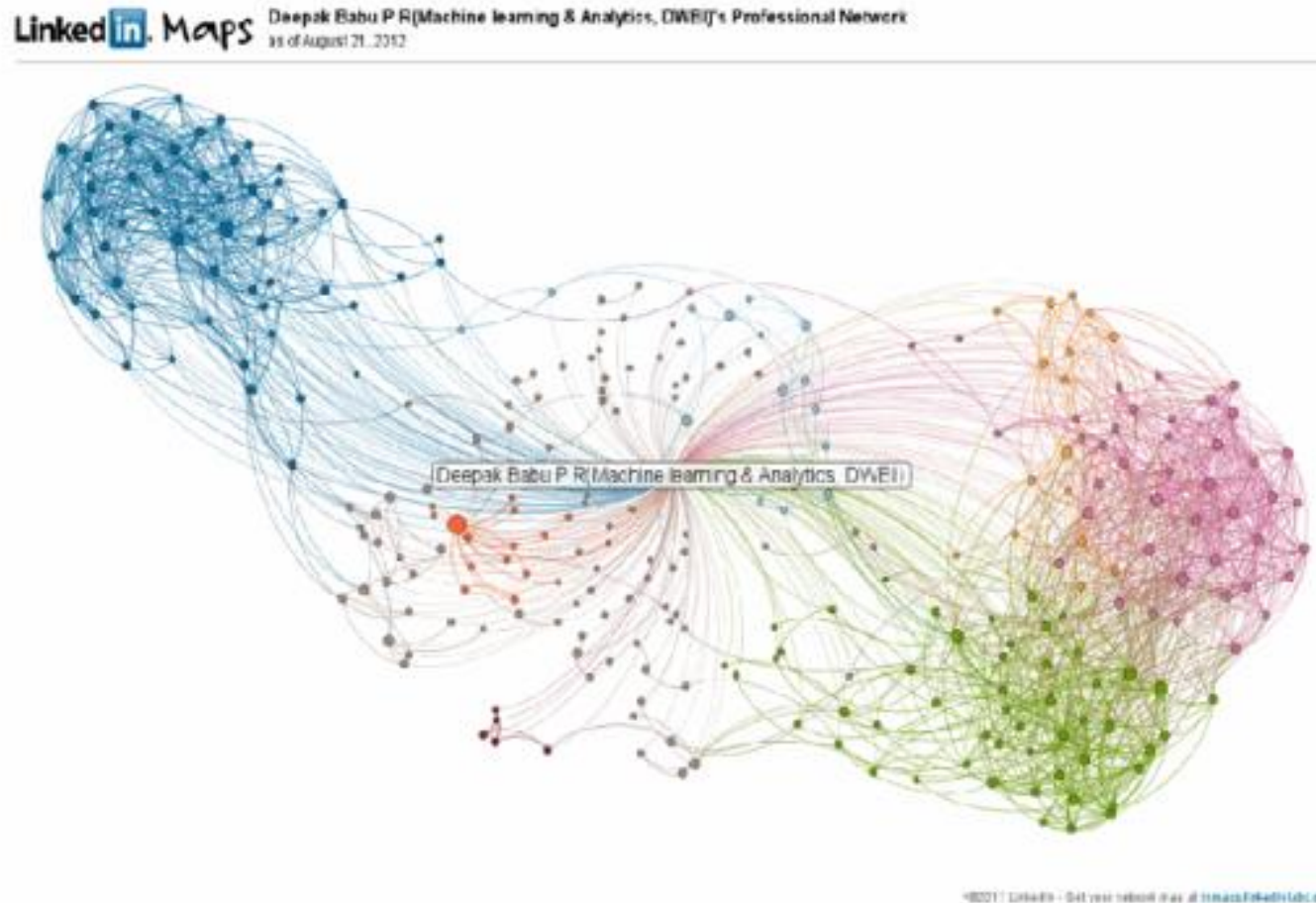


Nodes: users

Edges: interactions

Community detection:
Discover and group nodes tightly
connected

Social network



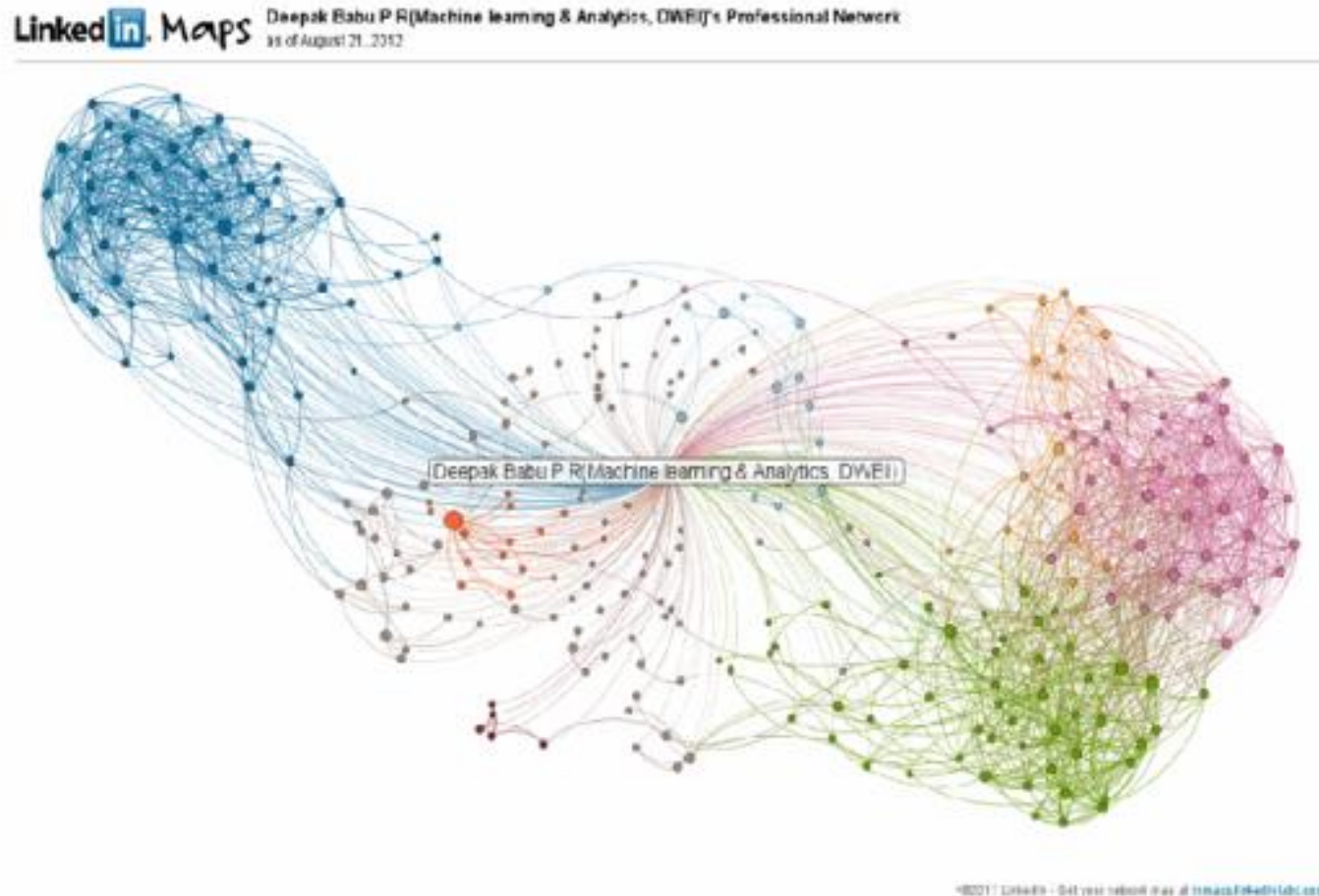
Nodes: users

Edges: interactions

Graph classification:

Categorize different graphs

Social network



Nodes: users

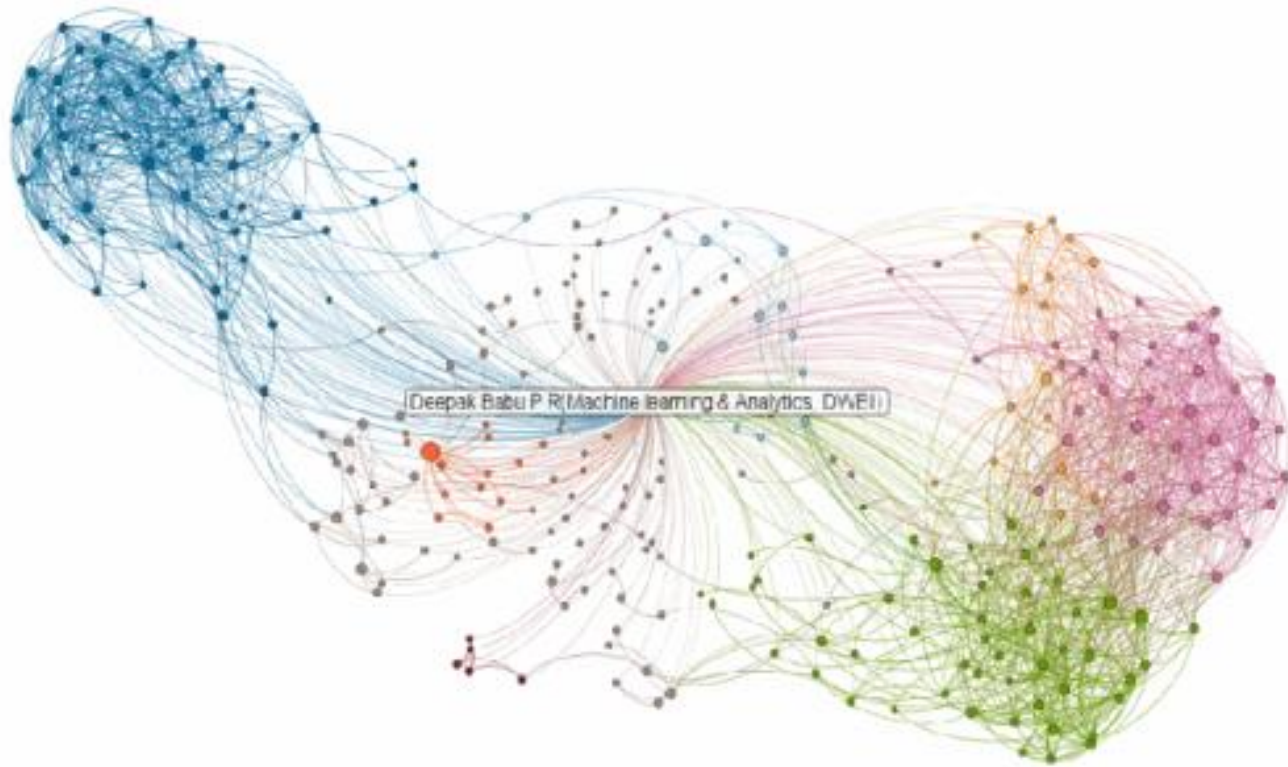
Edges: interactions

Graph classification:

Categorize different graphs
e.g., Molecule property
prediction

Social network

LinkedIn Maps Deepak Babu P R (Machine learning & Analytics, DWBI)'s Professional Network
as of August 21, 2012

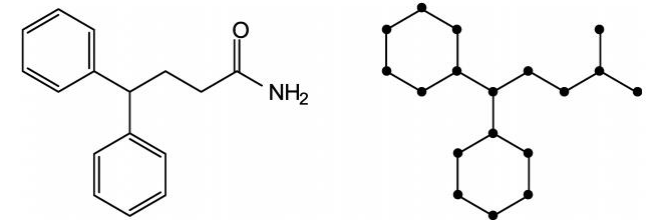


Nodes: users

Edges: interactions

Graph classification:

Categorize different graphs
e.g., Molecule property
prediction

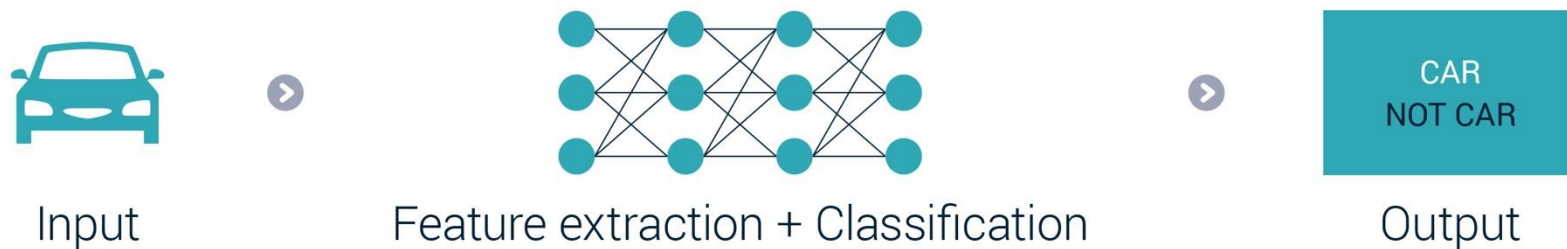


Machine learning tasks for graph data

Machine Learning

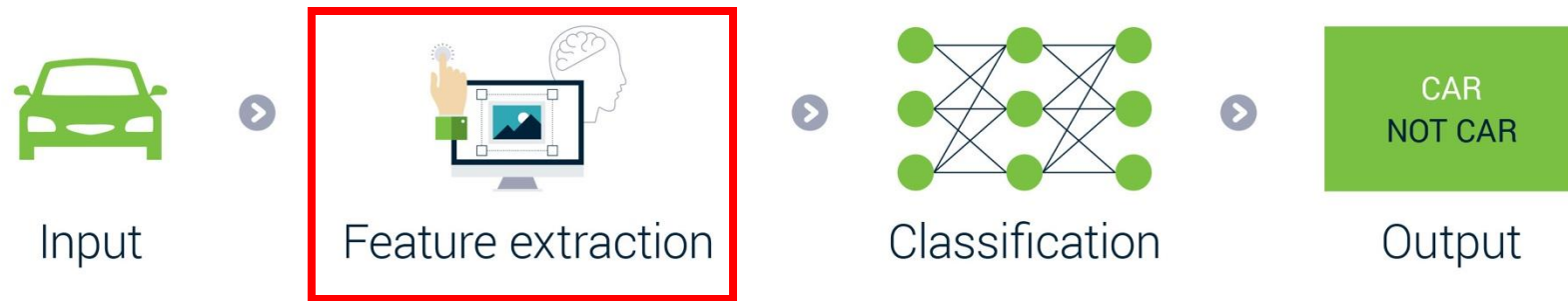


Deep Learning

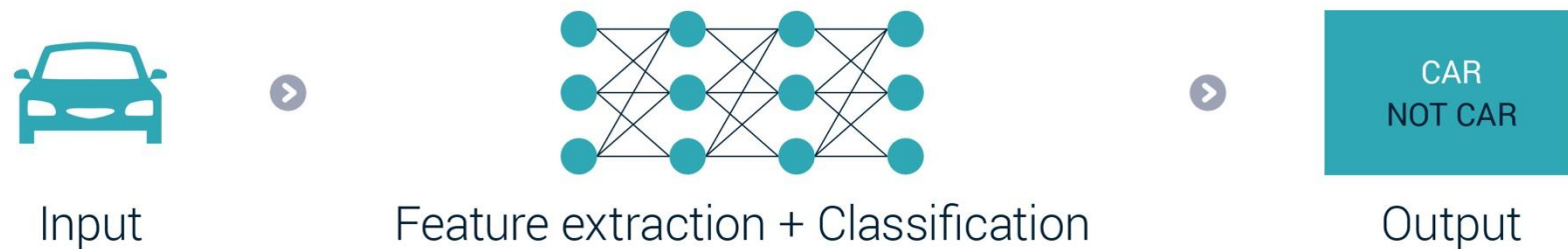


Machine learning tasks for graph data

Machine Learning

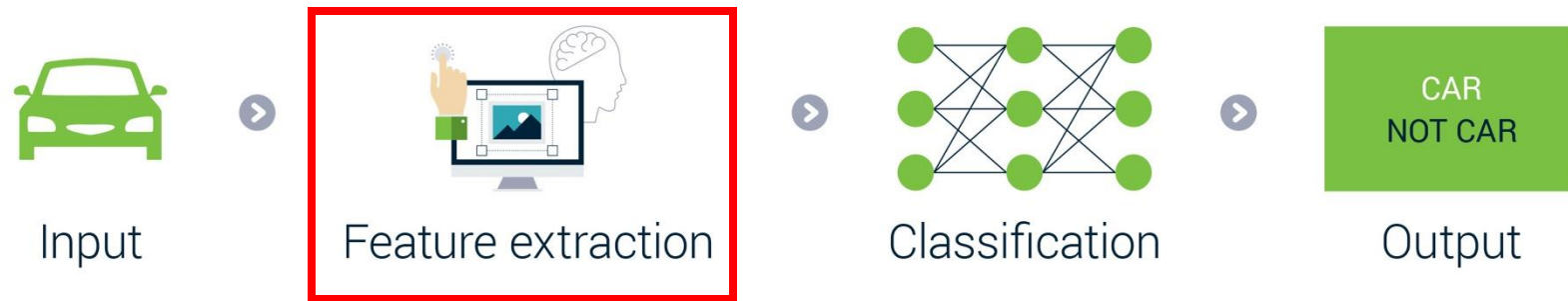


Deep Learning

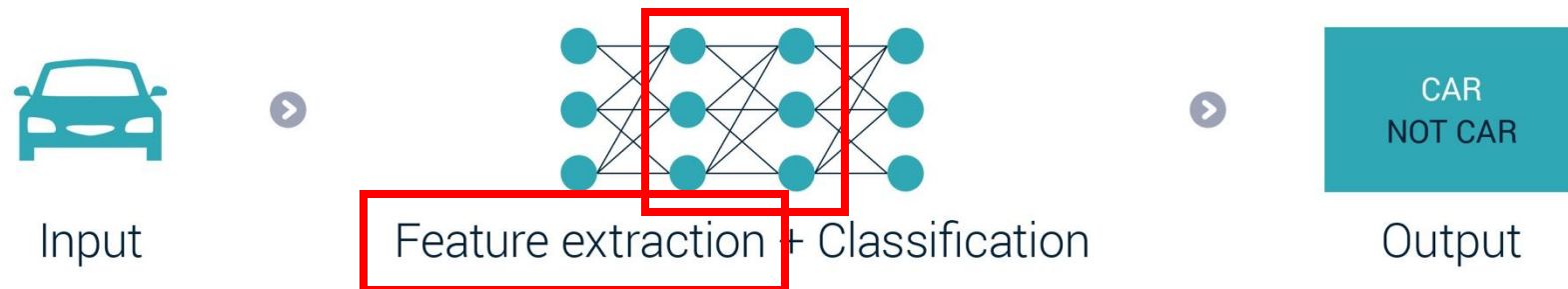


Machine learning tasks for graph data

Machine Learning



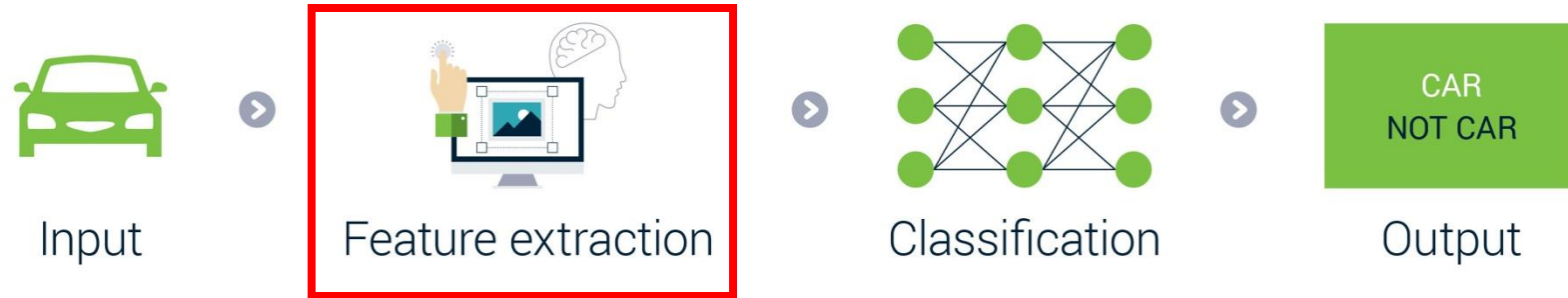
Deep Learning



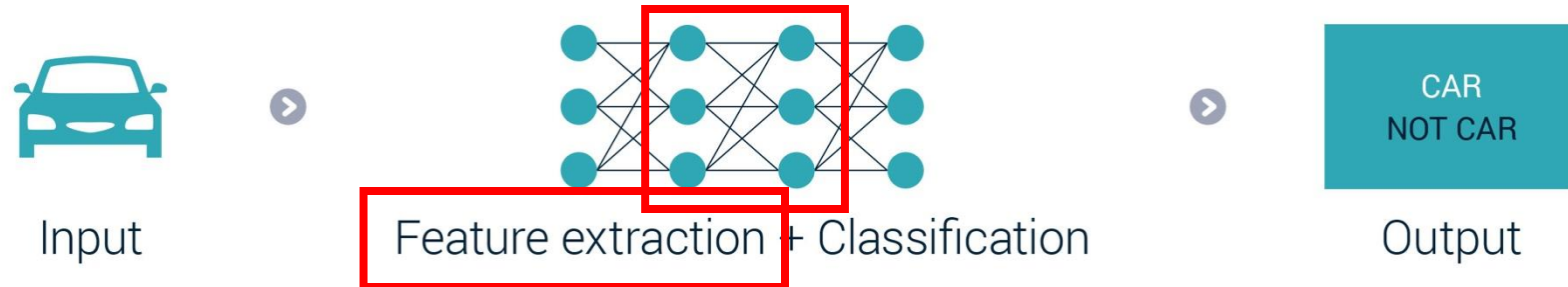
Machine learning tasks for graph data

Machine Learning

Consider correlations



Deep Learning



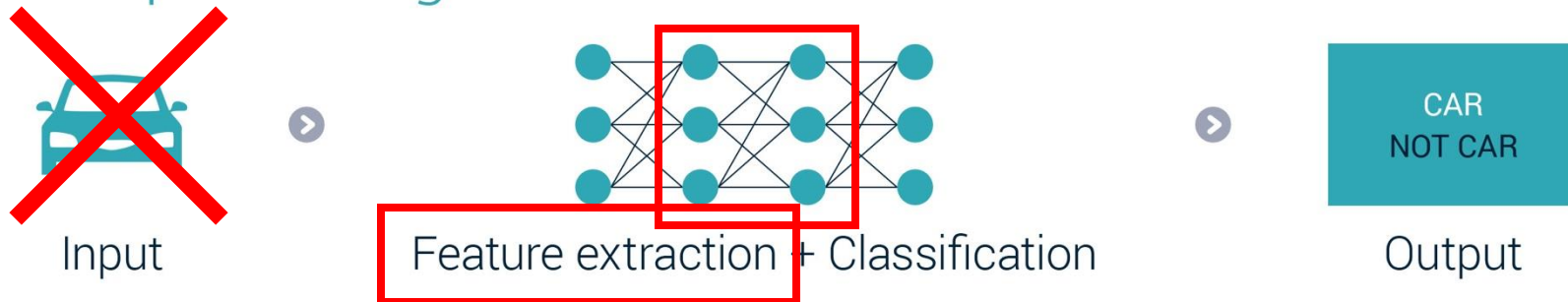
Machine learning tasks for graph data

Machine Learning

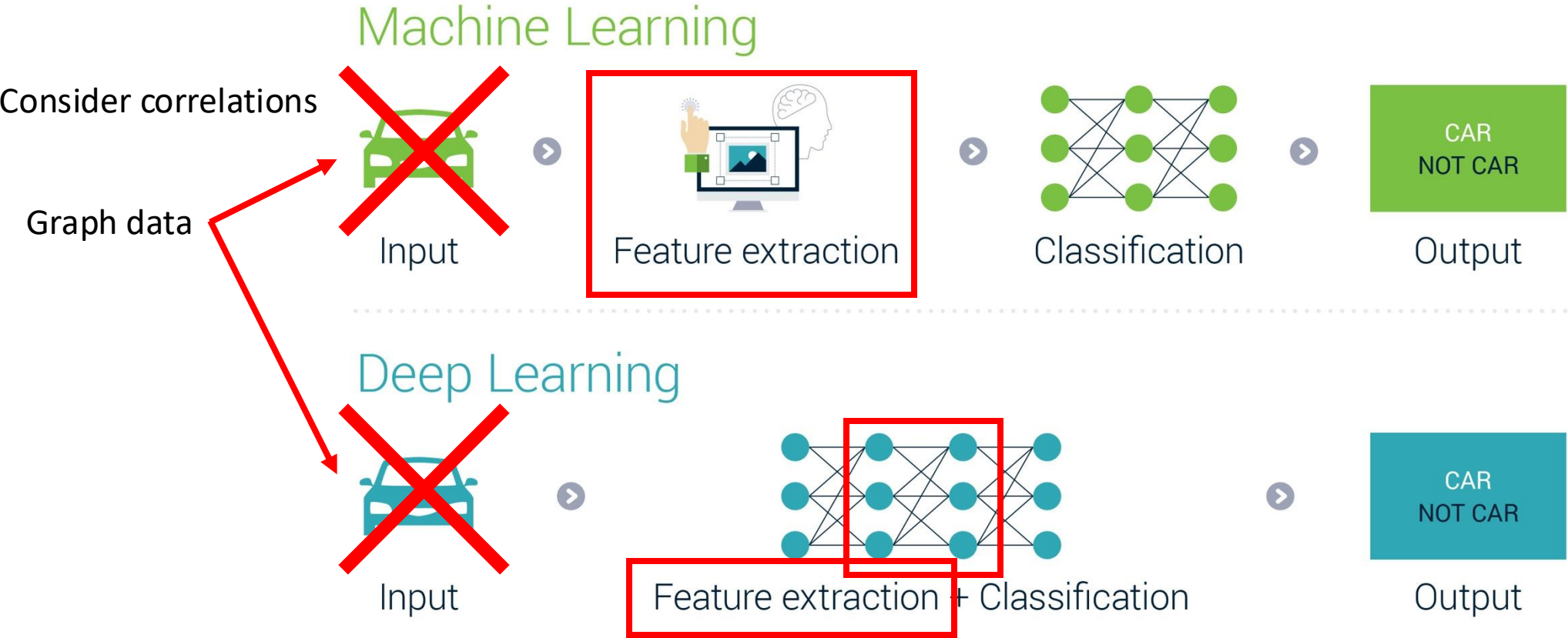
Consider correlations



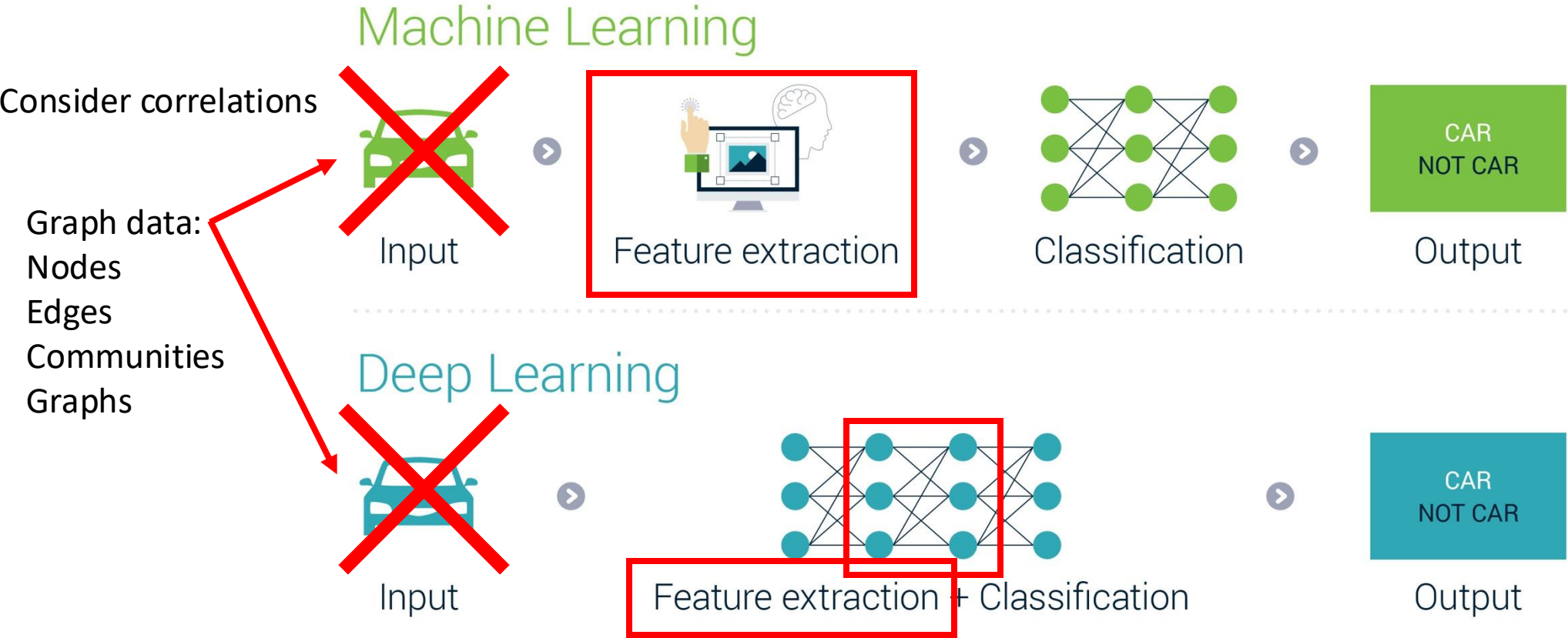
Deep Learning



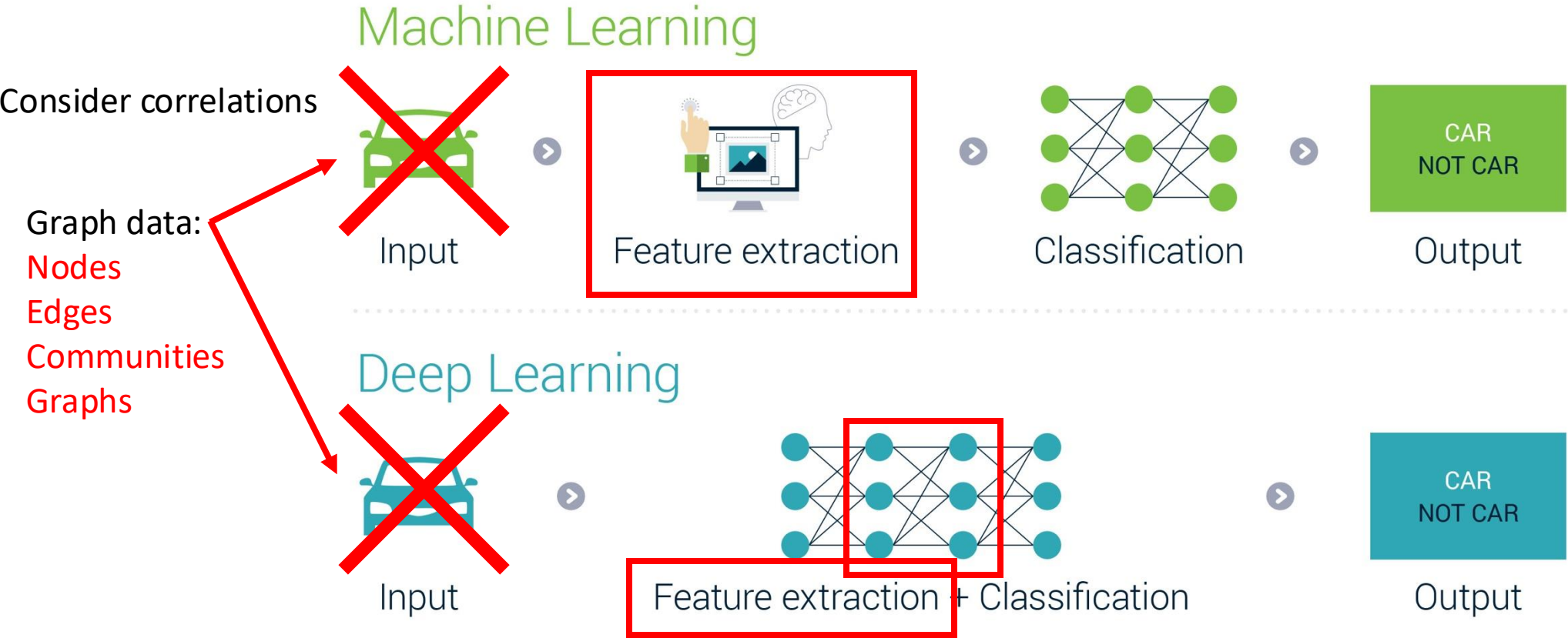
Machine learning tasks for graph data



Machine learning tasks for graph data



Machine learning tasks for graph data



Machine learning tasks for graph data

Machine Learning Q: how to learn node features?

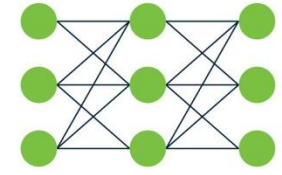
Consider correlations



Input



Feature extraction



Classification



Output

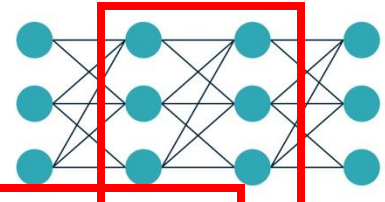
Graph data:

- Nodes
- Edges
- Communities
- Graphs

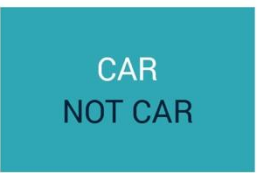


Input

Deep Learning



Feature extraction + Classification



Output

Machine learning tasks for graph data

Machine Learning

Q: how to learn node features? How to consider the correlation in graph?

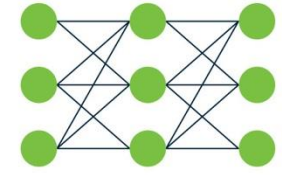
Consider correlations



Input



Feature extraction



Classification

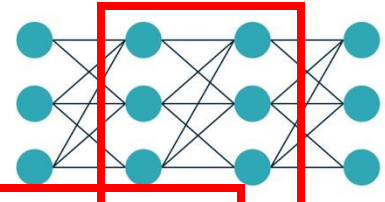


Output

Deep Learning



Input



Feature extraction + Classification



Output

Graph data:

- Nodes
- Edges
- Communities
- Graphs

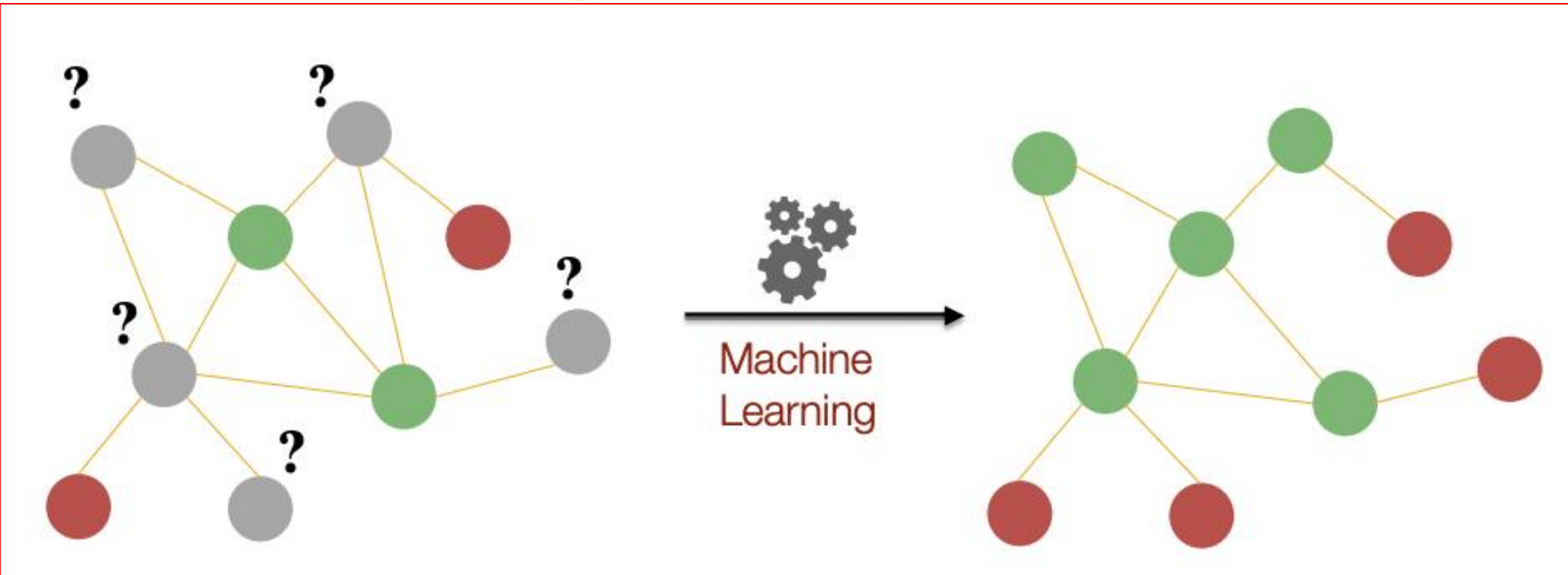


Machine learning tasks for graph data

Machine Learning

Q: how to learn node features? How to consider the correlation in graph?

Consider
Graph data
Nodes
Edges
Communities
Graphs



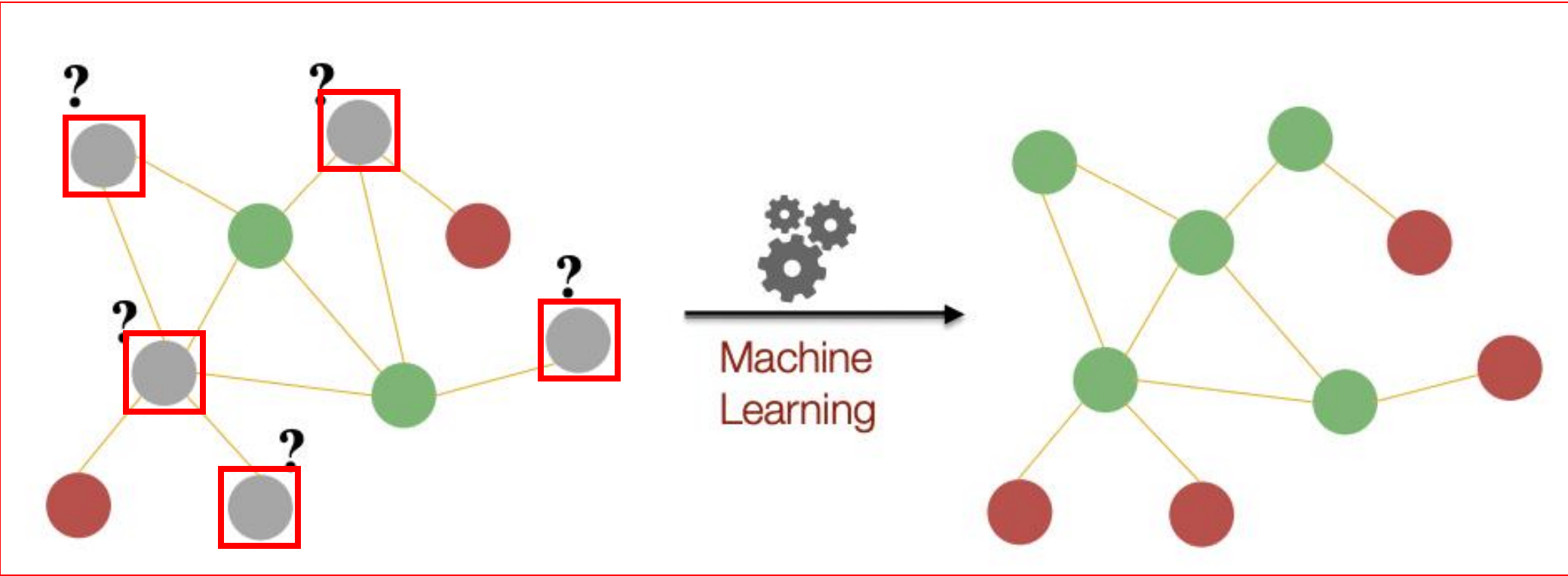
Machine learning tasks for graph data

Machine Learning

Q: how to learn node features? How to consider the correlation in graph?

Consider

- Graph data
- Nodes
- Edges
- Communities
- Graphs

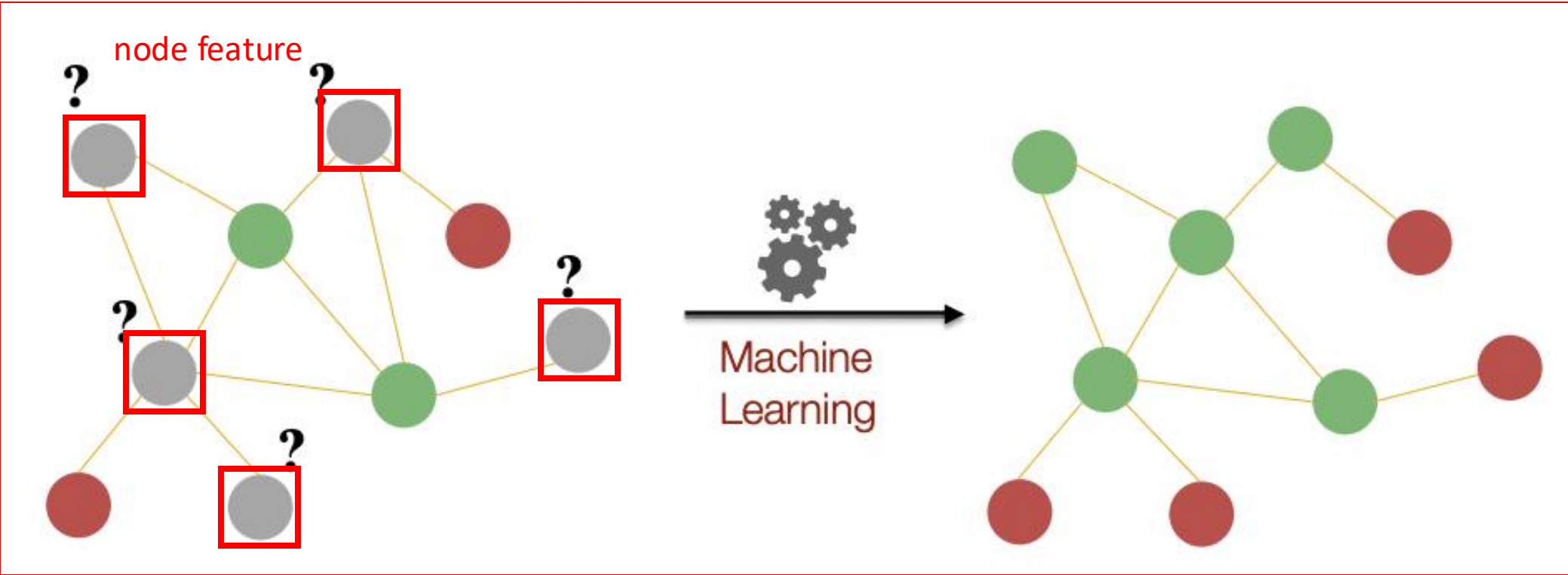


Machine learning tasks for graph data

Machine Learning

Q: how to learn node features? How to consider the correlation in graph?

Consider of
Graph data
Nodes
Edges
Communities
Graphs

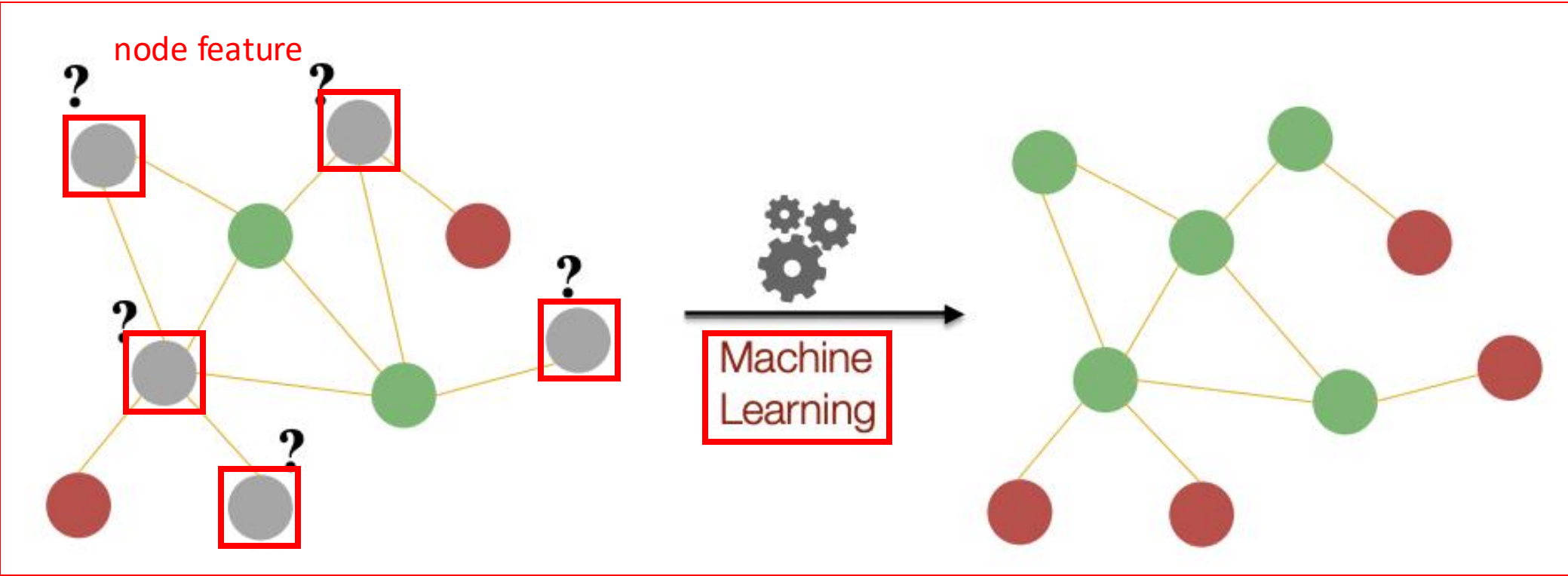


Machine learning tasks for graph data

Machine Learning

Q: how to learn node features? How to consider the correlation in graph?

Consider of
Graph data
Nodes
Edges
Communities
Graphs

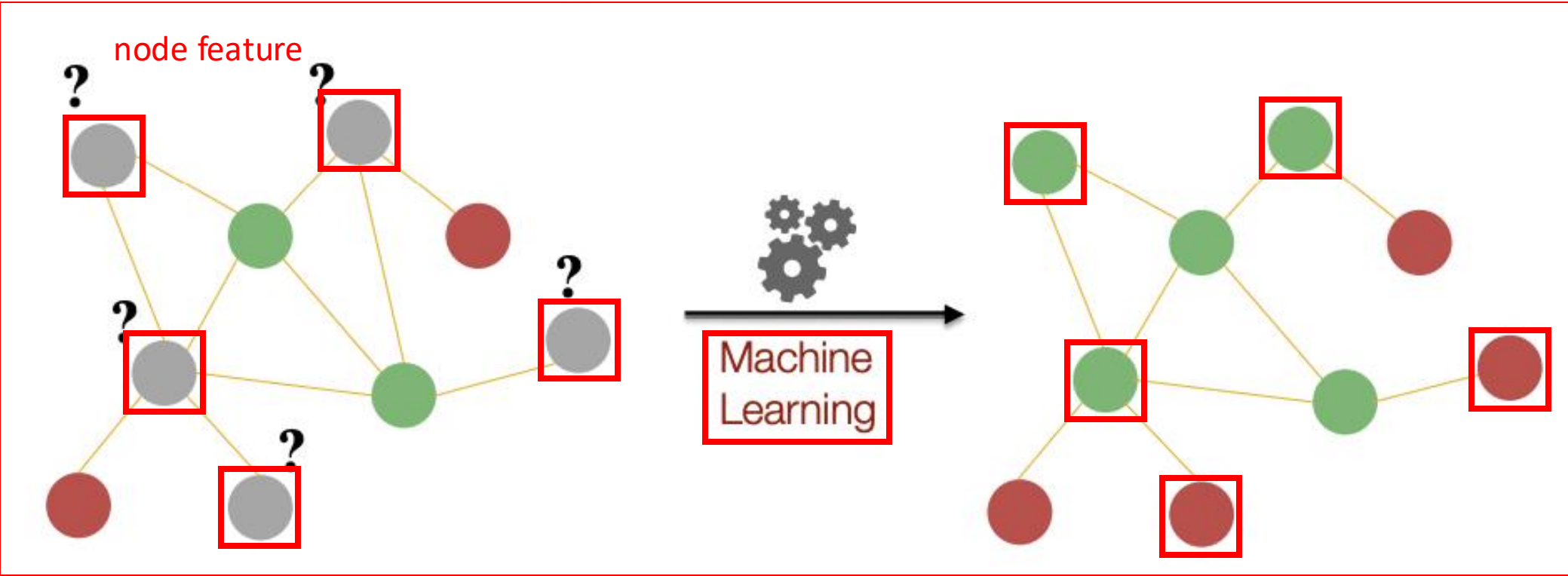


Machine learning tasks for graph data

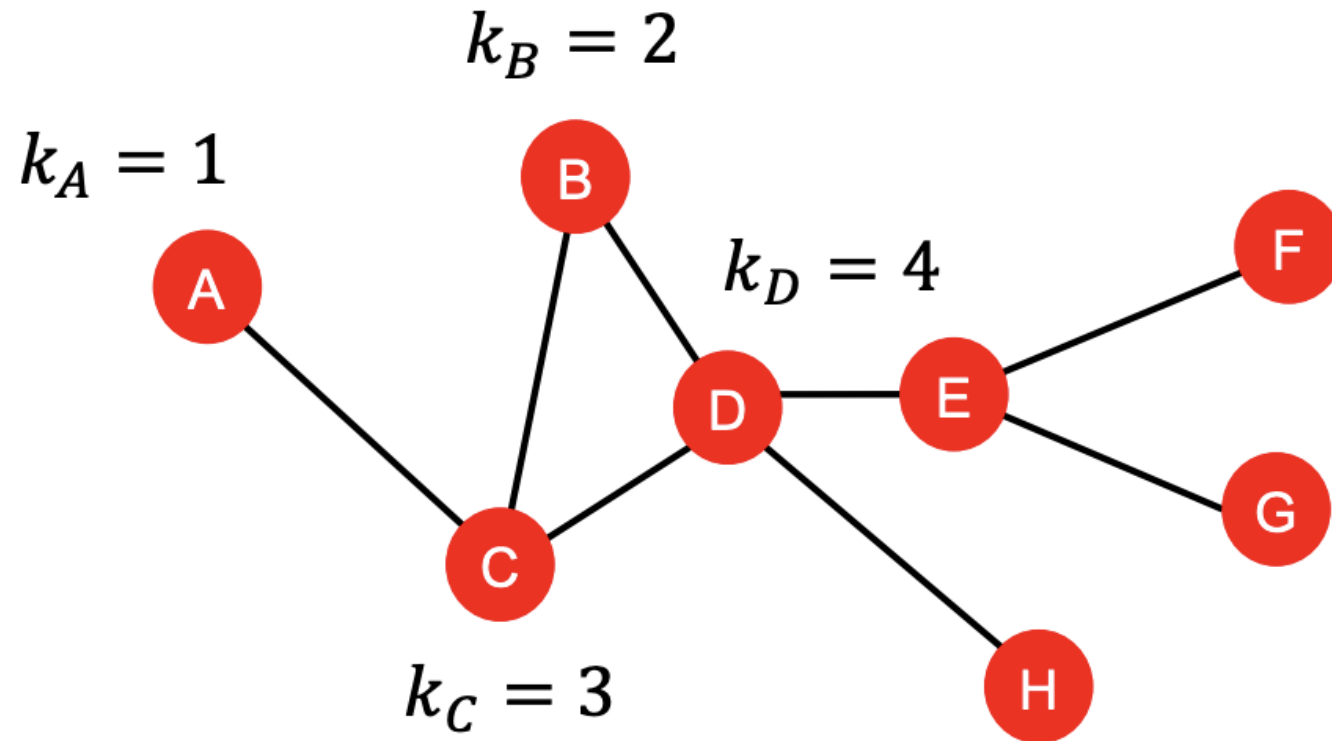
Machine Learning

Q: how to learn node features? How to consider the correlation in graph?

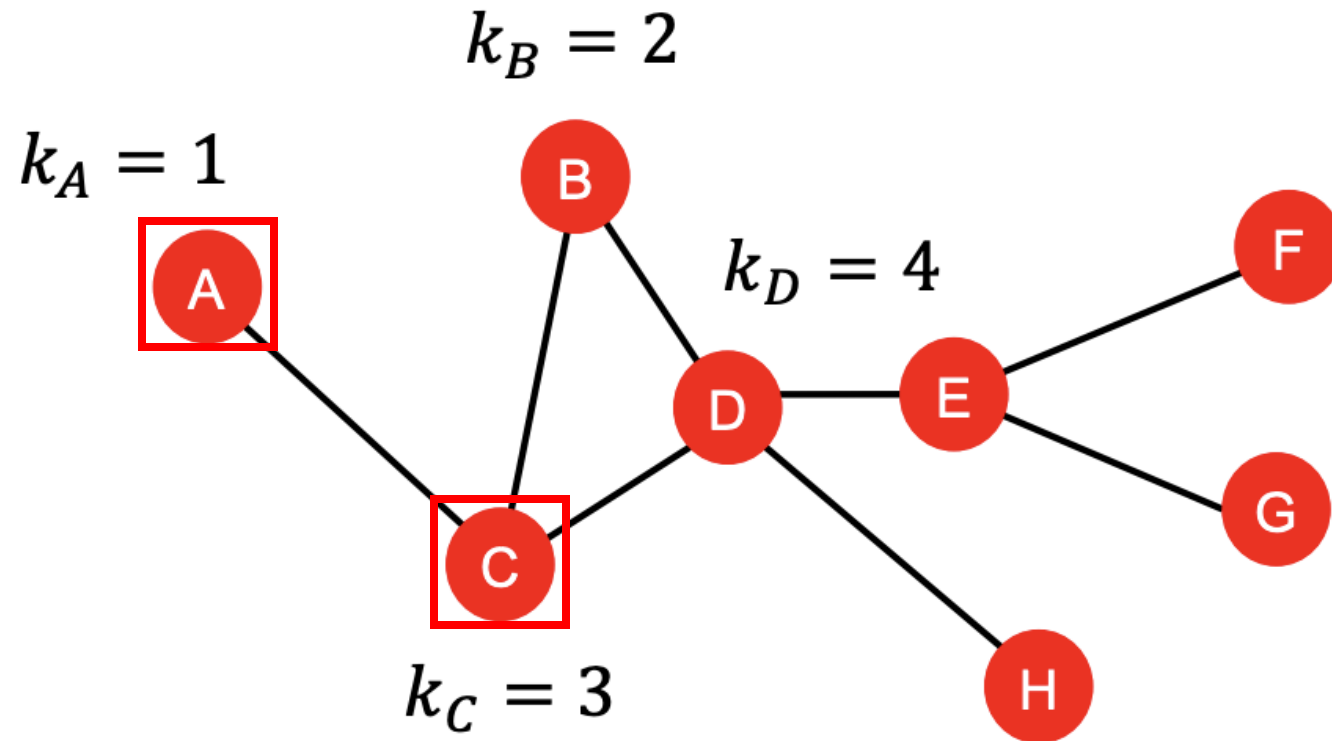
Consider of
Graph data
Nodes
Edges
Communities
Graphs



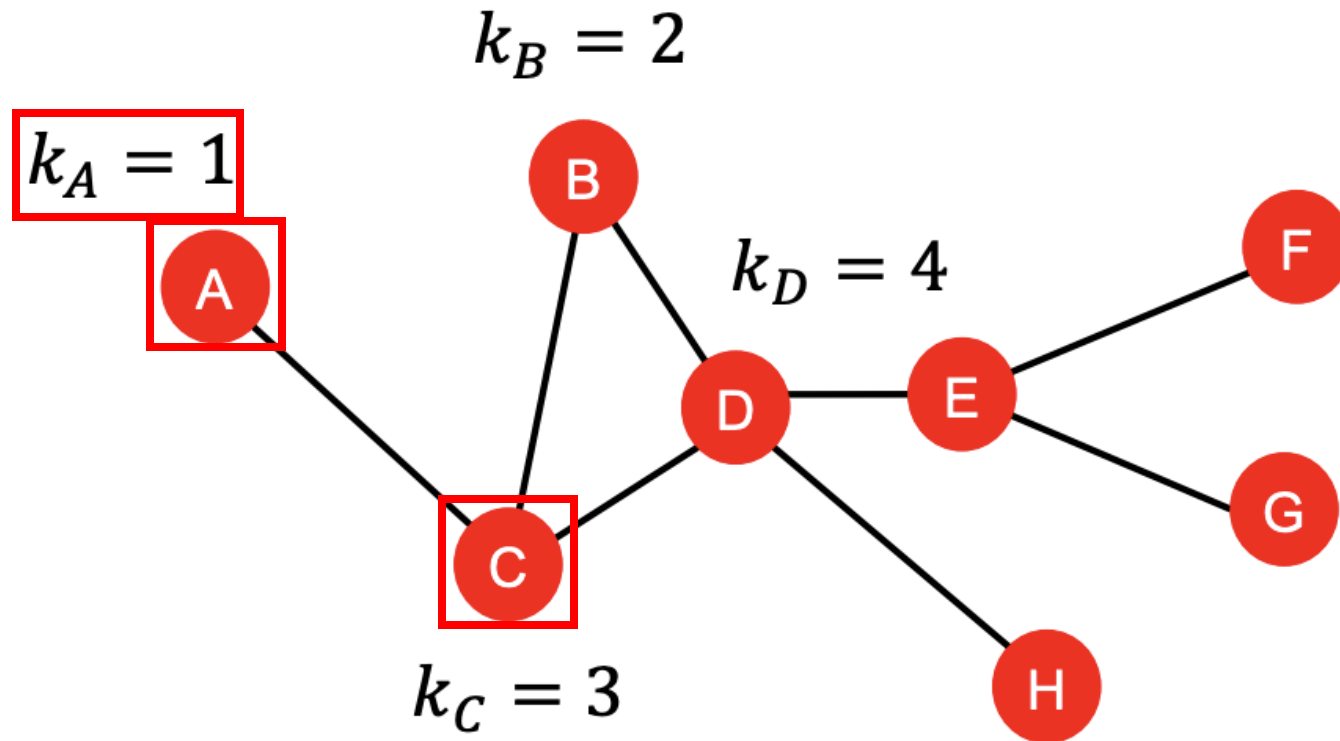
Node degree



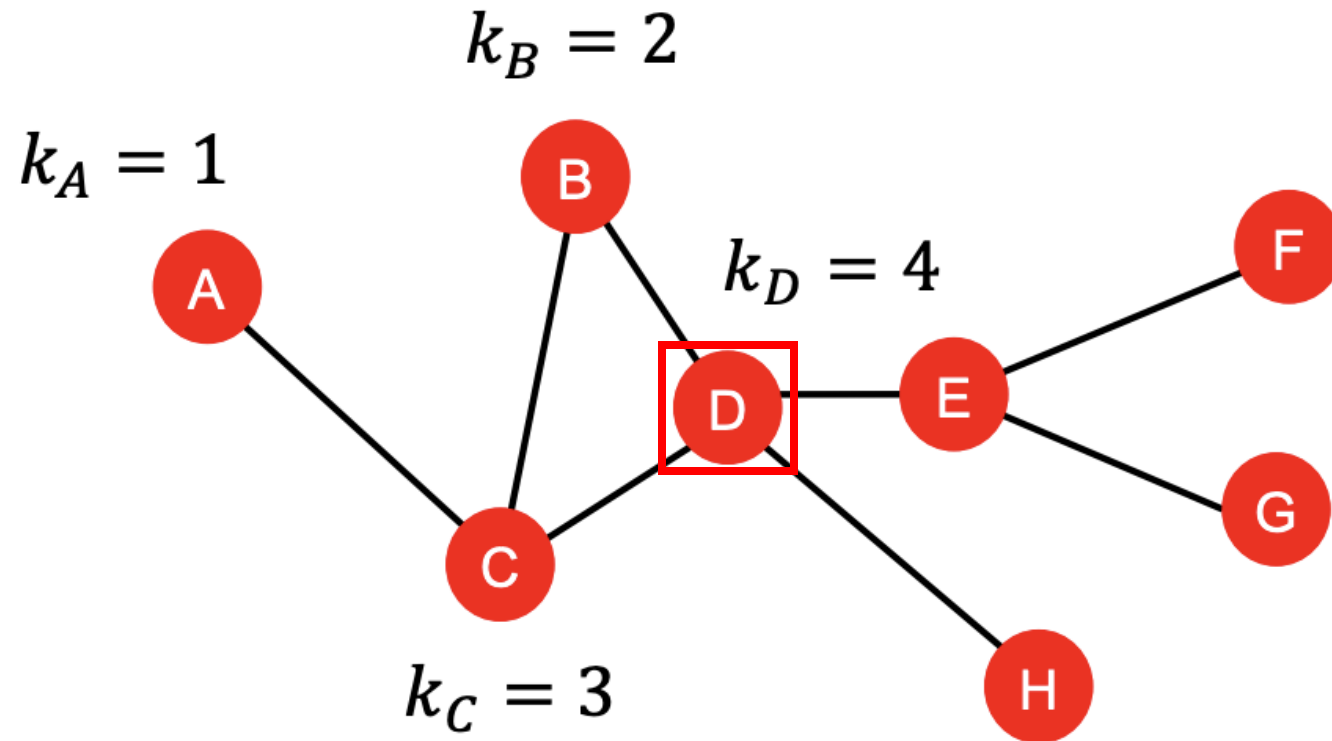
Node degree



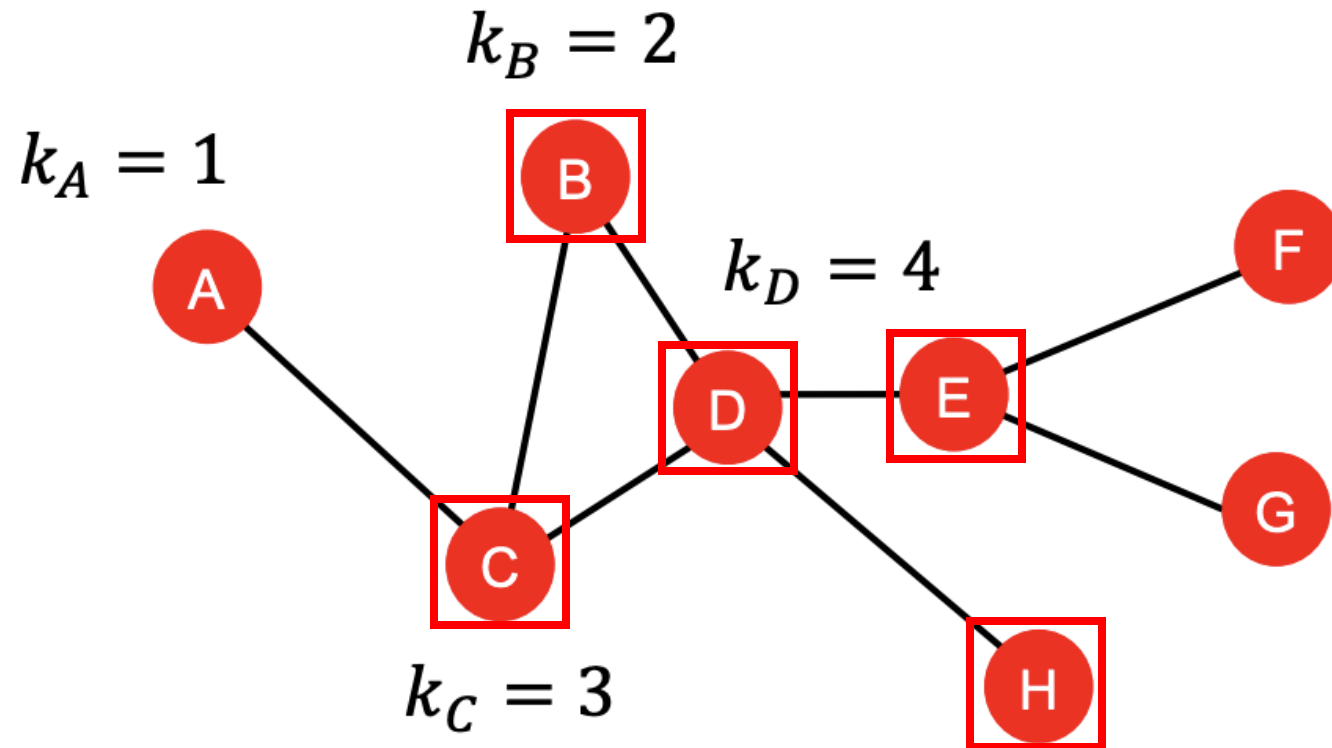
Node degree



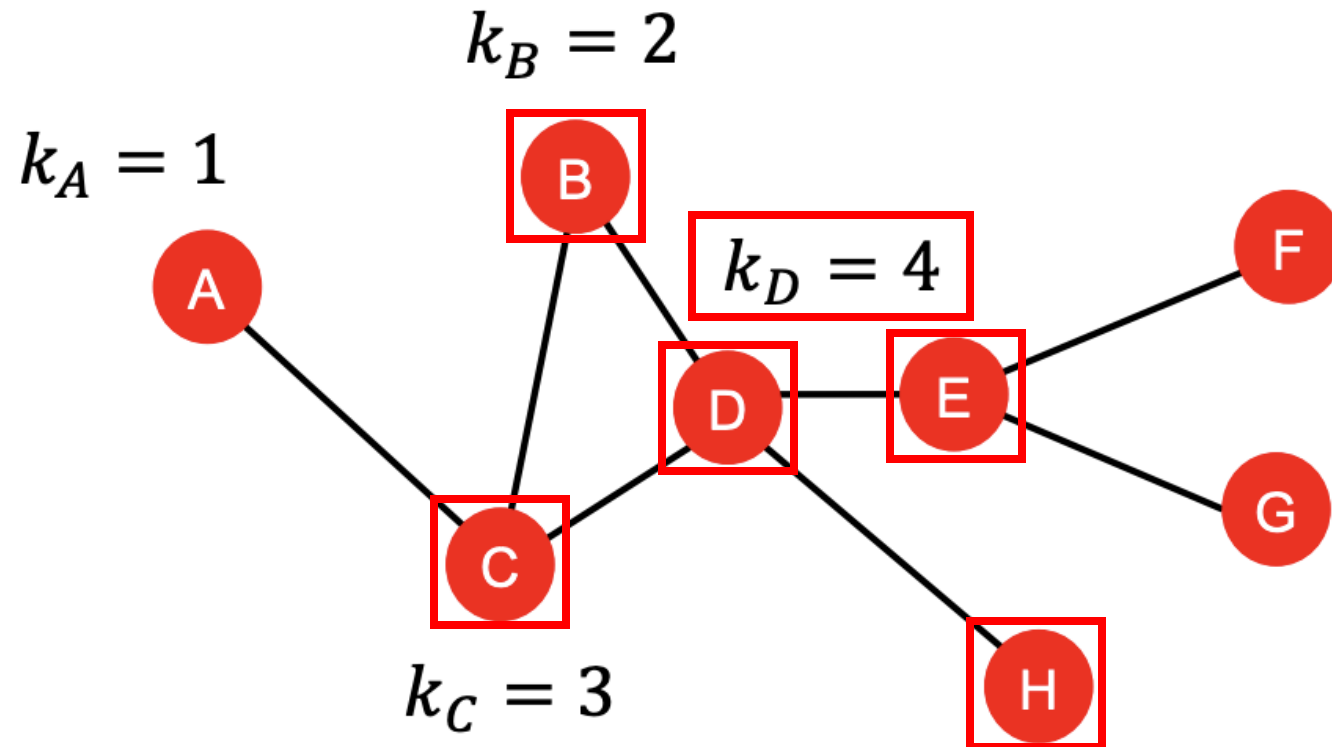
Node degree



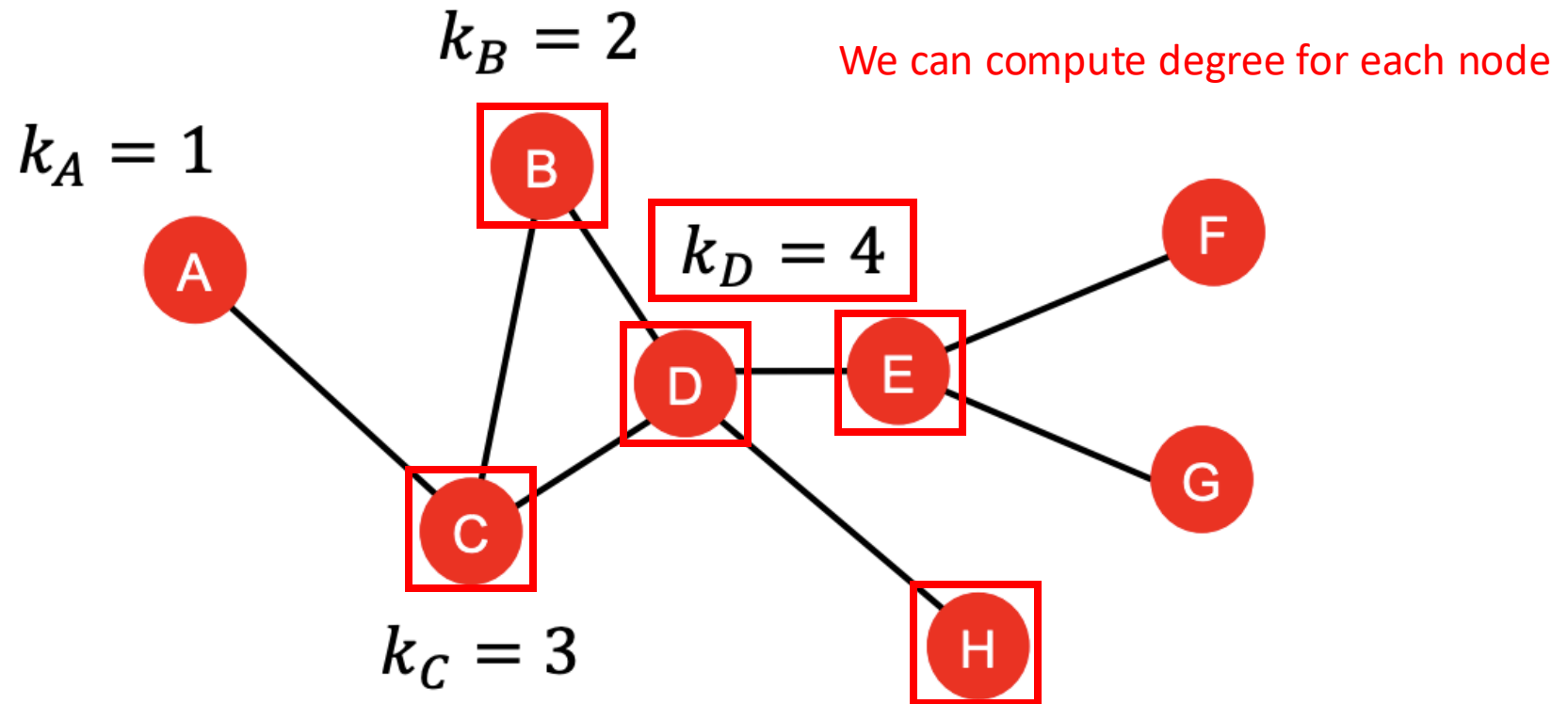
Node degree



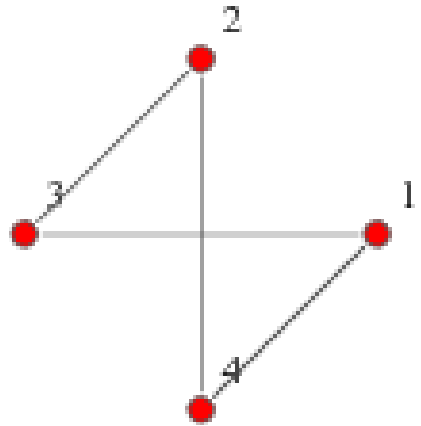
Node degree



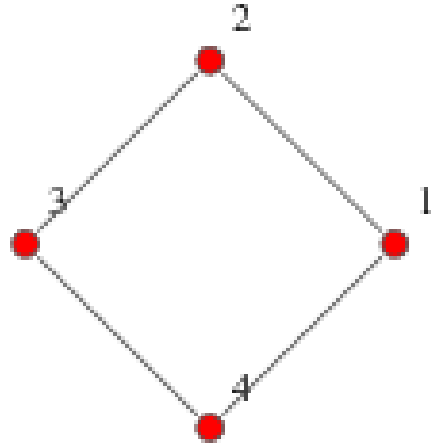
Node degree



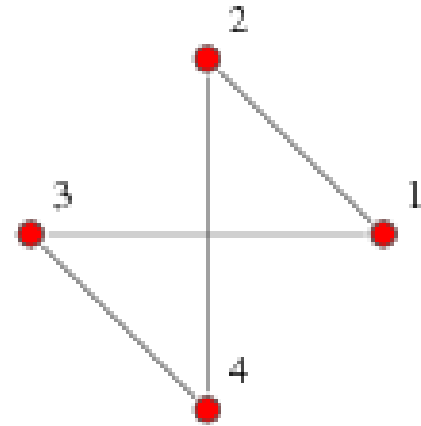
Adjacency matrix



$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

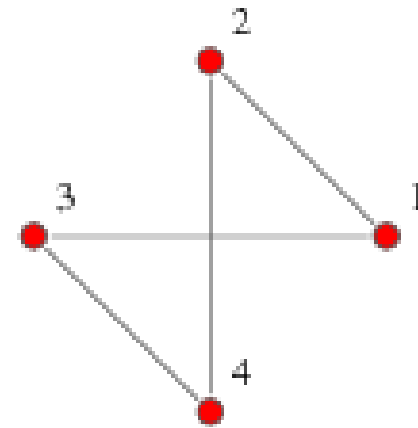
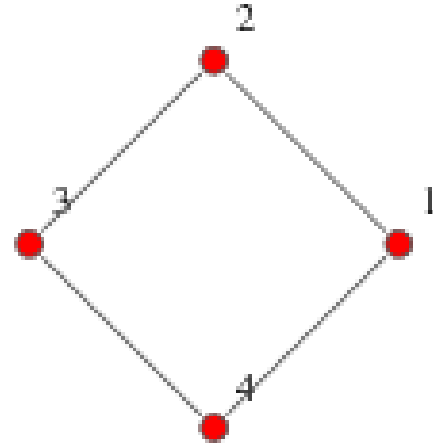
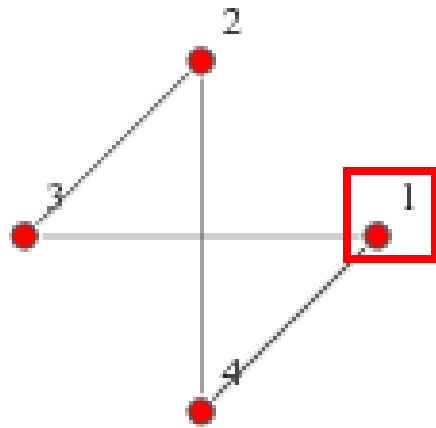


$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$



$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Adjacency matrix

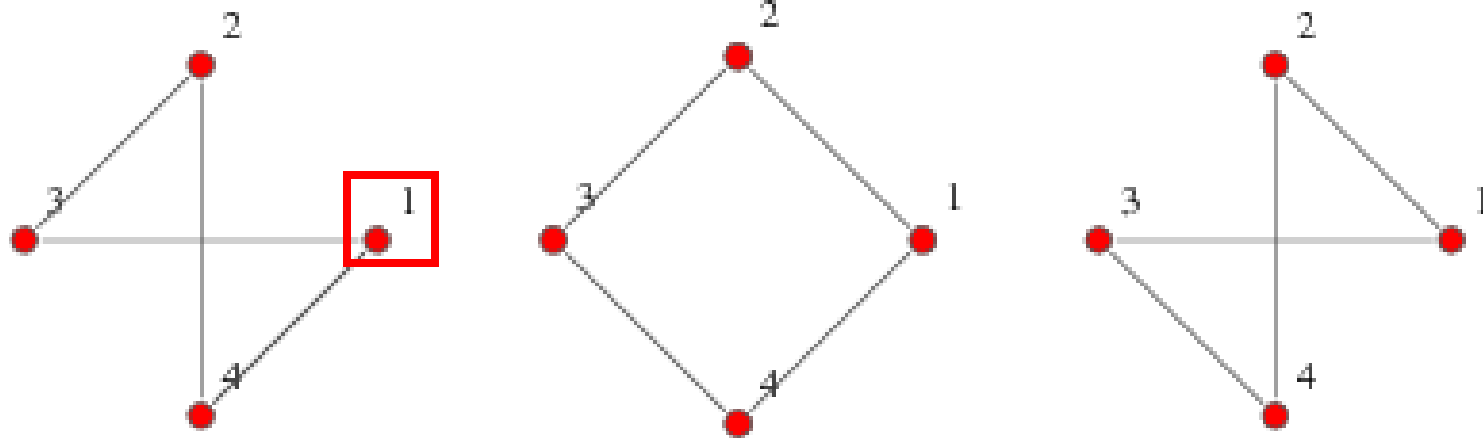


$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

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Adjacency matrix



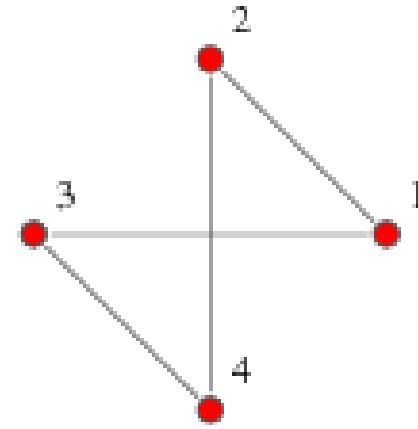
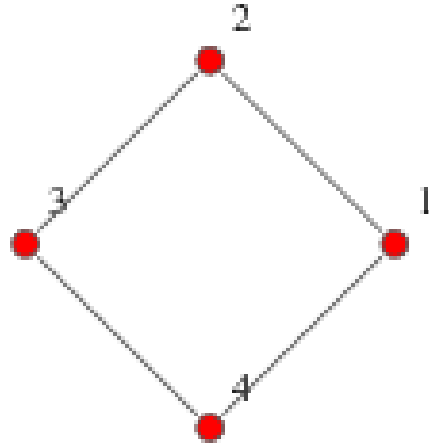
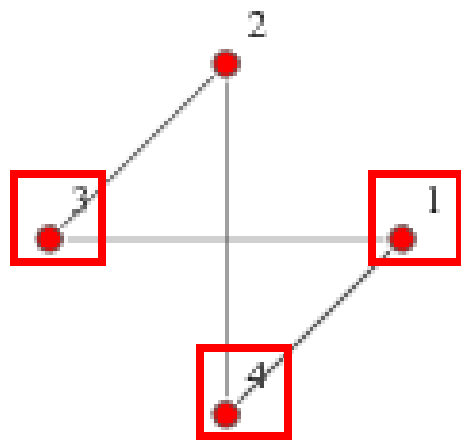
Q: which nodes are connected to node #1?

$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

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Adjacency matrix



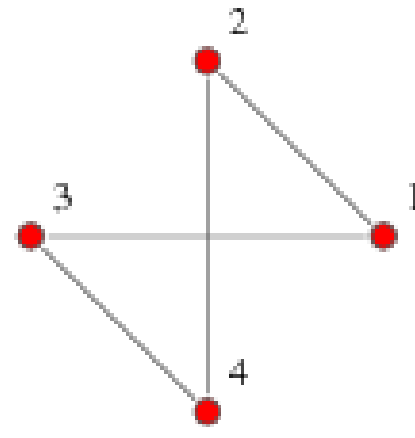
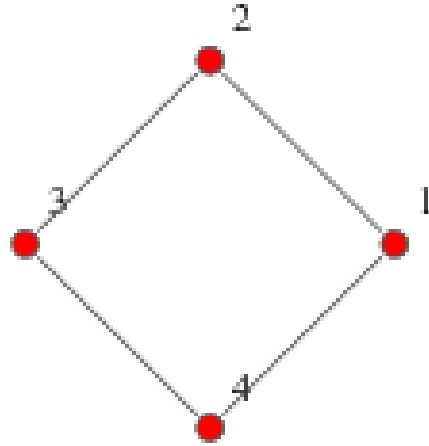
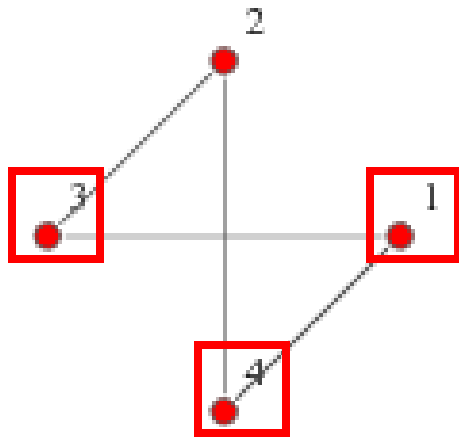
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$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Adjacency matrix



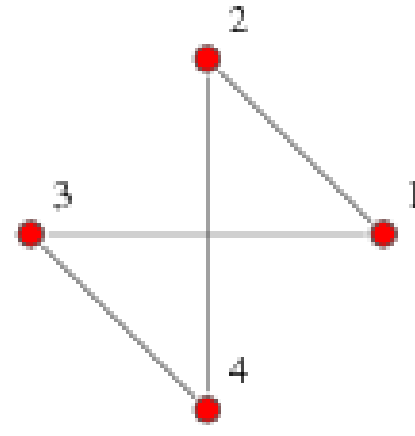
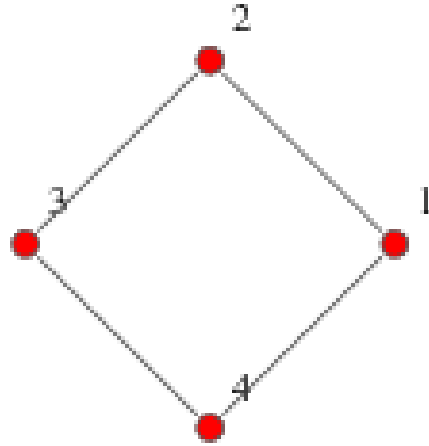
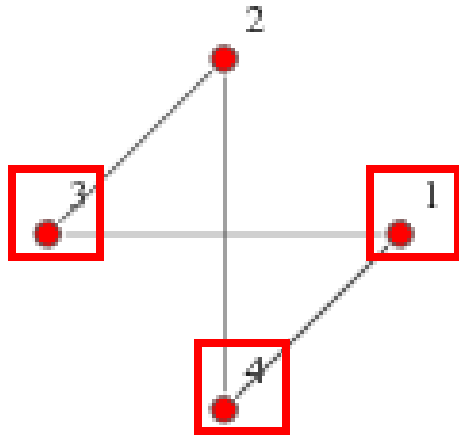
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$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Adjacency matrix



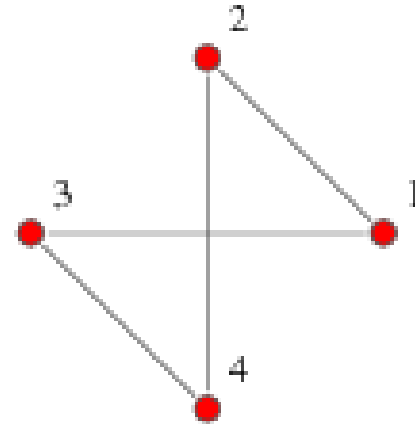
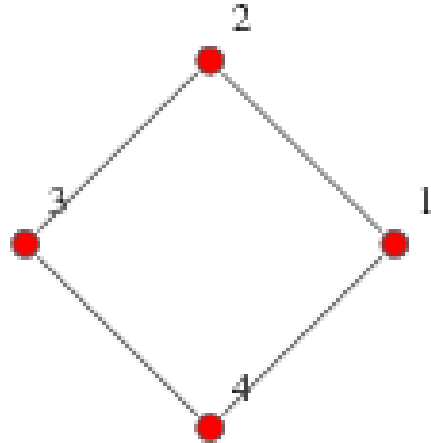
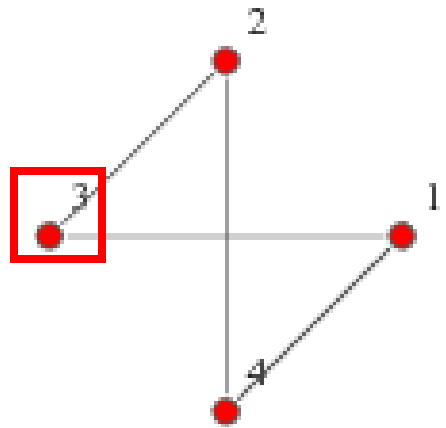
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Adjacency matrix



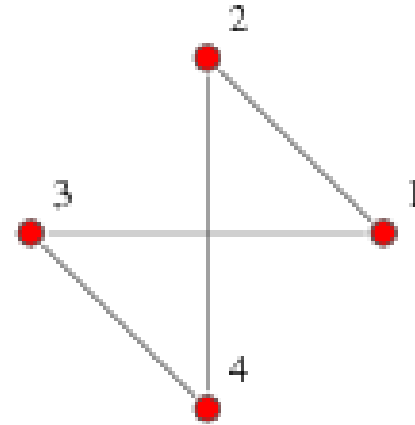
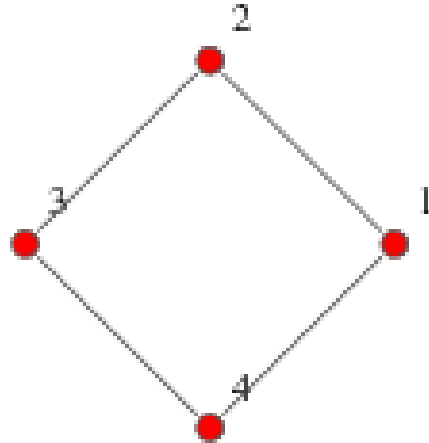
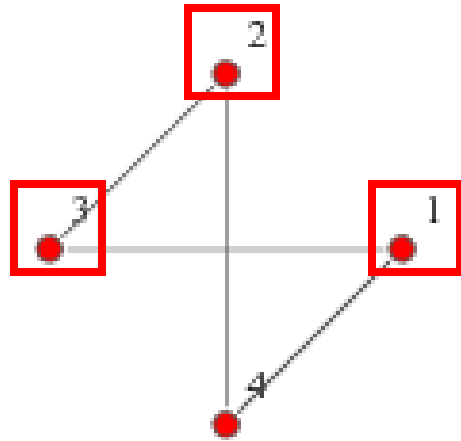
Q: which nodes are connected to node #3?

$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Adjacency matrix



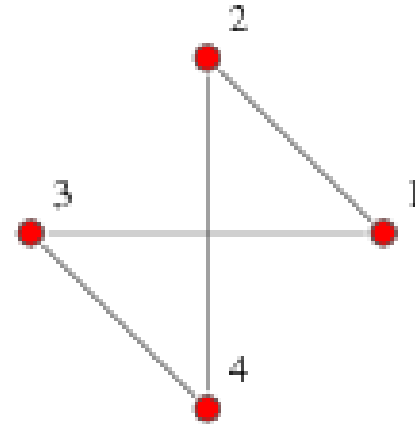
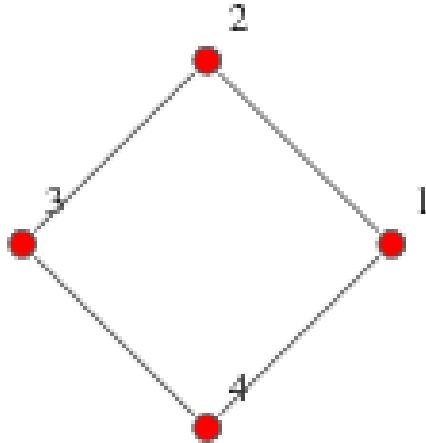
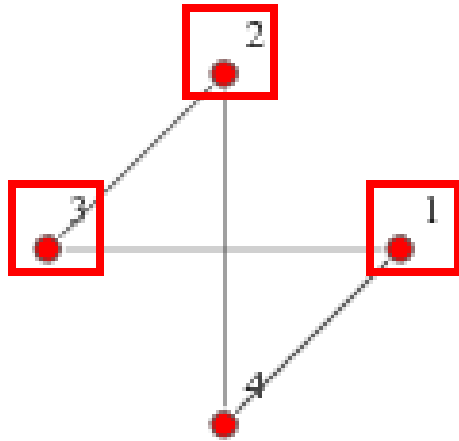
Q: which nodes are connected to node #3?

$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Adjacency matrix



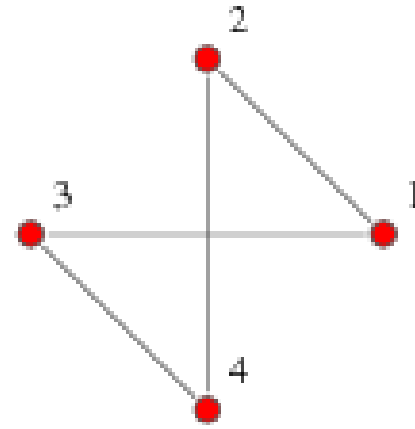
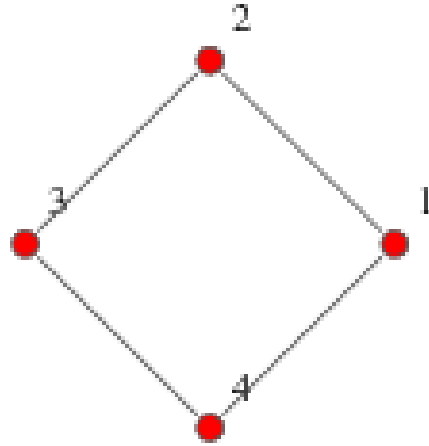
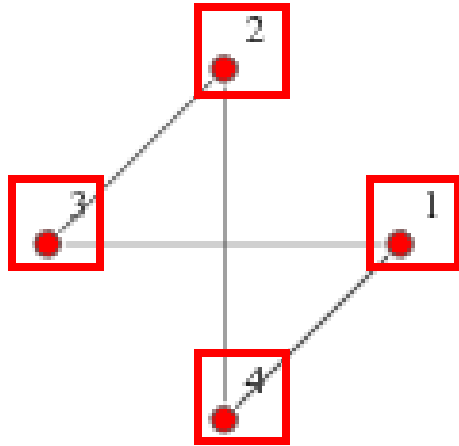
Q: which nodes are connected to node #3?

$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ \boxed{1} & \boxed{1} & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Adjacency matrix

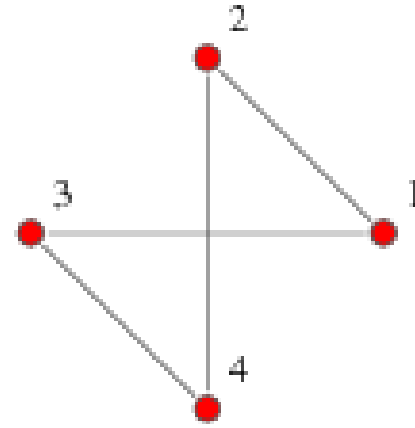
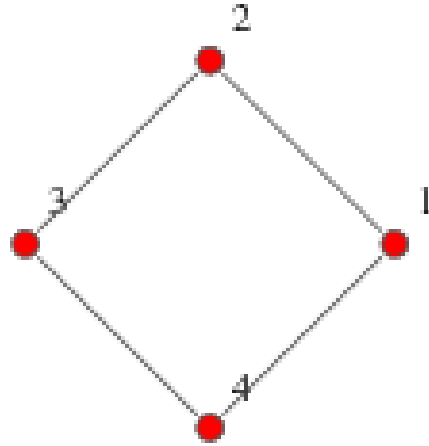
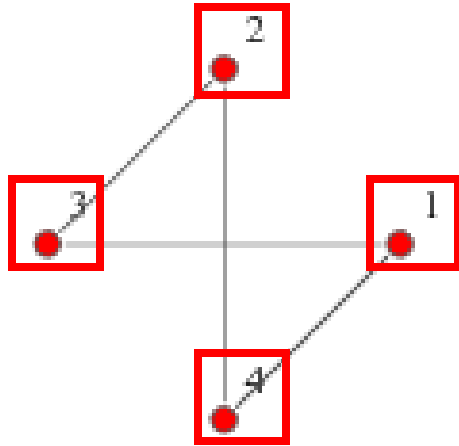


$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

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Adjacency matrix



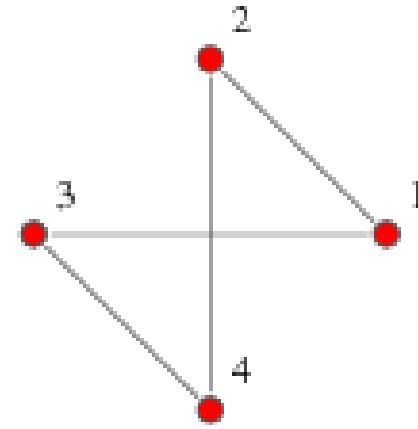
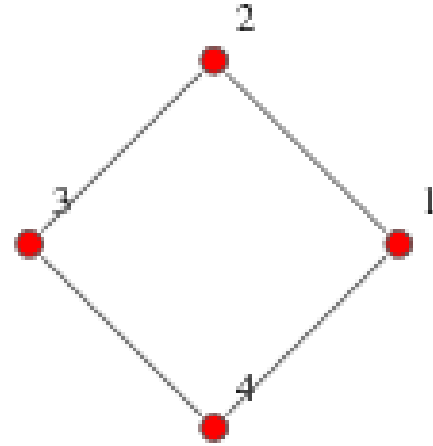
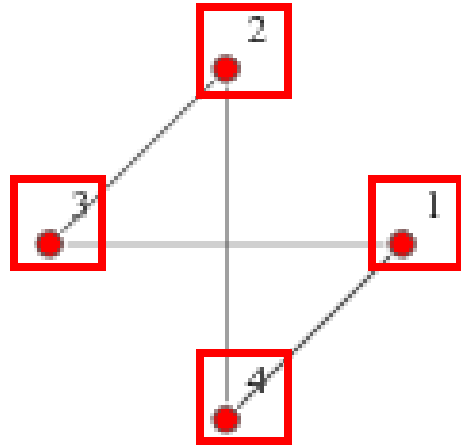
$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Q: What do entries on diagonal stand for?

Adjacency matrix

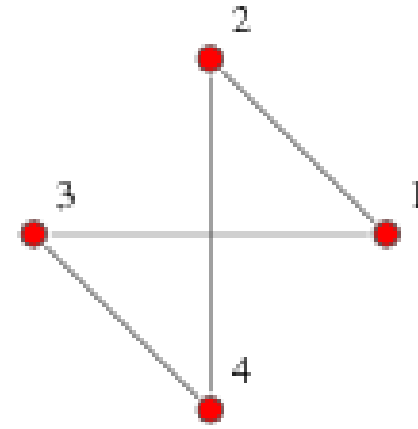
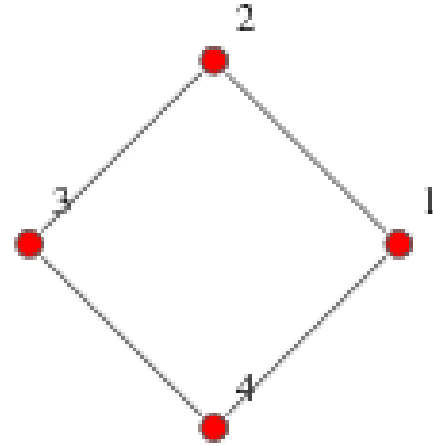
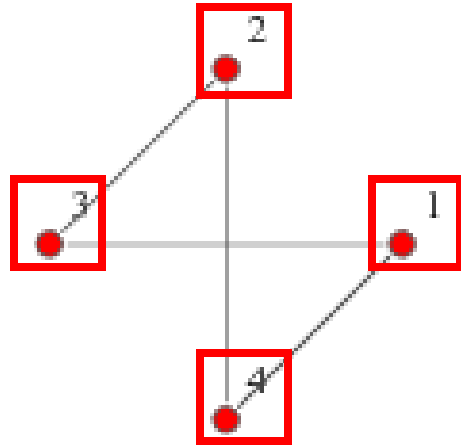


$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

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Adjacency matrix

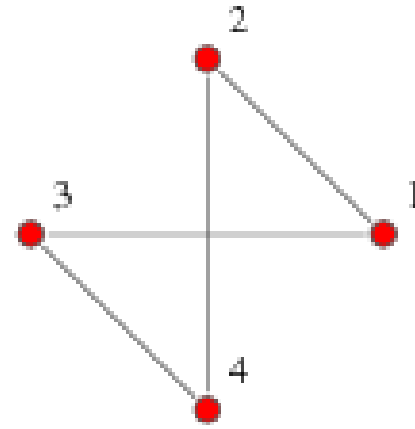
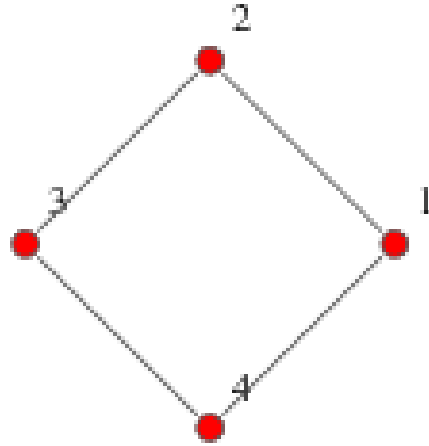
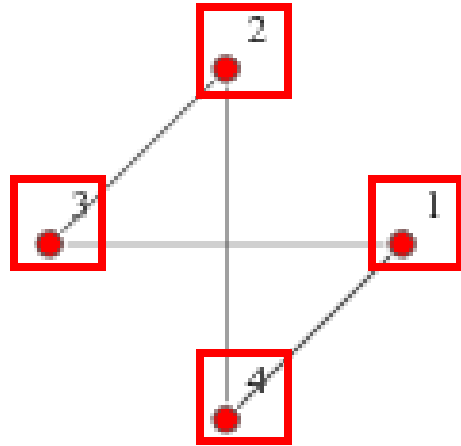


$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

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Adjacency matrix



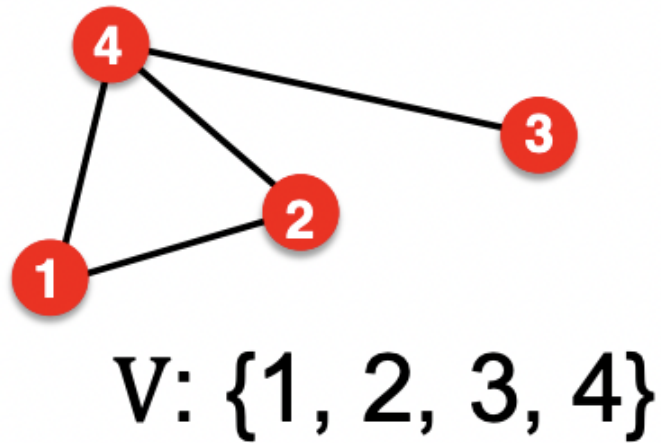
Symmetric

$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

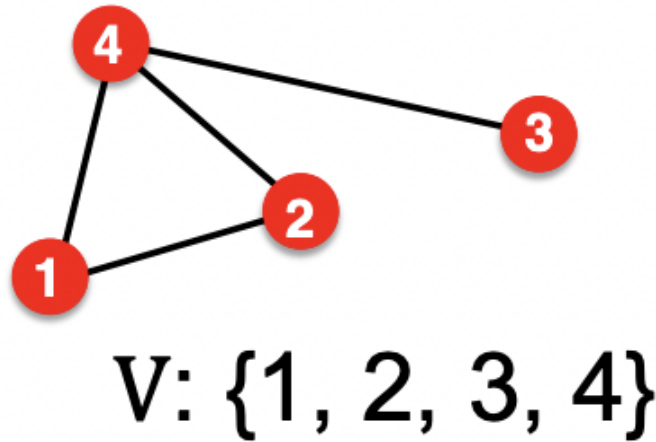
$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Encoder-decoder for graph data



$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Encoder-decoder for graph data



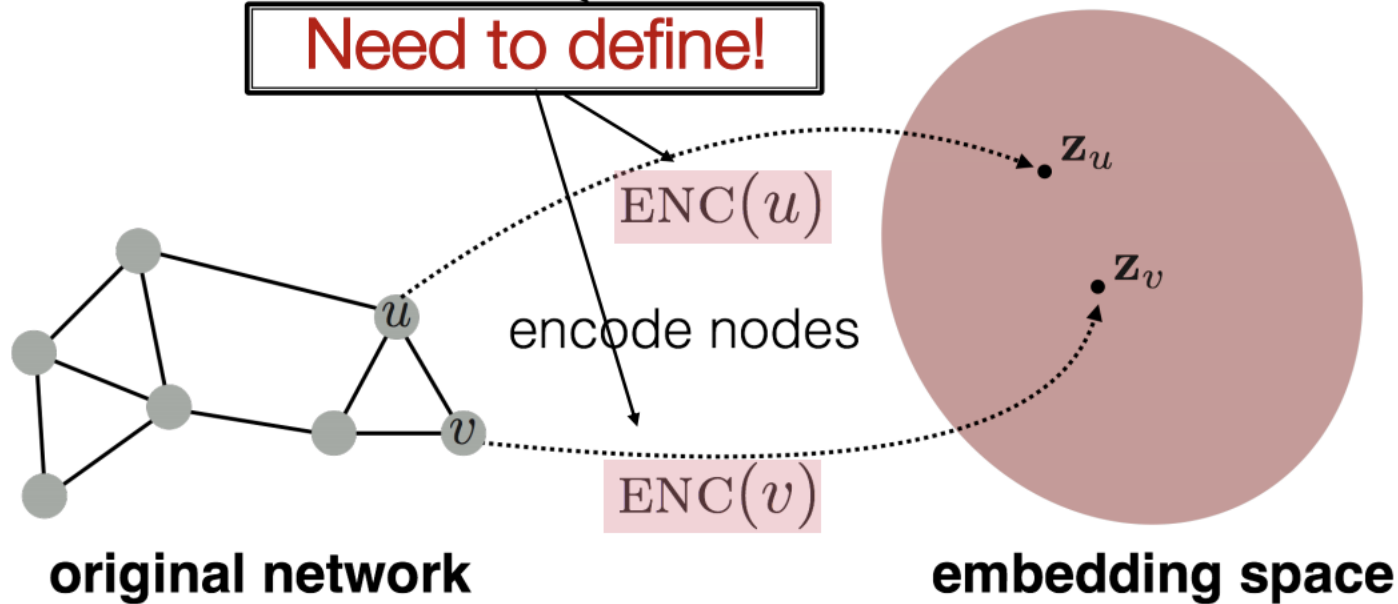
$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Q: can we learn node features with the correlation in the adjacency matrix?

Encoder-decoder for graph data

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

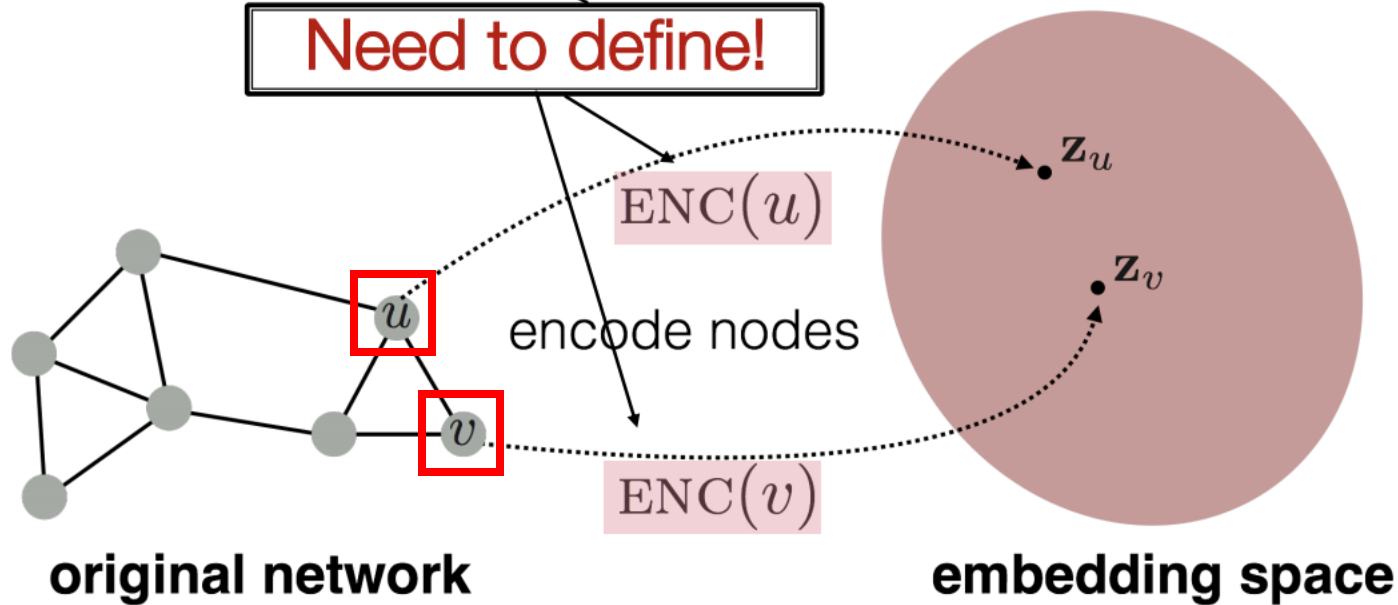
Need to define!



Encoder-decoder for graph data

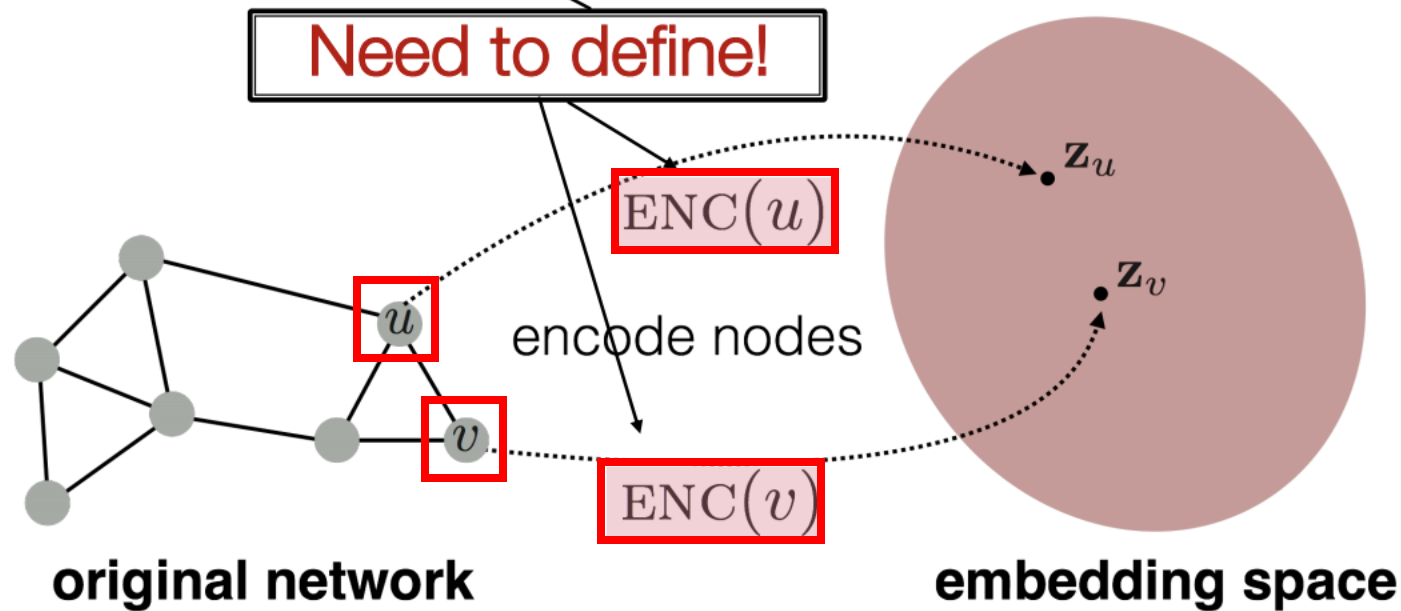
Goal: $\text{similarity}(u, v)$ in the original network $\approx \mathbf{z}_v^T \mathbf{z}_u$ Similarity of the embedding

Need to define!



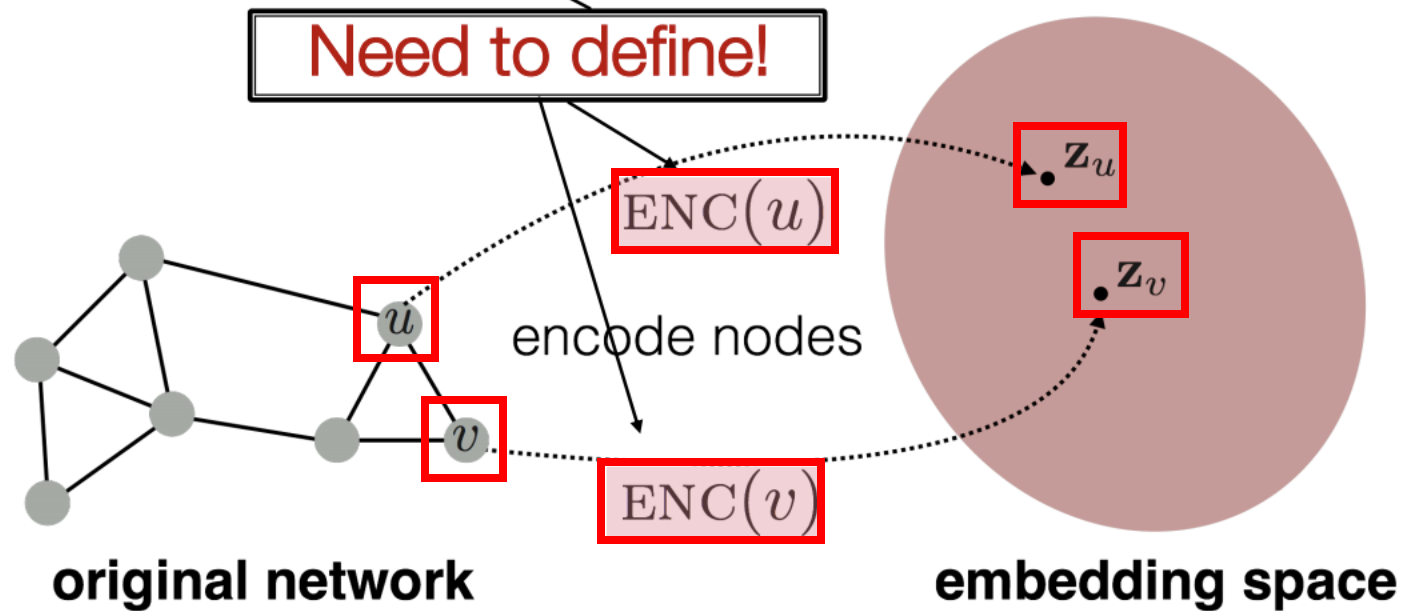
Encoder-decoder for graph data

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



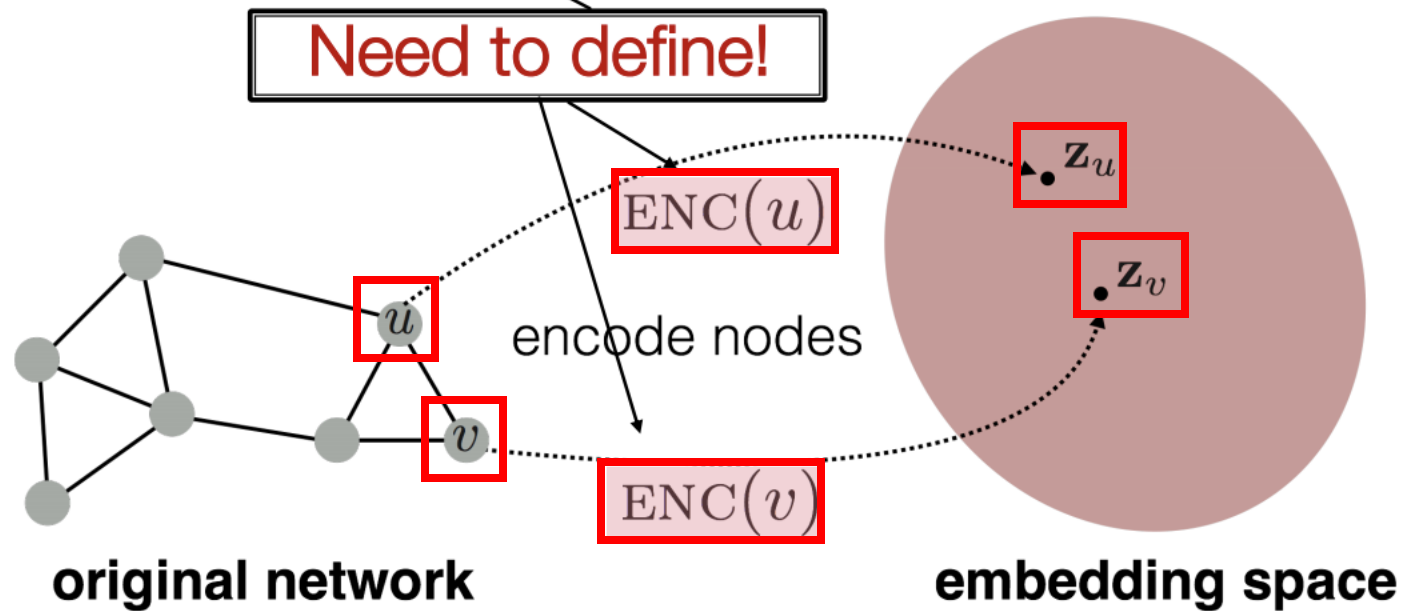
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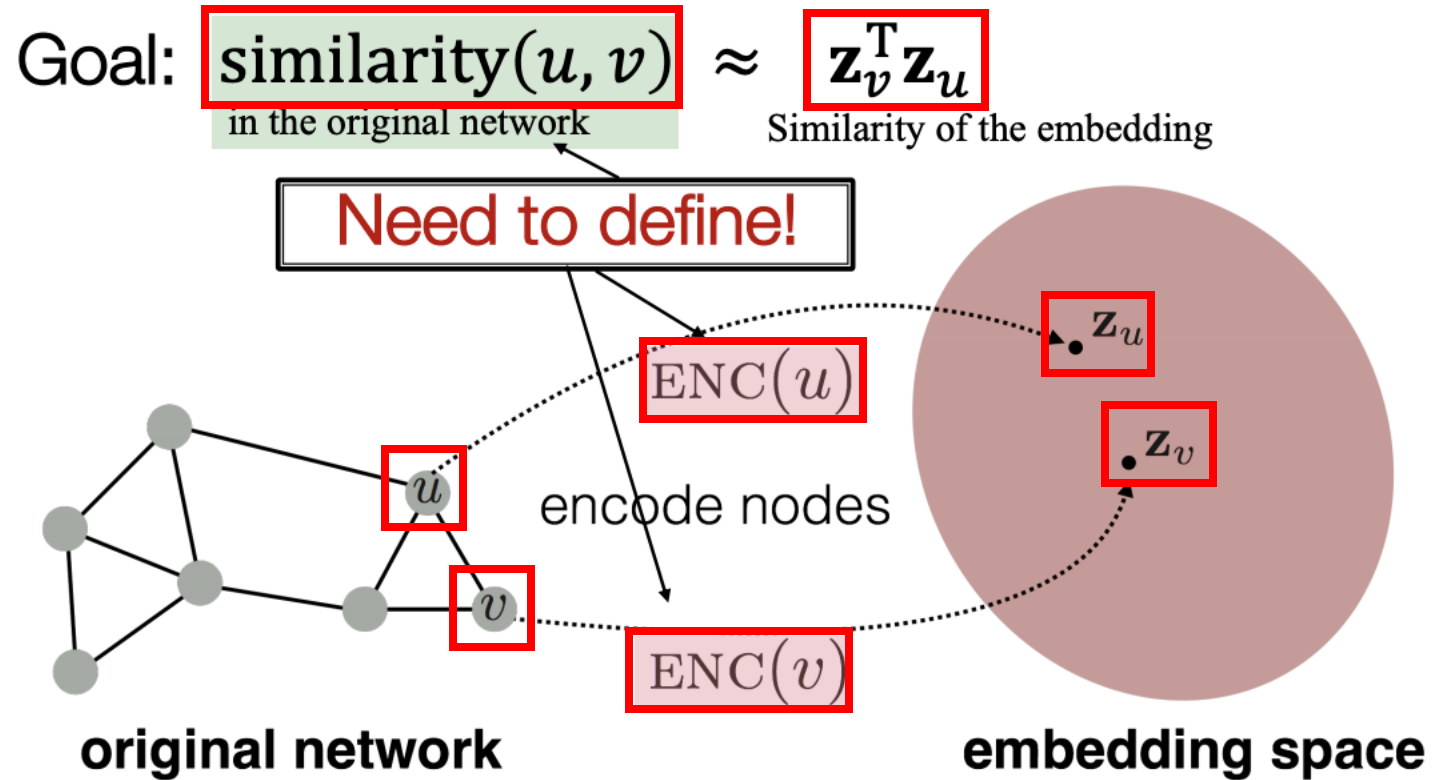


Encoder-decoder for graph data

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



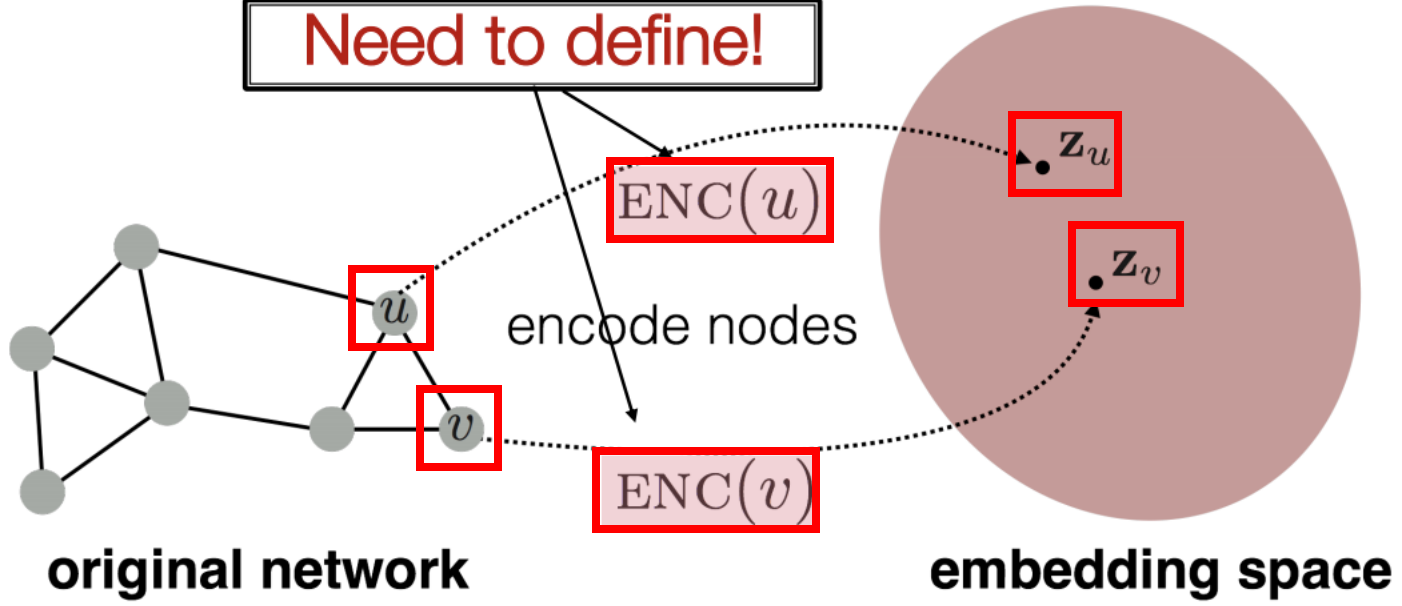
Encoder-decoder for graph data



Encoder-decoder for graph data

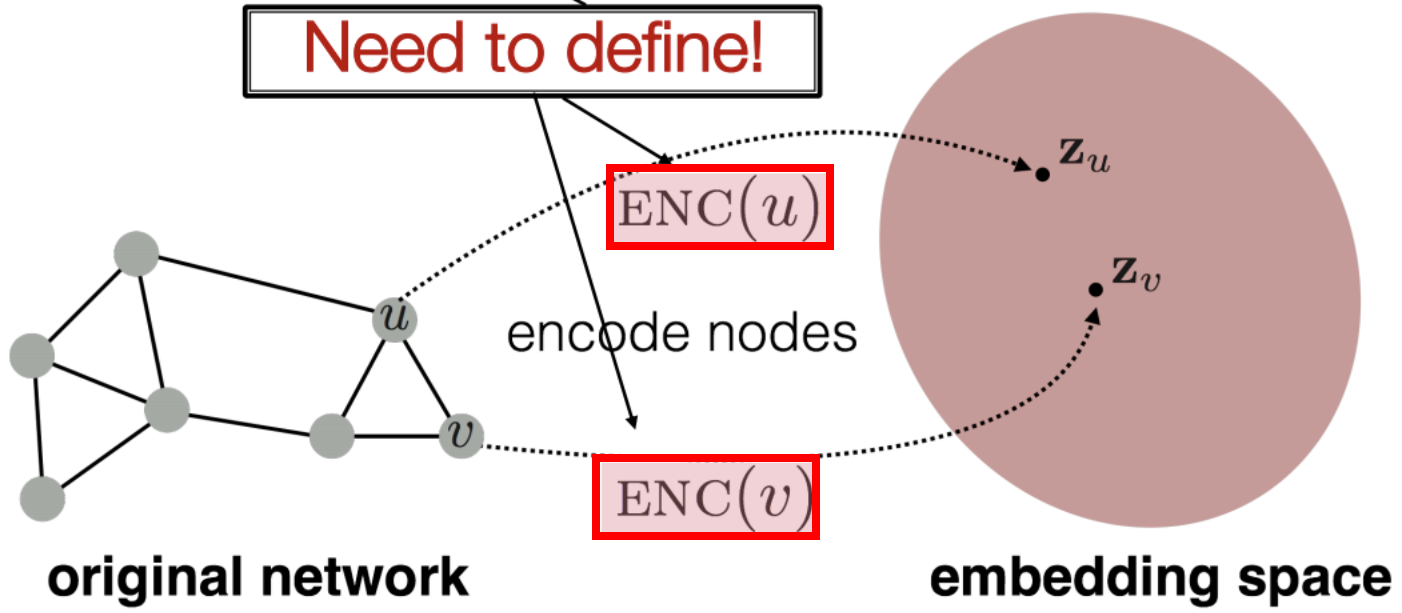
Goal: $\text{similarity}(u, v)$ in the original network $\approx \mathbf{z}_v^T \mathbf{z}_u$ Similarity of the embedding $u = k_1, v = k_2$

Need to define!



Encoder-decoder for graph data

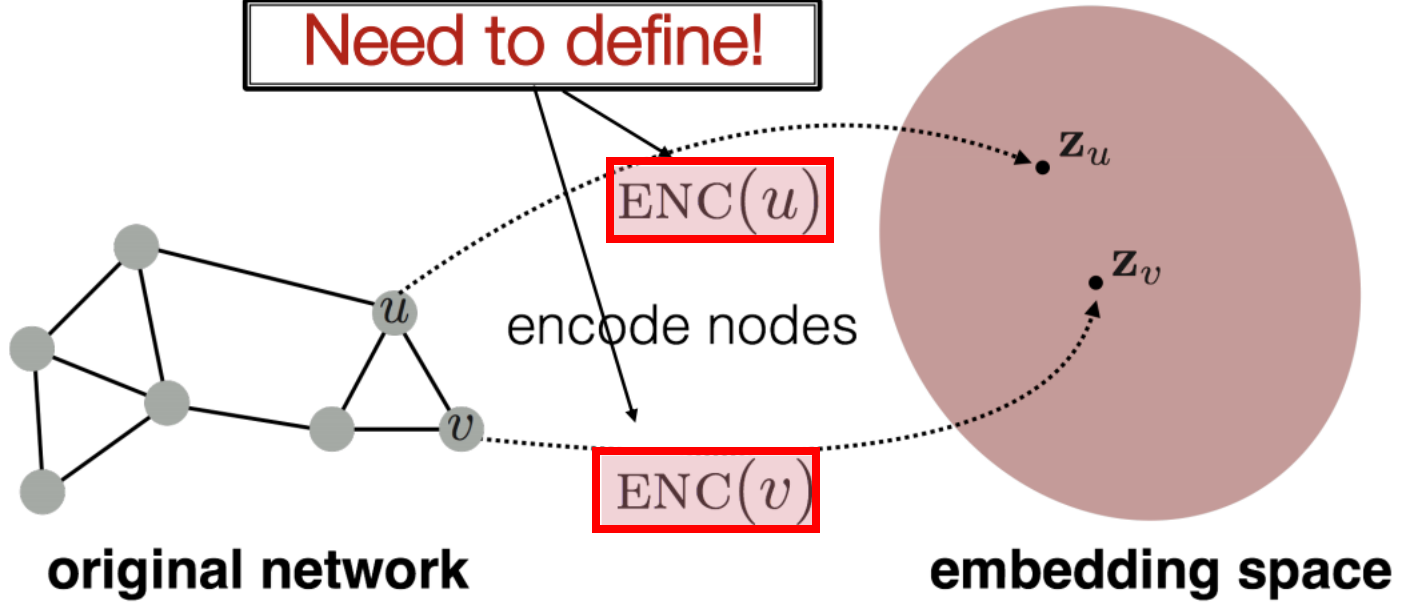
Goal: $\text{similarity}(u, v)$ in the original network $\approx \mathbf{z}_v^T \mathbf{z}_u$ Similarity of the embedding $u = k_1, v = k_2$ Q: how to learn ENC?



Encoder-decoder for graph data

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

Need to define!



Q: how to learn ENC?

$$\text{ENC}(v) = \mathbf{z}_v = \mathbf{Z} \cdot v$$

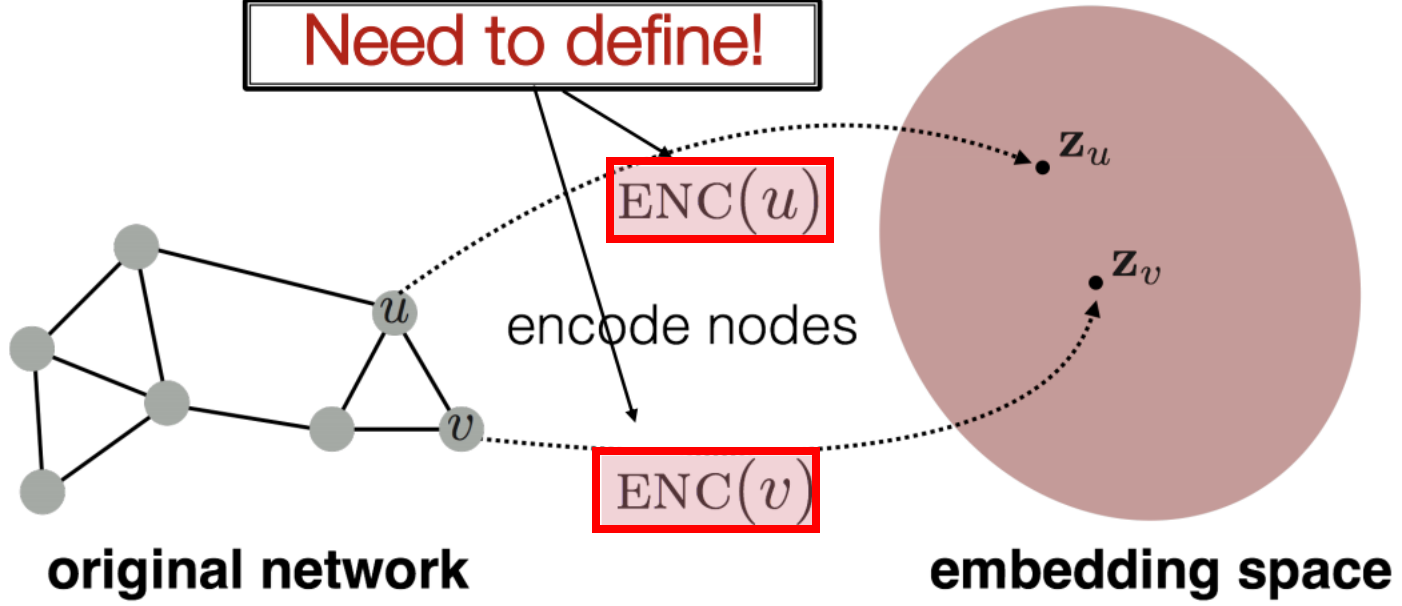
$\mathbf{Z} \in \mathbb{R}^{d \times |\mathcal{V}|}$ matrix, each column is a node embedding [what we learn / optimize]

$v \in \mathbb{I}^{|\mathcal{V}|}$ indicator vector, all zeroes except a one in column indicating node v

Encoder-decoder for graph data

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

Need to define!



Q: how to learn ENC?
Linear transformation

$$\text{ENC}(v) = \mathbf{z}_v = \mathbf{Z} \cdot v$$

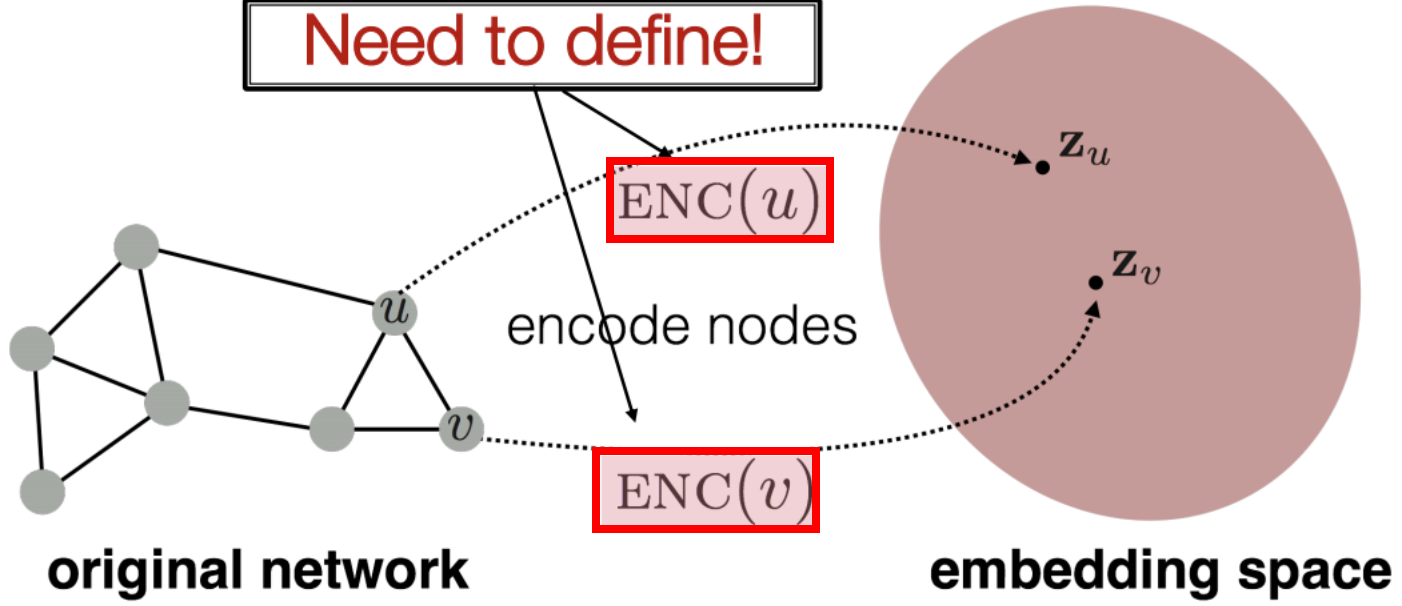
$\mathbf{Z} \in \mathbb{R}^{d \times |\mathcal{V}|}$ matrix, each column is a node embedding [what we learn / optimize]

$v \in \mathbb{I}^{|\mathcal{V}|}$ indicator vector, all zeroes except a one in column indicating node v

Encoder-decoder for graph data

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

Need to define!



Q: how to learn ENC?
Linear transformation

$$\text{ENC}(v) = \mathbf{z}_v = \mathbf{Z} \cdot v$$

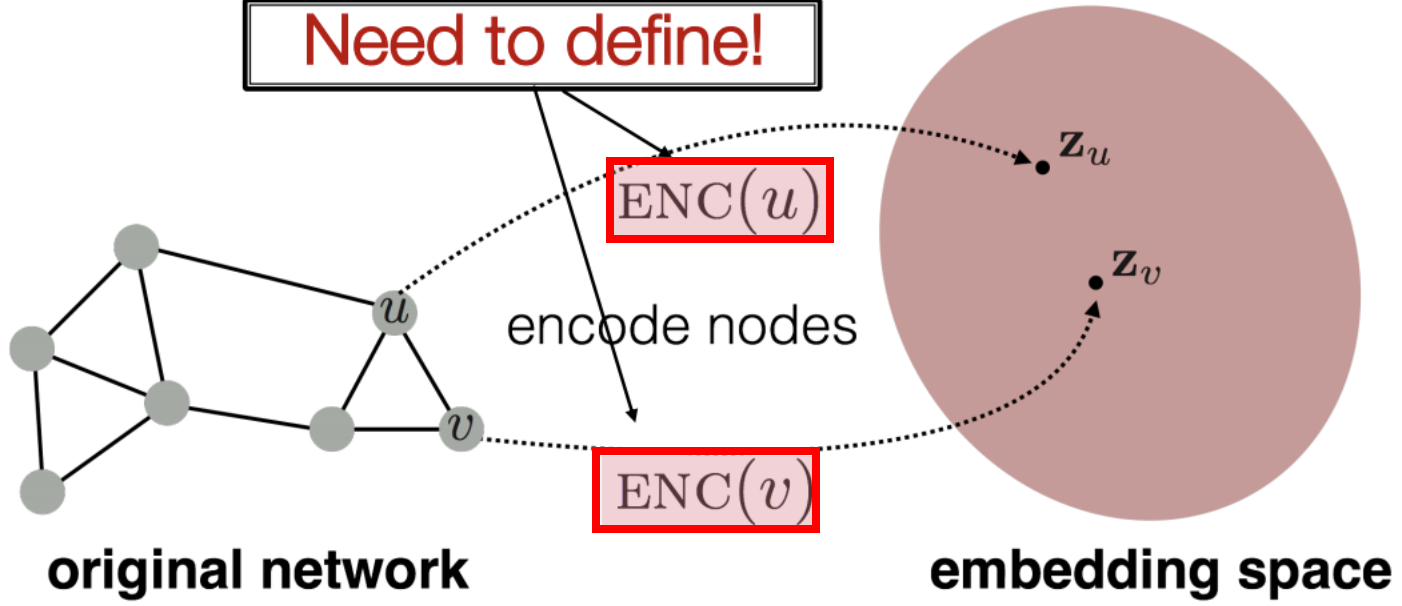
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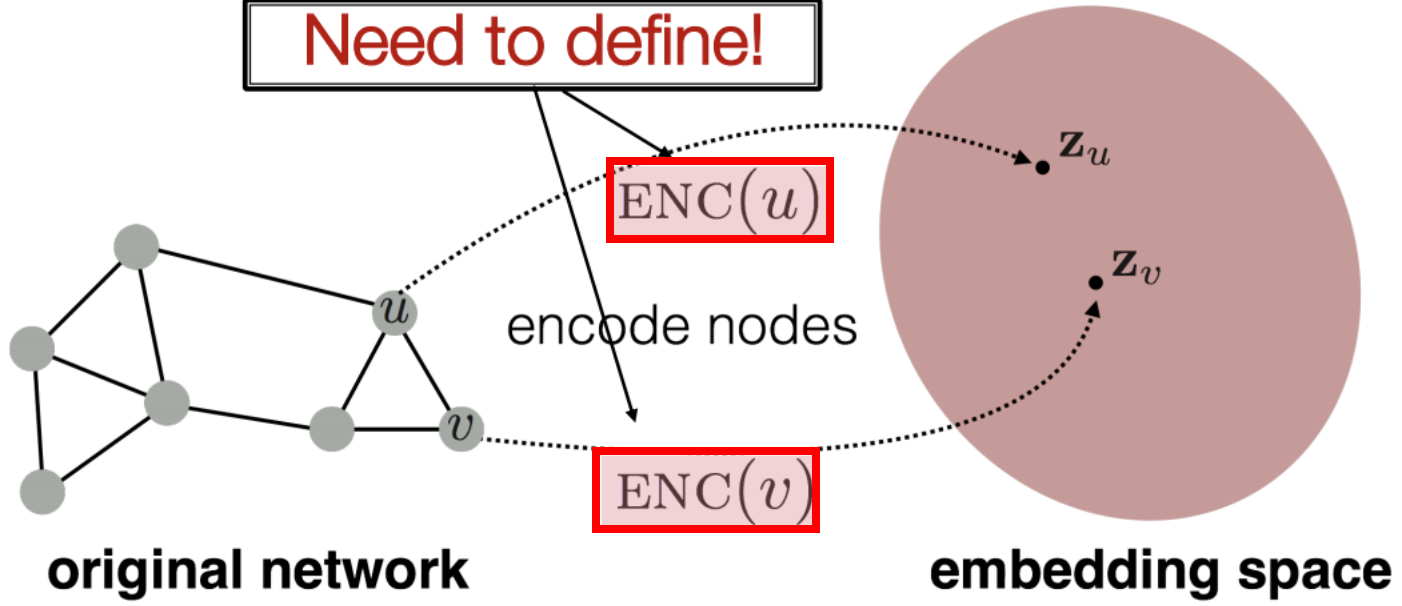
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One-hot labels

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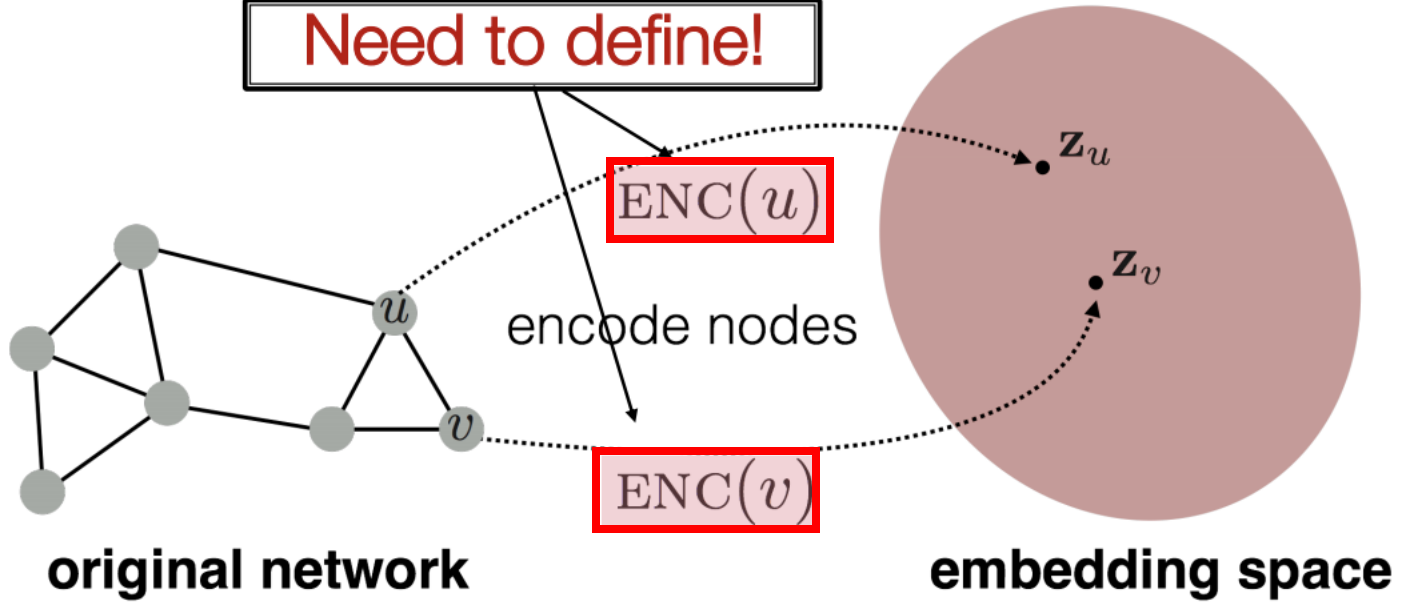
$$v \in \mathbb{I}^{|\mathcal{V}|}$$

Binary	Gray code	One-hot
000	000	00000001
001	001	00000010
010	011	00000100
011	010	00001000
100	110	00010000
101	111	00100000
110	101	01000000
111	100	10000000

Encoder-decoder for graph data

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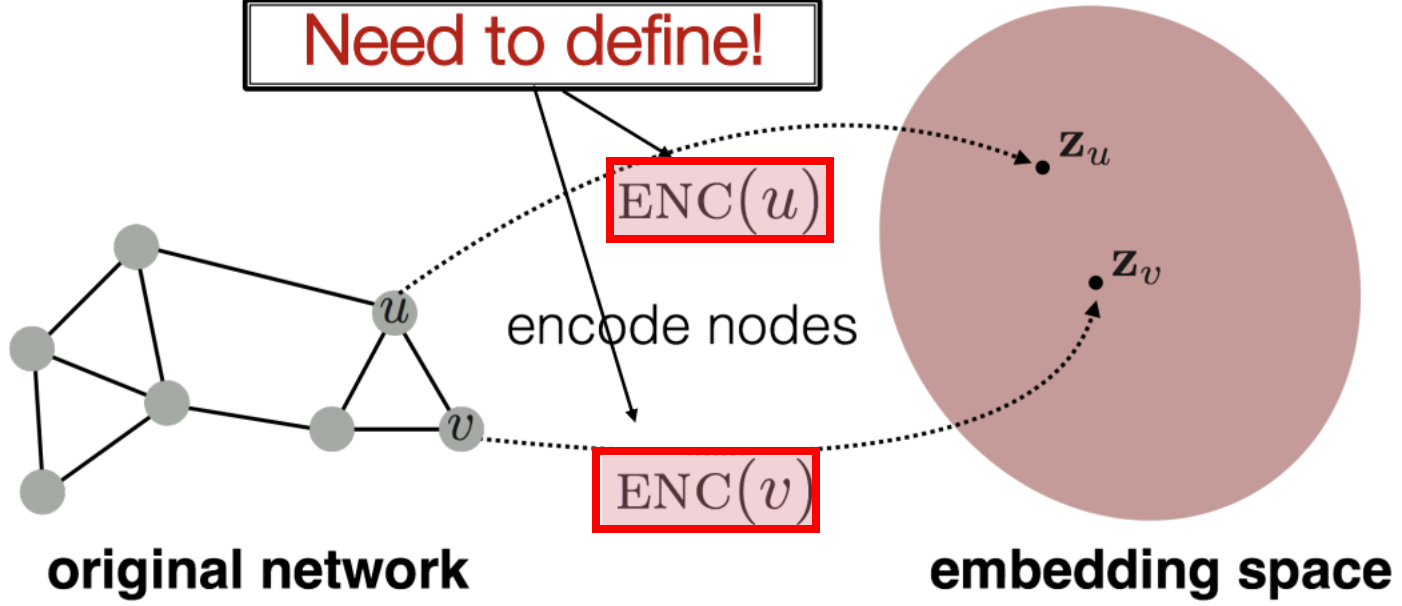
Each node

Binary	Gray code	One-hot
000	000	00000001
001	001	00000010
010	011	00000100
011	010	00001000
100	110	00010000
101	111	00100000
110	101	01000000
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Encoder-decoder for graph data

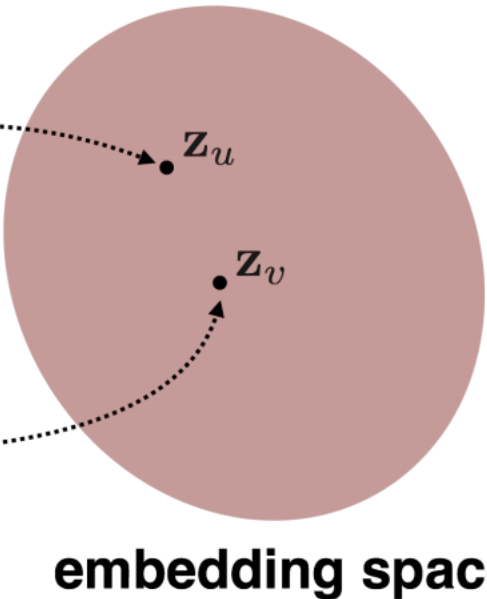
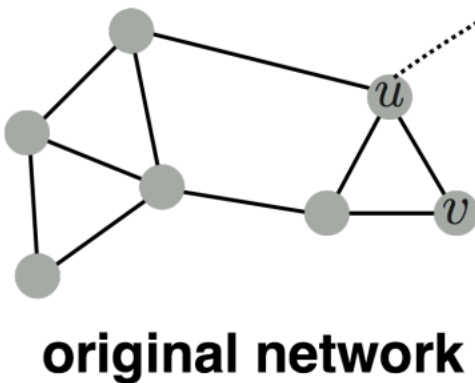
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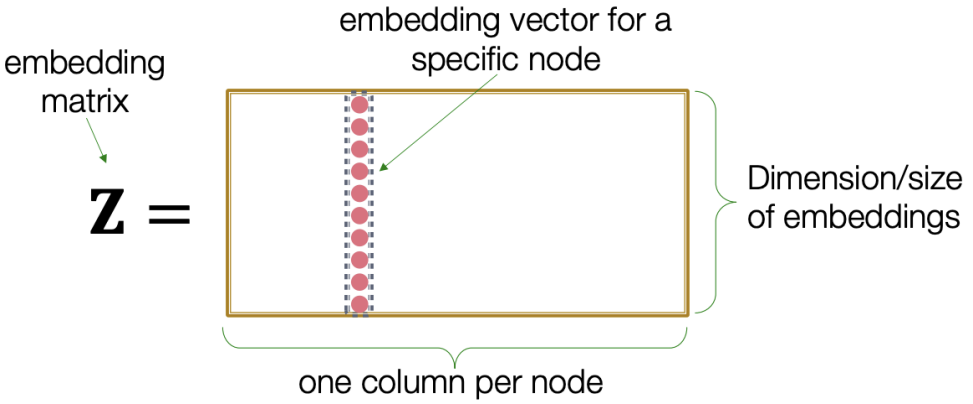
$\text{ENC}(u)$

encode nodes

$\text{ENC}(v)$



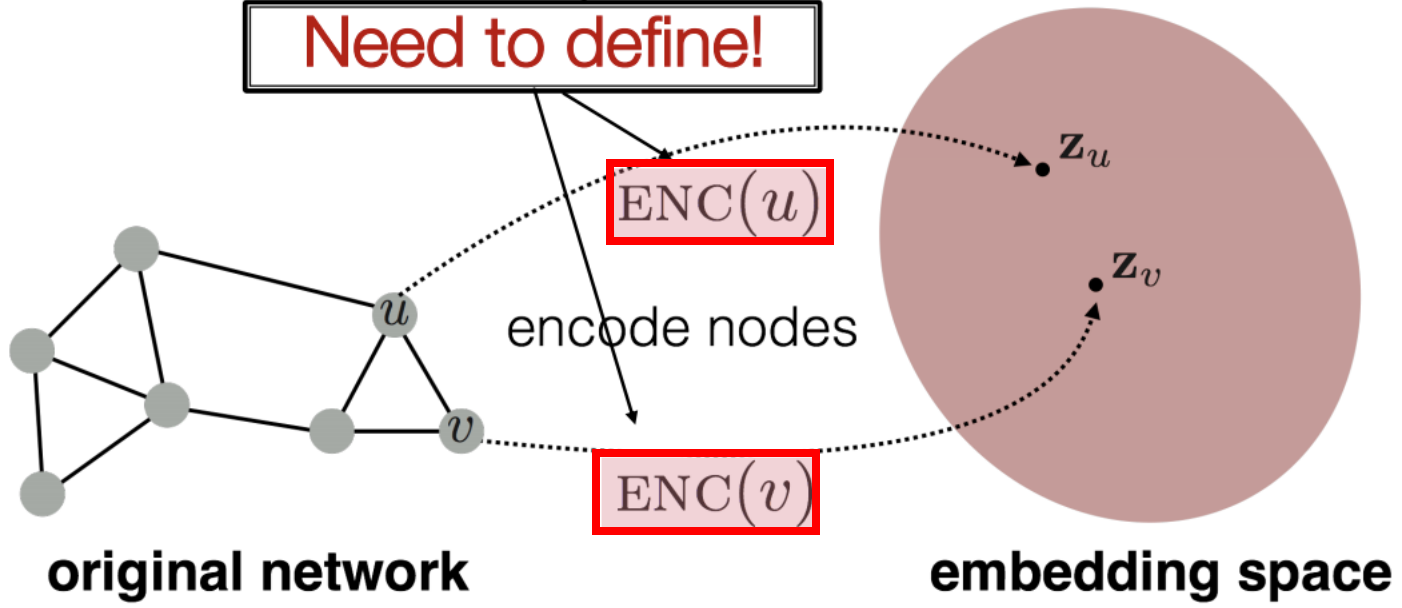
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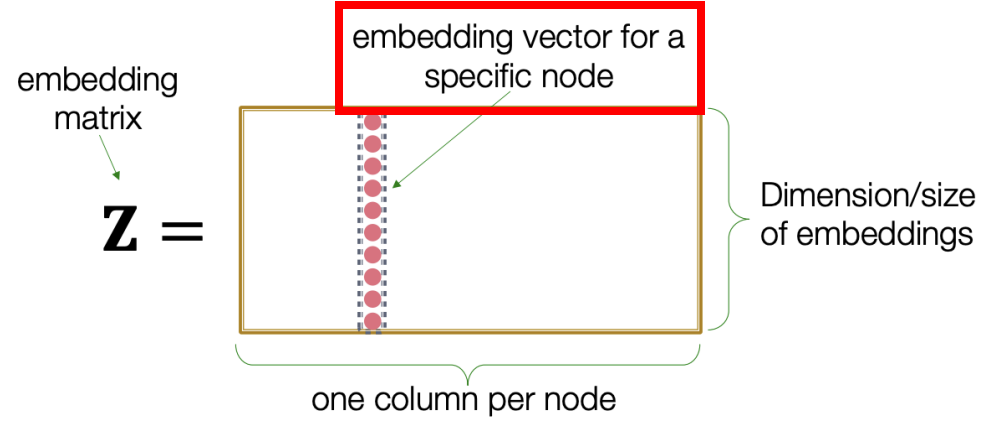
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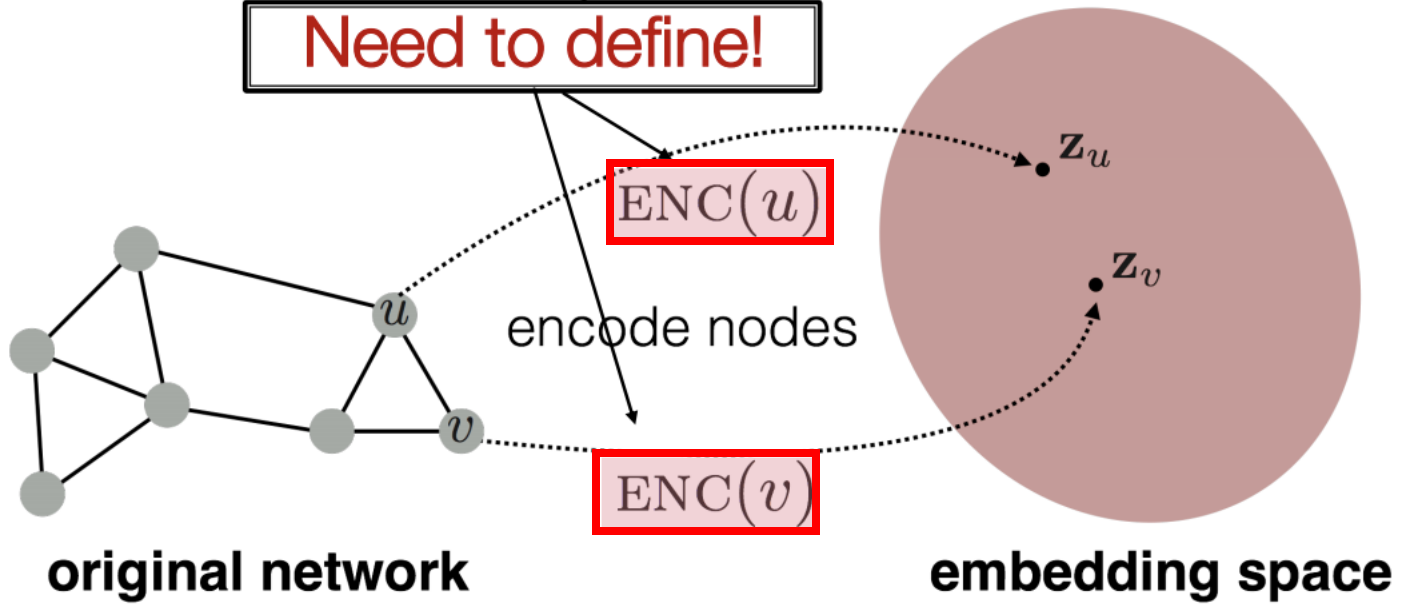
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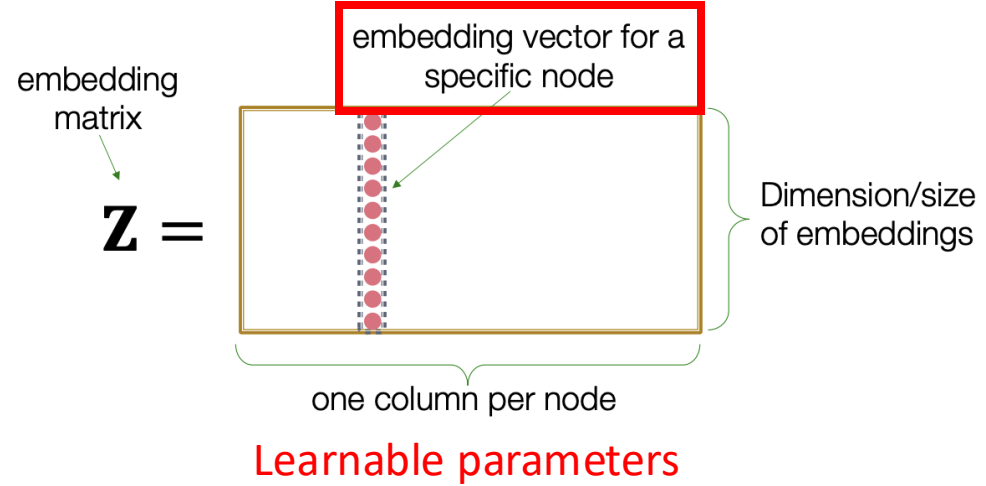
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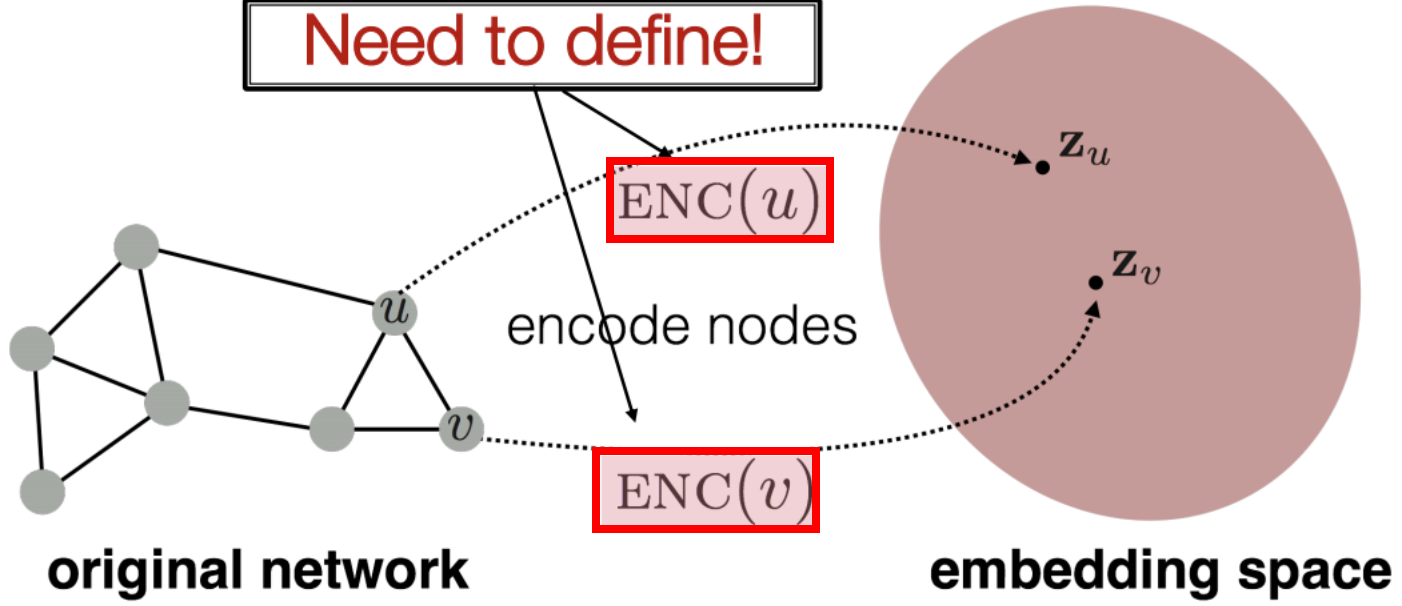
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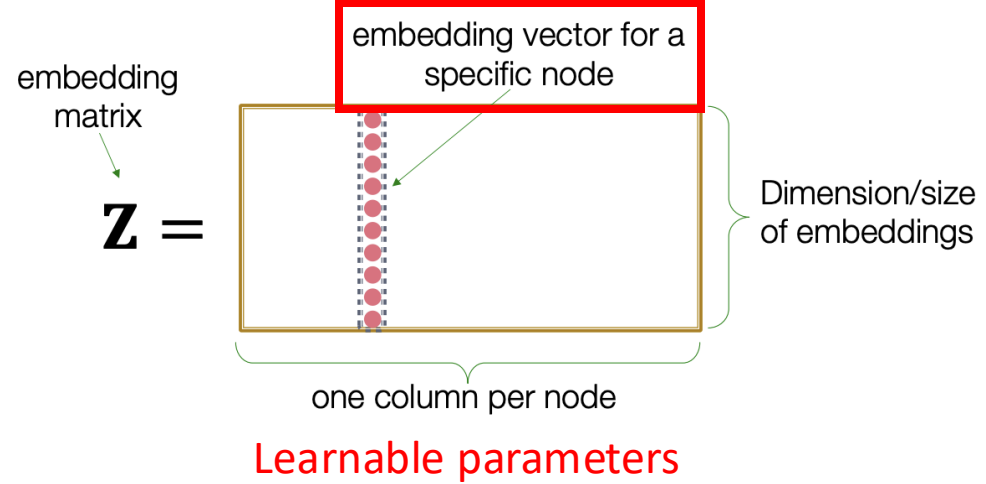
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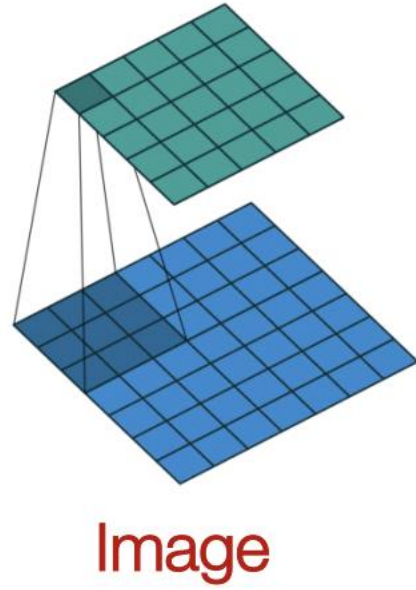


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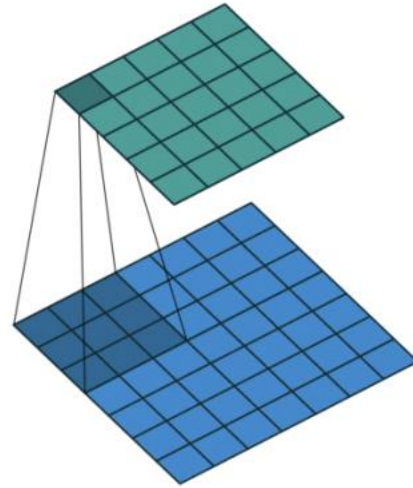


Q: how can we replace linear node embedding with nonlinear functions?

Graph neural networks



Graph neural networks



Image

Q: can we use convolution operation on graph?

Graph convolutional neural networks