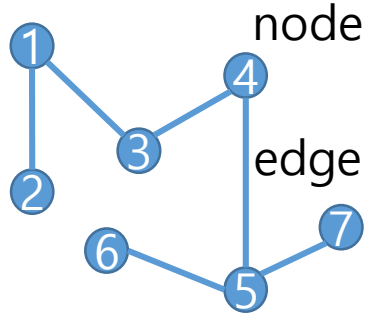
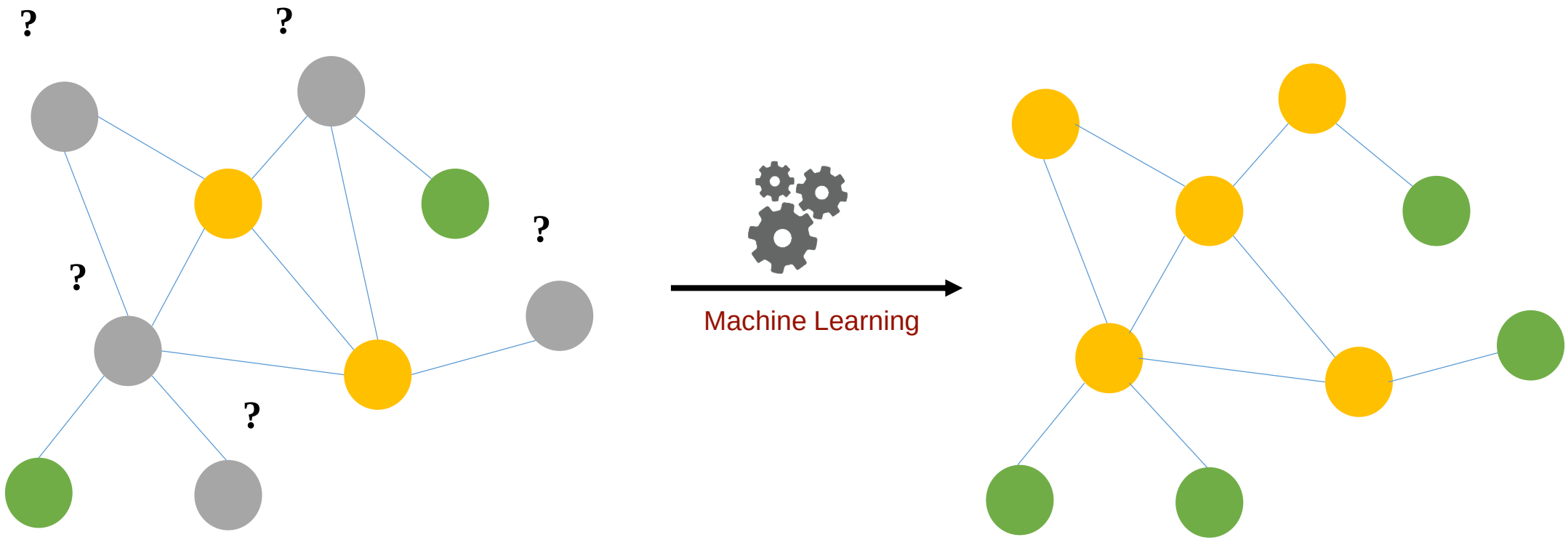
Revisit: Machine Learning with Graphs

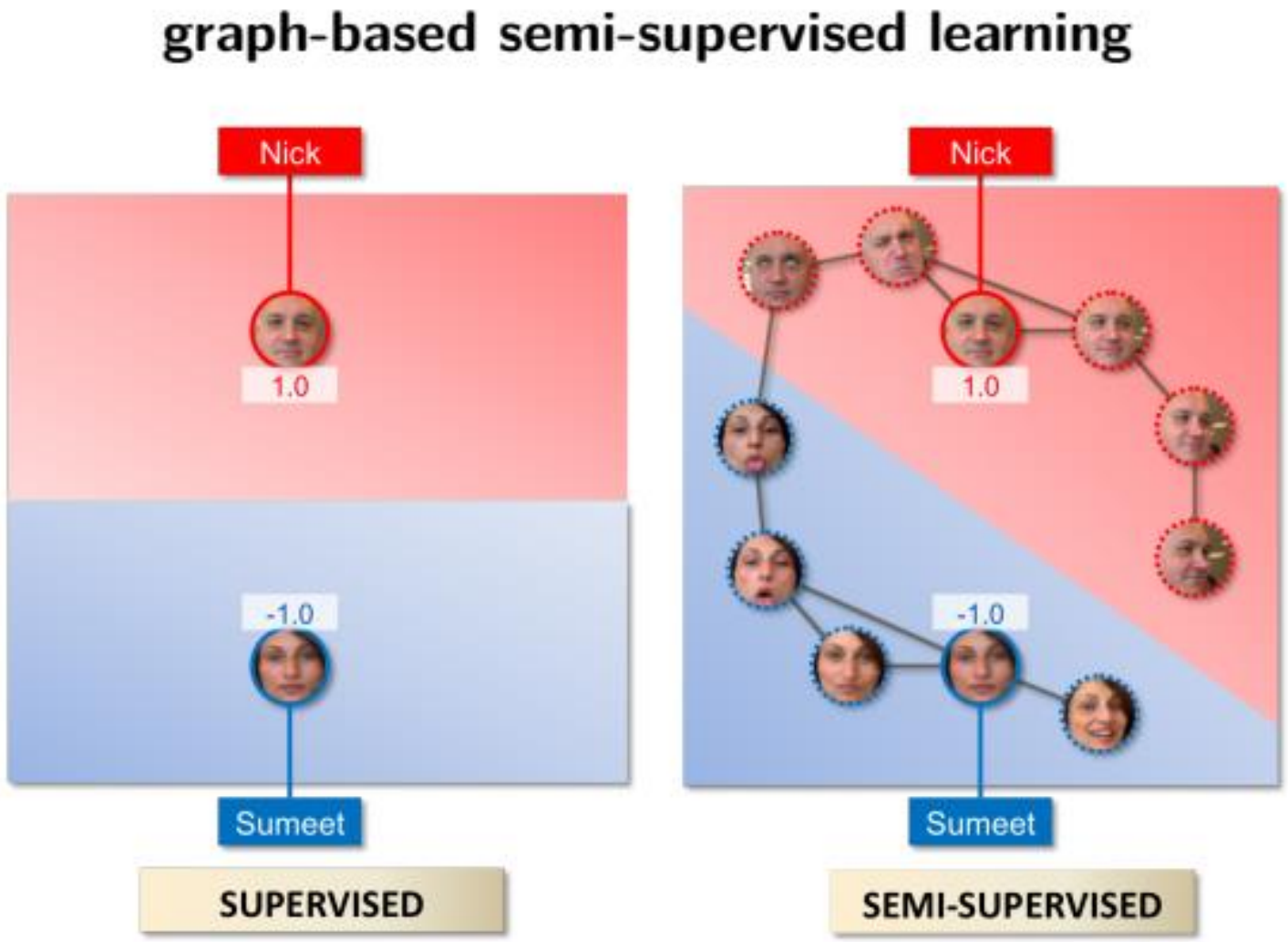
- Node classification (semi-supervised Learning)
  - Predict a type of a given node
- Link prediction
  - Predict whether two nodes are linked
- Community detection (node clustering, unsupervised learning)
  - Identify densely linked clusters of nodes
- Network similarity
  - How similar are two (sub)networks
- Ranking
  - Page ranking in Web



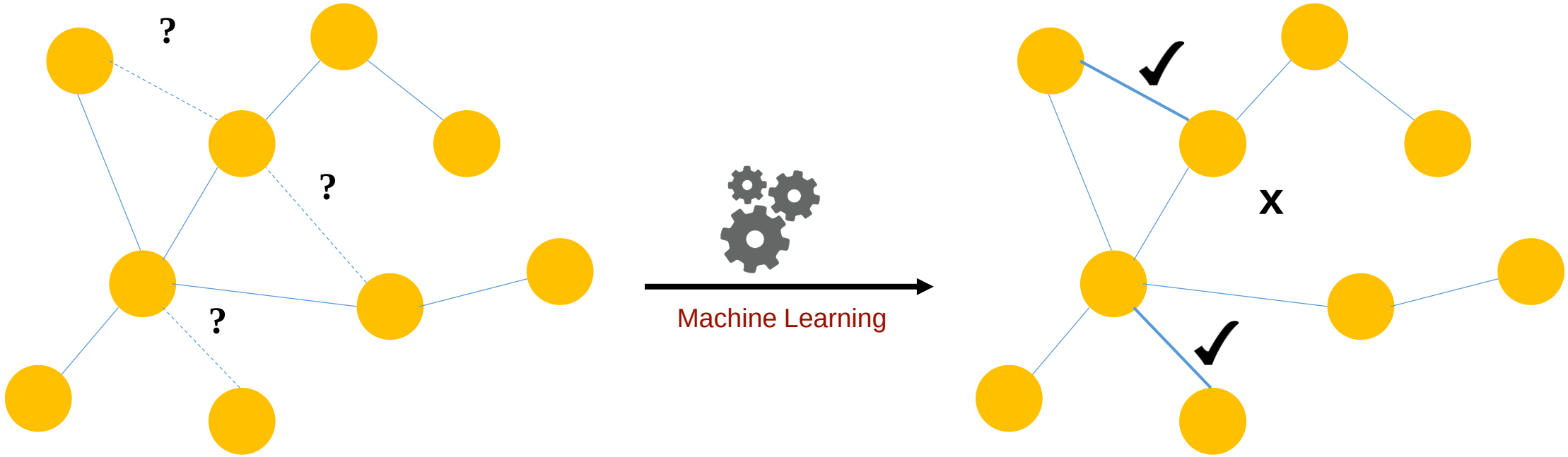
Example: Node Classification



Example: Node Classification

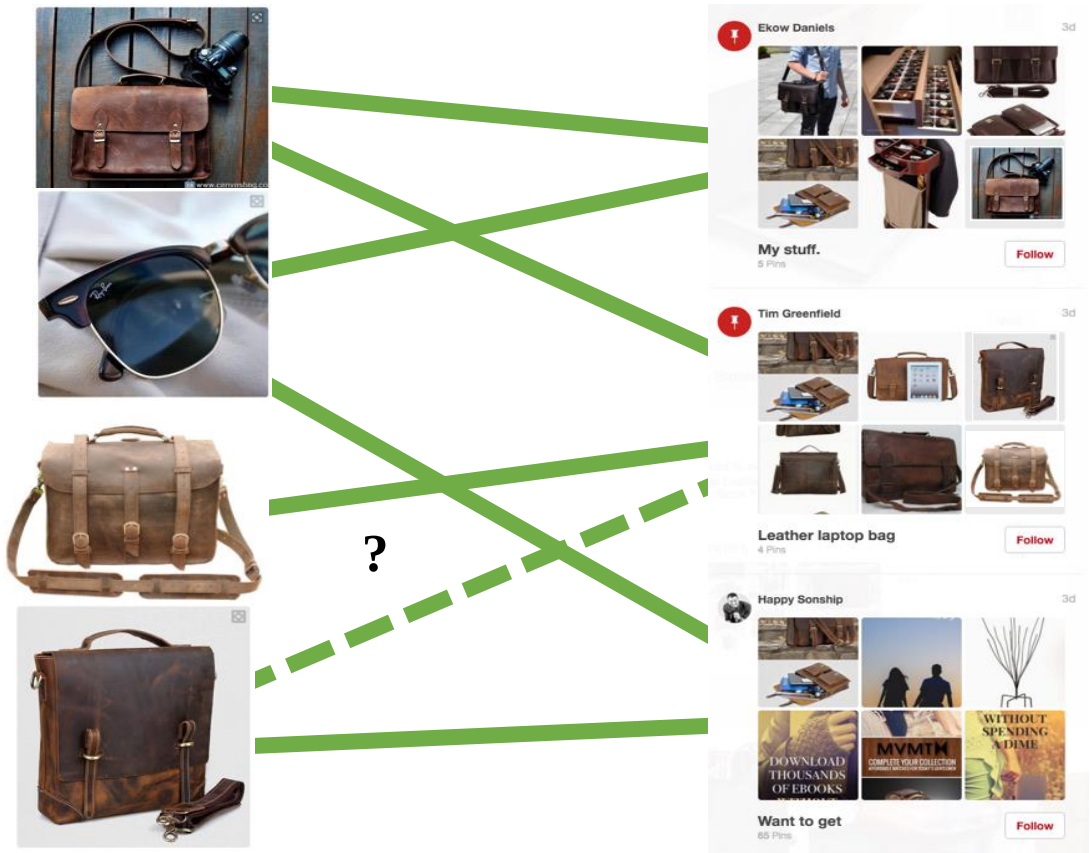


Example: Link Prediction



Example: Link Prediction

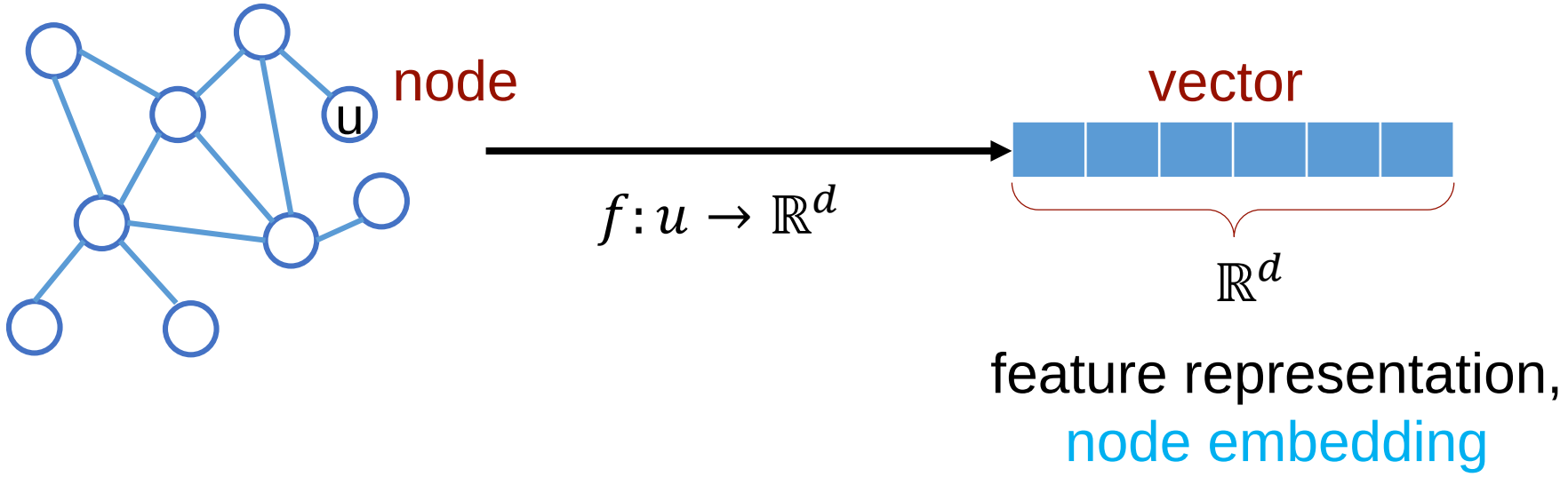
Content recommendation is link prediction!



Feature Learning in Graphs

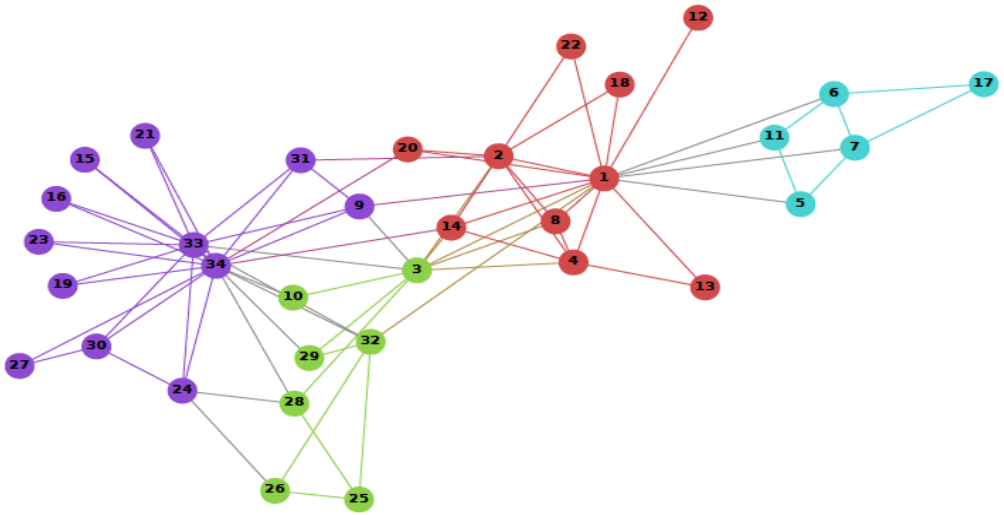
Goal:

Efficient feature learning for machine learning in networks!

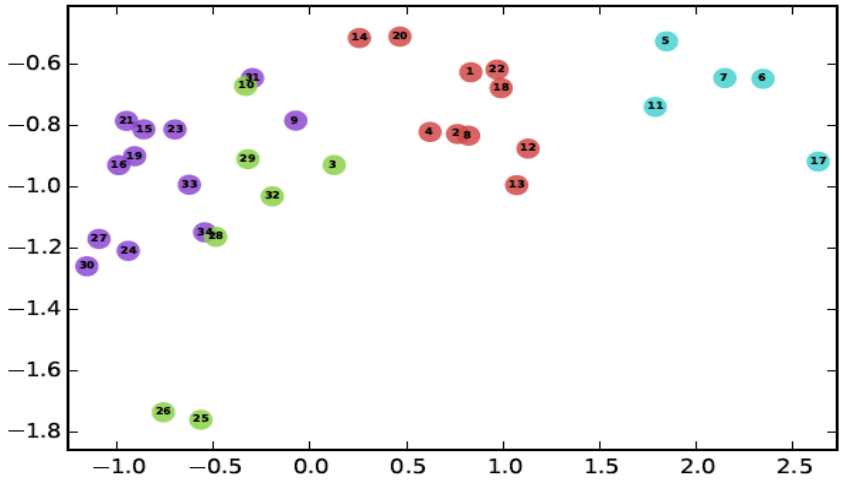


feature representation,
node embedding

Example: Feature Learning in Graphs



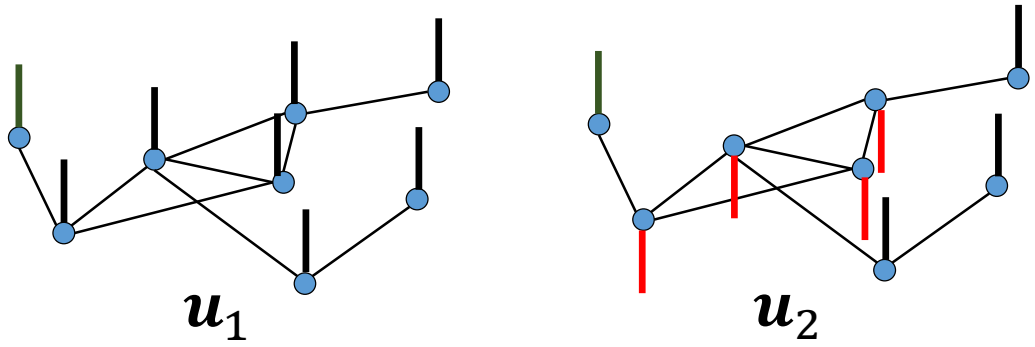
Graph input



representation
in feature space
(node embedding)

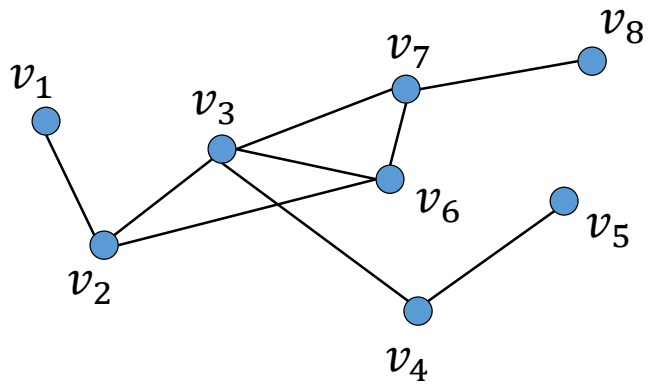
Graph Laplacian (Spectral Graph Theory)

$$\boldsymbol{L = D - W}$$



Graphs and Graph Signals

AAAI 2020 Tutorial (Yao Ma, et al.): Spectral graph theory. American Mathematical Soc.; 1997.

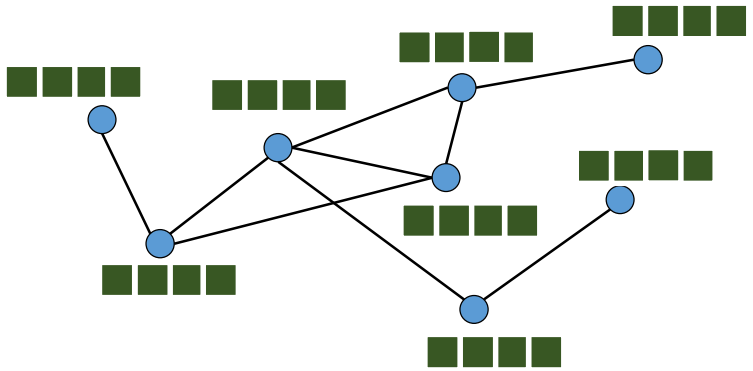


$$\mathcal{V} = \{v_i | \; i = 1, \dots, N\}$$

$$\mathcal{E} = \{e_{ij} | i, j = 1, \dots, N\}$$

$$\mathcal{G}(\mathcal{V}, \mathcal{E}) = \{\mathcal{V}, \mathcal{E}\}$$

Graphs and Graph Signals (Functions)



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$$\mathcal{E} = \{e_{ij} | i, j = 1, \dots, N\}$$

$$\mathcal{G}(\mathcal{V}, \mathcal{E}) = \{\mathcal{V}, \mathcal{E}\}$$

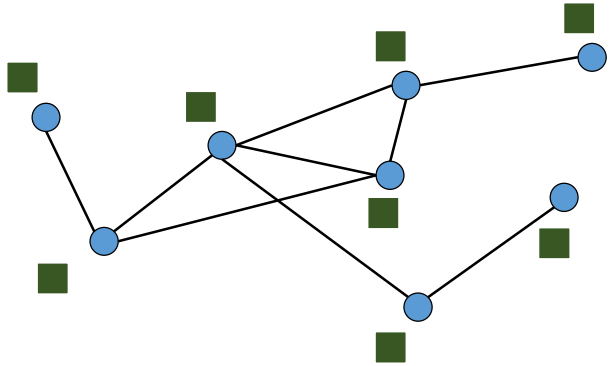
Graph Signal: $f : \mathcal{V} \rightarrow \mathbb{R}^{N \times d}$

$N \times d$ dim. Matrix

GNN input Matrix

$$\mathcal{V} \longrightarrow \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \end{bmatrix} = f = \begin{bmatrix} 2 & 3 & \dots & 2 \\ 1 & 5 & \dots & 4 \\ & & & \\ . & . & . & \\ . & . & . & \\ . & . & . & \\ 2 & 6 & \dots & 3 \\ 1 & 4 & \dots & 5 \end{bmatrix}$$

Graphs and Graph Signals



$$\mathcal{V} = \{v_i | \; i = 1, \dots, N\}$$

$$\mathcal{E} = \{e_{ij} | i, j = 1, \dots, N\}$$

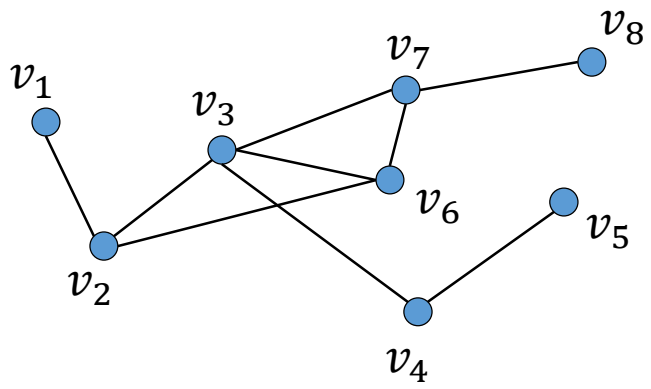
$$\mathcal{G}(\mathcal{V}, \mathcal{E}) = \{\mathcal{V}, \mathcal{E}\}$$

Graph Signal: $f : \mathcal{V} \rightarrow \mathbb{R}^N$

$N \times 1$ vector for simplicity

$$\mathcal{V} \longrightarrow \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \\ f_6 \\ f_7 \\ f_8 \end{bmatrix} = f = \begin{bmatrix} 2 \\ 5 \\ 1 \\ \vdots \\ 6 \\ 4 \\ 3 \end{bmatrix}$$

Matrix Representations of Graphs



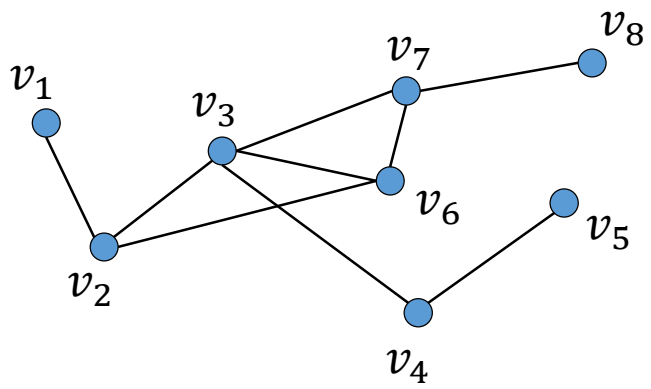
Adjacency Matrix: $A[i,j] = 1$ if v_i is adjacent to v_j

$A[i,j] = 0$, otherwise

Adjacency Matrix or Affinity Matrix

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

Matrix Representations of Graphs



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$A[i,j] = 0$, otherwise

Degree Matrix: $\mathbf{D} = \mathrm{diag}(degree(v_1), \ldots, degree(v_N))$

Degree Matrix

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & -1 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & -1 & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

$\boldsymbol{D}$ Adjacency Matrix $\boldsymbol{A}$ Laplacian Matrix $\boldsymbol{L}$

Laplacian Matrix as an Operator

Laplacian matrix is a difference operator:

$$\boldsymbol{h = Lf = (D - A)f = Df - Af}$$

Laplacian Matrix as an Operator

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$$\boldsymbol{h = Lf = (D - A)f = Df - Af}$$

$$\boldsymbol{h_i = L_i\, f = (D_i - A_i)f = D_i f - A_i f}$$

$$\boldsymbol{D} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

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

$$f = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_j \\ \vdots \\ N \end{bmatrix}$$

Laplacian Matrix as an Operator

Laplacian matrix is a difference operator:

$$\boldsymbol{h = Lf = (D - A)f = Df - Af}$$

$$h_i = \boldsymbol{L_i f = (D_i - A_i)f = D_i f - A_i f}$$

$$\boldsymbol{= D_{i,i} f_i - A_i f}$$

$$\boldsymbol{D} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

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$$h_6 = \mathbf{4}f_6 - f_2 - f_3 - f_5 - f_7$$
$$= (f_6 - f_2) + (f_6 - f_3) + (f_6 - f_5) + (f_6 - f_7)$$

$$\boldsymbol{D} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

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$$\boldsymbol{= D_{i,i} f_i - A_i f}$$

$$h_i = \sum_{v_j \in \mathcal{N}(v_i)} (f_i - f_j)$$

meaning?

$$h_6 = \mathbf{4}f_6 - f_2 - f_3 - f_5 - f_7$$
$$= (f_6 - f_2) + (f_6 - f_3) + (f_6 - f_5) + (f_6 - f_7)$$

$$\boldsymbol{D} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

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meaning?

$$h_6 = (f_6 - f_2) + (f_6 - f_3) + (f_6 - f_5) + (f_6 - f_7)$$
$$= 2.1 - 3.5 + 5.3 - 4.2$$

$$\boldsymbol{D} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

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$$f = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_j \\ \vdots \\ N \end{bmatrix}$$

Laplacian Matrix as an Operator

Laplacian quadratic form:

$$\boldsymbol{h = Lf}, \quad h_i = \sum_{\boldsymbol{v_j \in \mathcal{N}(v_i)}} (f_i - f_j)$$

$$\boldsymbol{f^T L f} = \sum_{\boldsymbol{i}} f_i h_i = \sum_{\boldsymbol{i}} \sum_{\boldsymbol{v_j \in \mathcal{N}(v_i)}} f_i (f_i - f_j)$$

$$\boldsymbol{D} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

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$$= \frac{\boldsymbol{1}}{\boldsymbol{2}} \sum_{\boldsymbol{i,j}} \boldsymbol{A(i,j)} f_i (f_i - f_j) + \frac{\boldsymbol{1}}{\boldsymbol{2}} \sum_{\boldsymbol{i,j}} \boldsymbol{A(j,i)} f_i (f_i - f_j)$$

Laplacian Matrix as an Operator

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

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$$= \frac{\boldsymbol{1}}{\boldsymbol{2}} \sum_{\boldsymbol{i,j}} \boldsymbol{A(i,j)} f_i \left(f_i - f_j\right) - \frac{\boldsymbol{1}}{\boldsymbol{2}} \sum_{\boldsymbol{i,j}} \boldsymbol{A(i,j)} f_j (f_i - f_j)$$

Laplacian Matrix as an Operator

Laplacian quadratic form:

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$$= \frac{\boldsymbol{1}}{\boldsymbol{2}} \sum_{\boldsymbol{i,j}} \boldsymbol{A(i,j)} f_i \left(f_i - f_j\right) - \frac{\boldsymbol{1}}{\boldsymbol{2}} \sum_{\boldsymbol{i,j}} \boldsymbol{A(i,j)} f_j (f_i - f_j)$$

$$= \frac{\boldsymbol{1}}{\boldsymbol{2}} \sum_{\boldsymbol{i,j}} \boldsymbol{A(i,j)} \left(f_i - f_j\right)^{\boldsymbol{2}}$$

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

➡ The smaller, the similar the connected nodes

Summary: Laplacian Matrix as an Operator

Laplacian matrix is a difference operator:

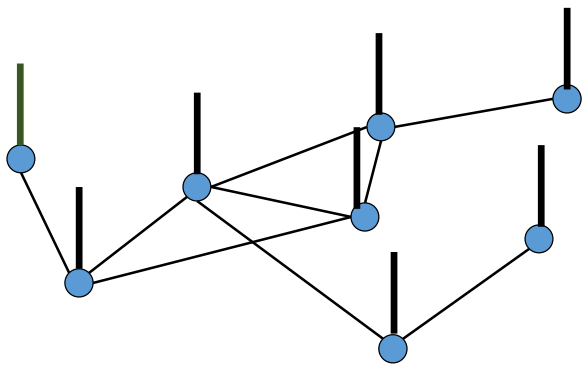
$$\boldsymbol{h = Lf = (D - A)f = Df - Af}$$

$$\boldsymbol{h(i)} = \sum_{\boldsymbol{v_j \in \mathcal{N}(v_i)}} (f_i - f_j)$$

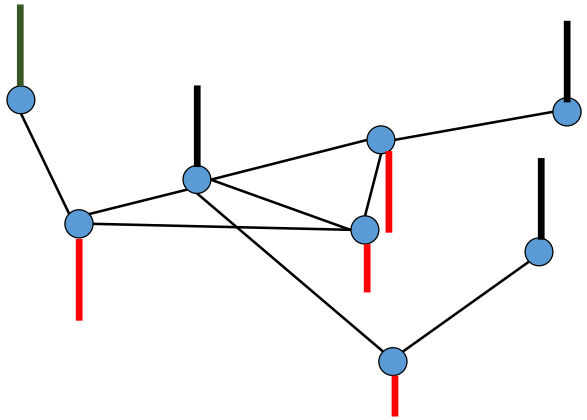
Laplacian quadratic form:

$$\boldsymbol{f^T Lf} = \frac{\boldsymbol{1}}{\boldsymbol{2}} \sum_{\boldsymbol{i,j}} \boldsymbol{A(i,j)} \left(f_i - f_j\right)^{\boldsymbol{2}}$$

- It can represent
  "Smoothness" or "Frequency" of the signal f
- The smaller, the similar the connected nodes.
  Can be a cost function for link prediction.
- Spectral Graph Theory



Low frequency graph signal



High frequency graph signal