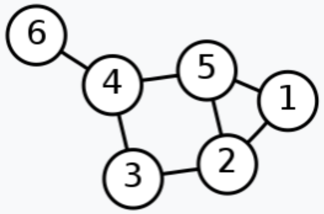
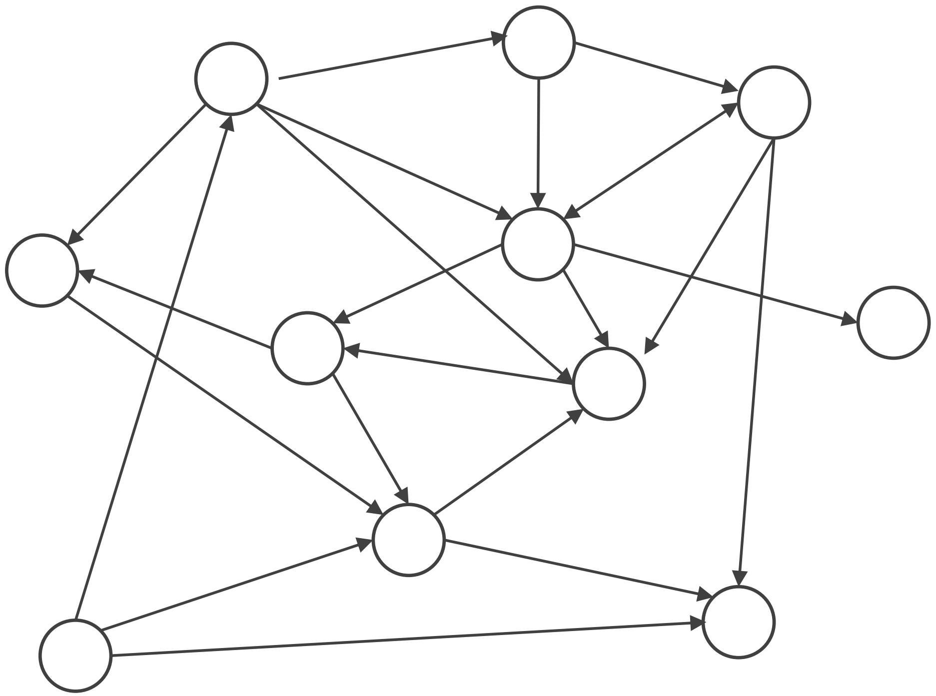
Revisiting graphs

Labelled graph	Degree matrix	Adjacency matrix	Laplacian matrix
	$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 3 & -1 & -1 \\ -1 & -1 & 0 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$

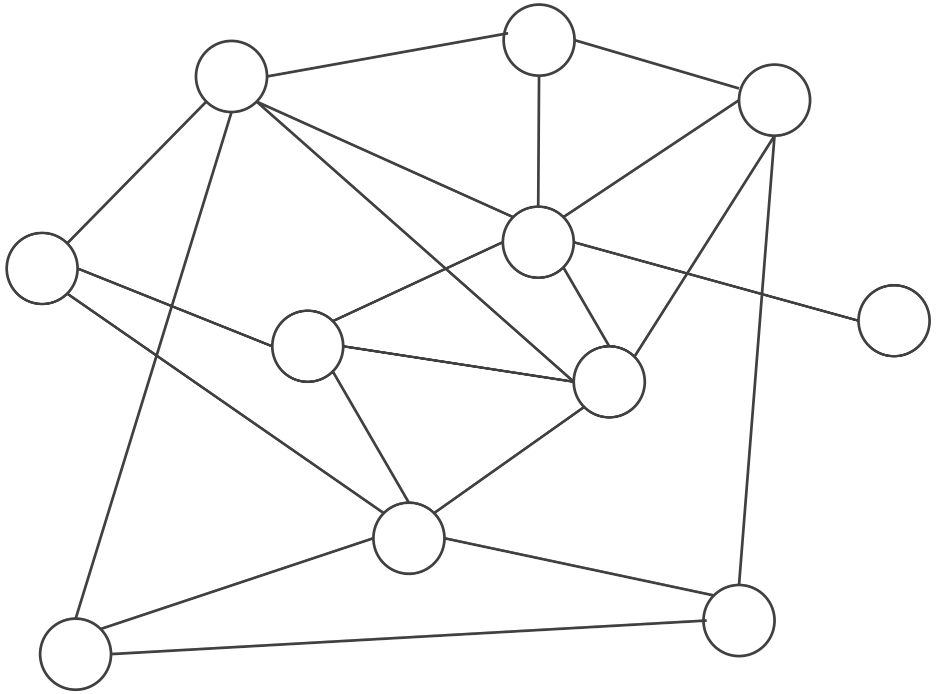
Directed graphs

- Vertices $\mathcal{V} = \{1, \dots, n\}$
- Edges $\mathcal{E} = \{(i, j): i, j \in \mathcal{V}\} \subseteq \mathcal{V} \times \mathcal{V}$ (directed)



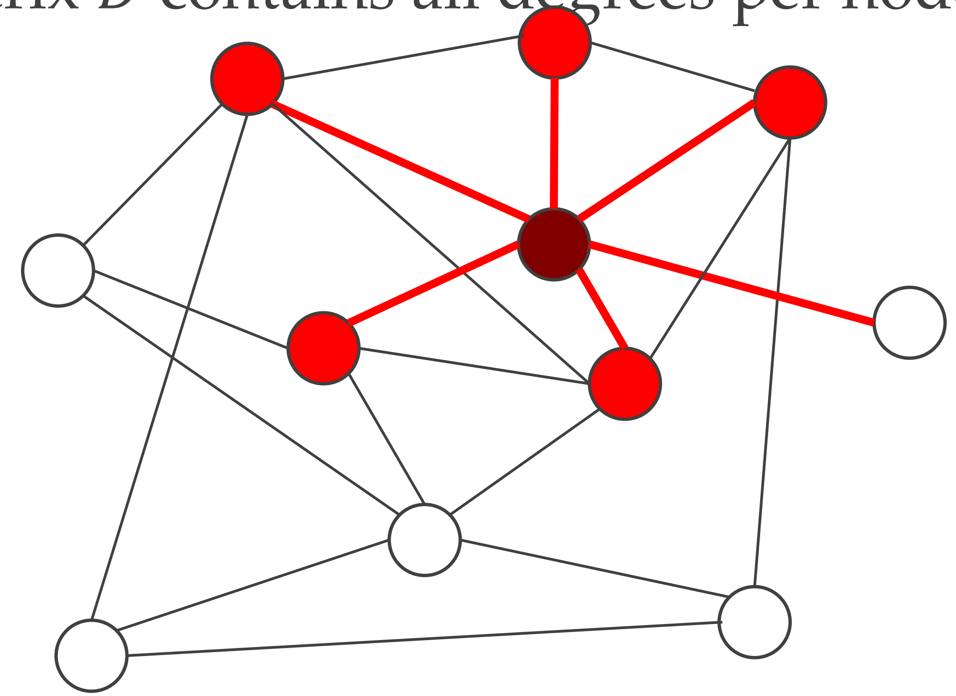
Undirected graphs

- Vertices $\mathcal{V} = \{1, \ldots, n\}$
- Edges $\mathcal{E} = \{(i, j): i, j \in \mathcal{V}\} \subseteq \mathcal{V} \times \mathcal{V}$ (directed)
- Edges $\mathcal{E} = \{\{i, j\}: i, j \in \mathcal{V}\} \subseteq \mathcal{V} \times \mathcal{V}$ (undirected)



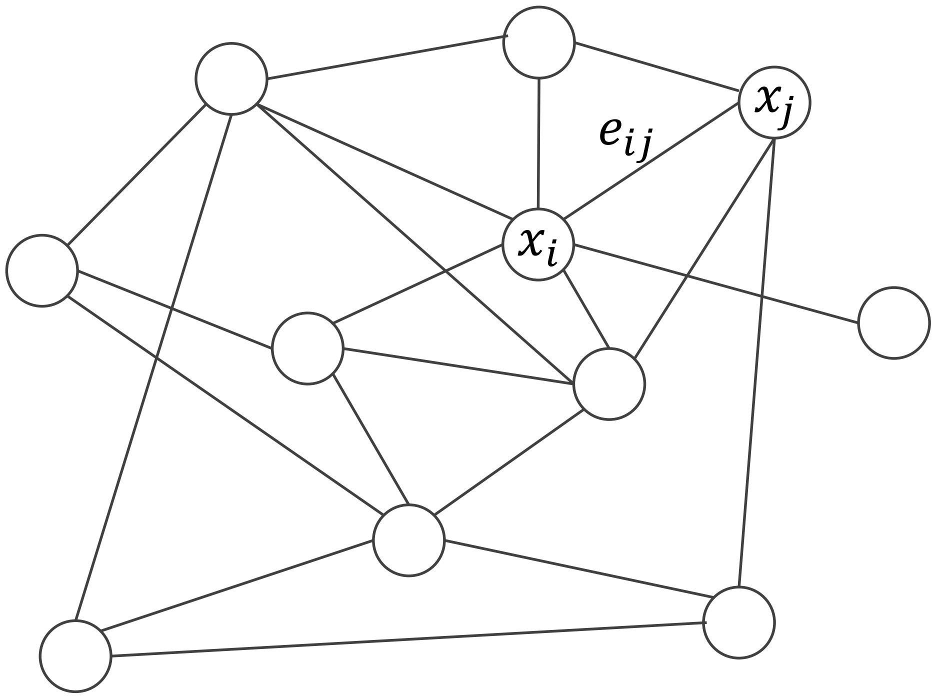
Graph neighborhood

- The neighborhood of a node is all nodes directly connected to it
$$\mathcal{N}(i) = \{j : (i, j) \in \mathcal{E}\}$$
- The degree of the node is the number of neighbors: $d_i = |\mathcal{N}(i)|$
  - The diagonal matrix D contains all degrees per node



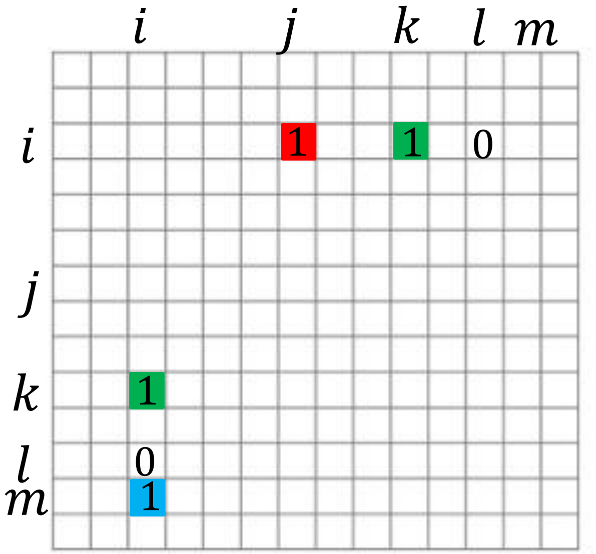
Attributes

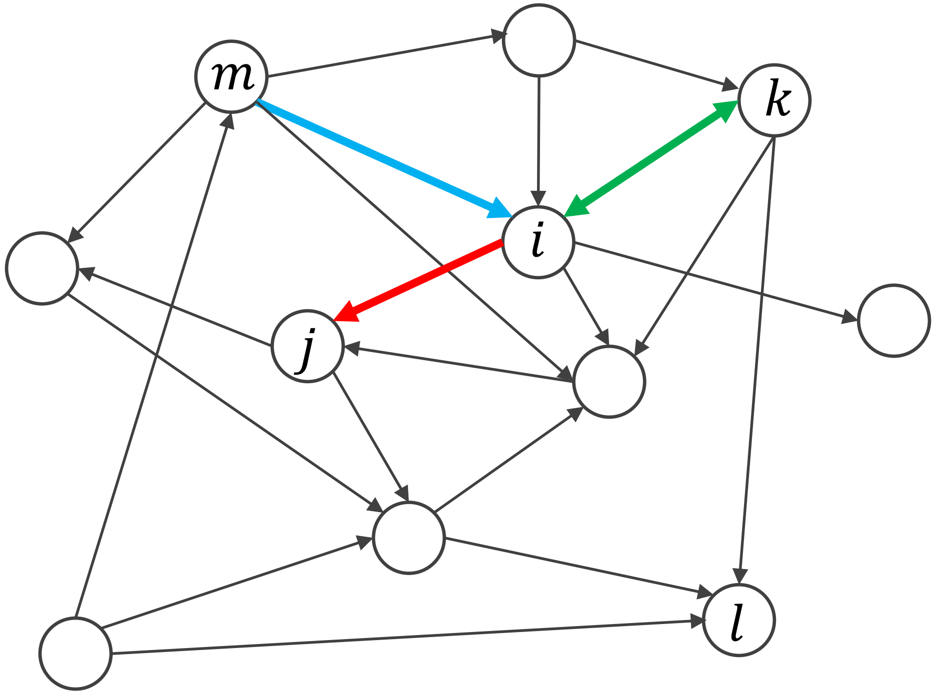
- Node features $\boldsymbol{x}: \mathcal{V} \rightarrow \mathbb{R}^d$, $X = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_n)$
- Edge features $\boldsymbol{e}_{ij}: \mathcal{E} \rightarrow \mathbb{R}^{d'}$
  - If $d' \in \mathbb{R}$ we simply have a weighted graph



Adjacency matrix

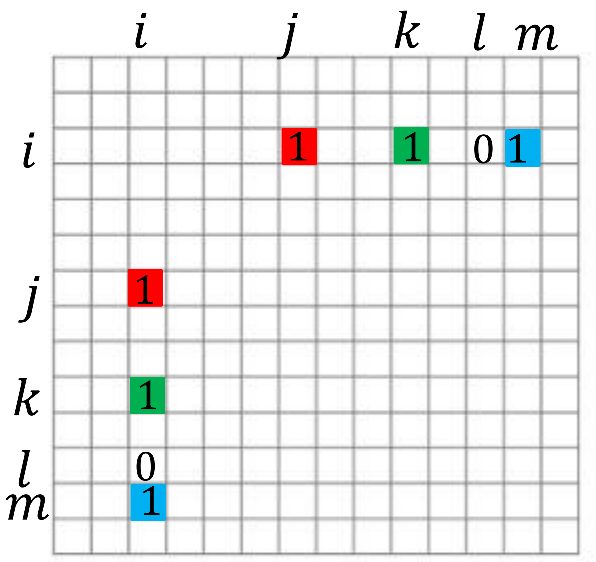
- An $n \times n$ matrix A, for n nodes
- $A_{ij} = \begin{cases} 1 \text{ if } (i,j) \in \mathcal{E} \\ 0 \text{ if } (i,j) \notin \mathcal{E} \end{cases}$

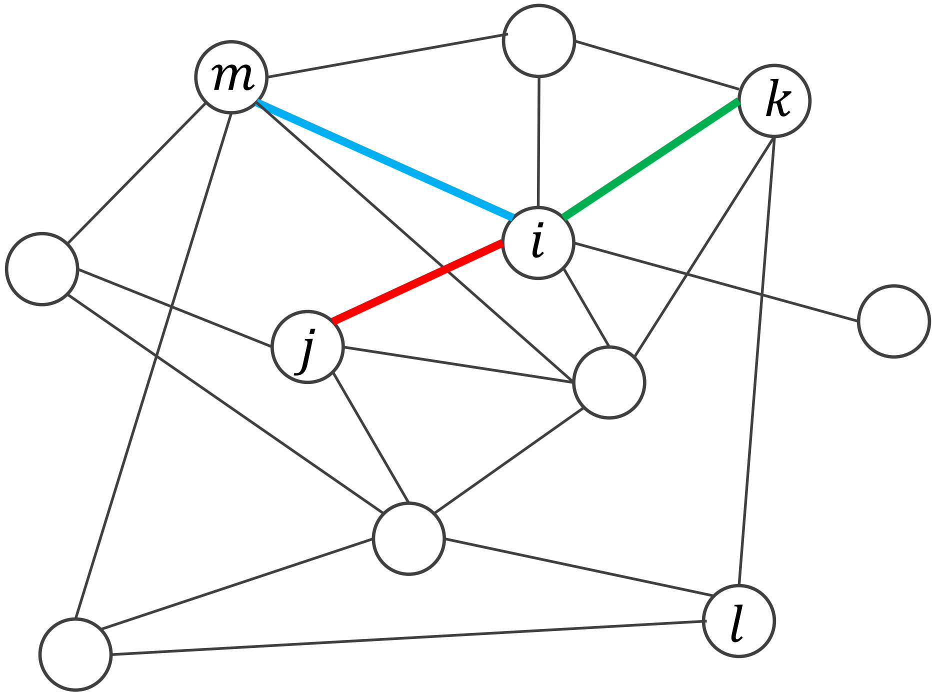




Adjacency matrix for undirected graphs

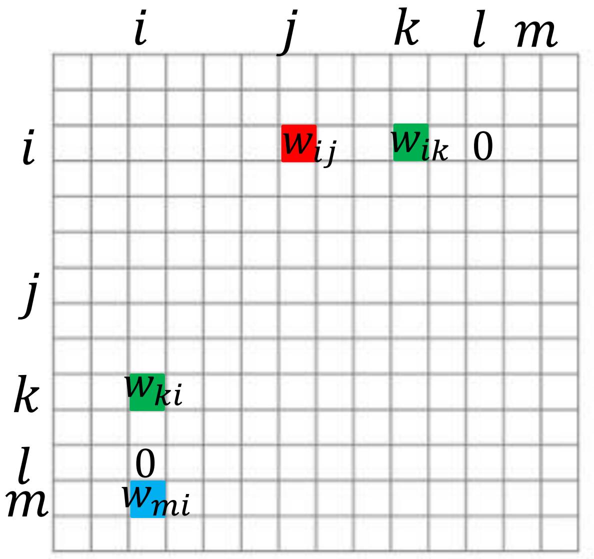
- The adjacency matrix is symmetric for undirected graphs

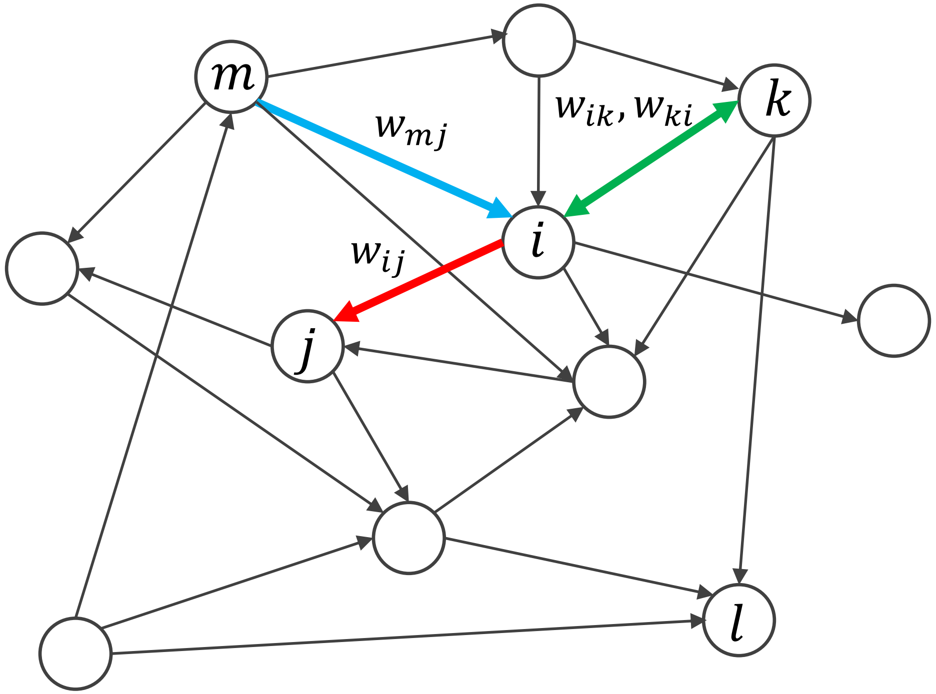




Weighted adjacency matrix

- When the edges have weights, so does the adjacency matrix





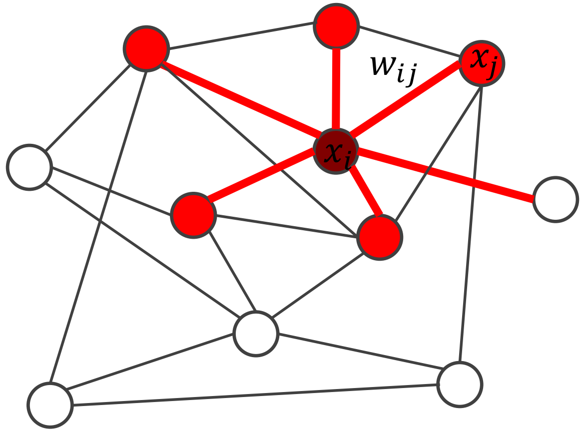
Graph Laplacian

- A matrix representation of a graph: $\Delta = D - A$
- Normalize to cancel out skewing by the degree matrix

$$\Delta = D^{-1}(D - A) = I - D^{-1}A$$

- Or for better symmetry

$$\Delta = D^{-1/2}(D - A)D^{-1/2} = I - D^{-1/2}AD^{-1/2}$$



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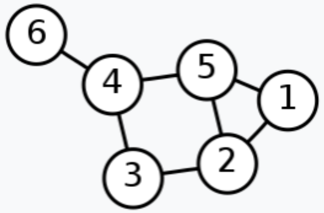
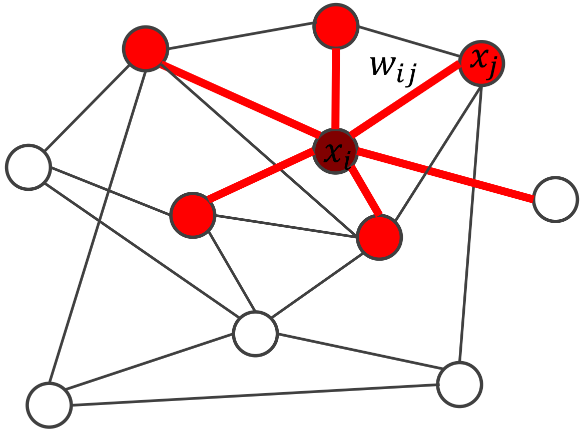
	$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1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

Local difference operator

- The local difference operator

$$(\Delta \boldsymbol{x})_i = \frac{1}{d_i} \sum_{j \in \mathcal{N}(i)} w_{ij} \, (\boldsymbol{x}_i - \boldsymbol{x}_j)$$

- A bit similar to a convolution



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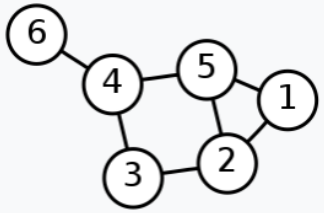	$\begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1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

Dirichlet energy

- Measures the smoothness of the signal in the graph

$$E(X) = \sum_{i \in \mathcal{V}} \frac{1}{d_i} \sum_{j \in \mathcal{N}(i)} w_{ij} \left\| x_i - x_j \right\|^2 = \mathrm{trace}(\mathbf{X \Delta X}^{\mathrm{T}})$$

- The bigger differences ($x_i - x_j$) between all possible neighbors
  - The bigger the ‘energy’ in our graph
  - The less smooth the graph is