Spectral Clustering: A Graph Cut Formulation

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Objective

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Define the graph partition formulation

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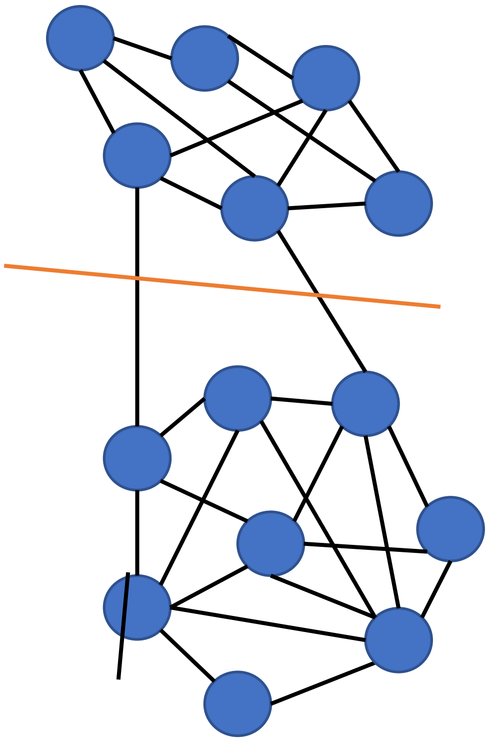
Learn how to solve simple graph partition

Clustering as Graph Partition/Cut

- Find a partition of a graph such that the edges between different groups have a very low weight while the edges within a group have high weight.

- E.g., minimum cut

CutSize = 2



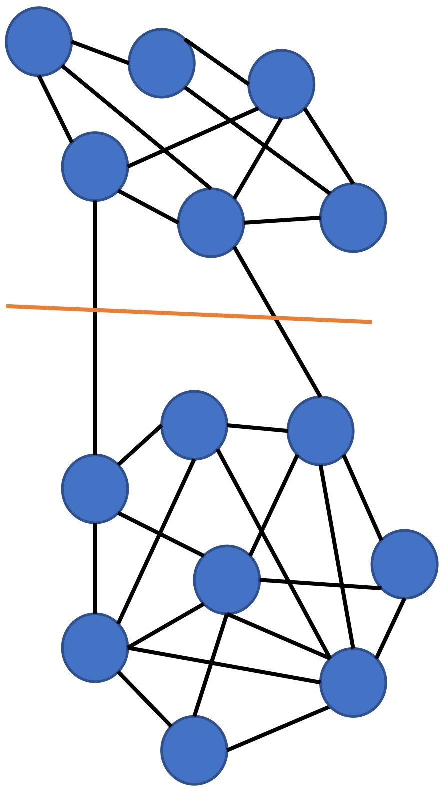
- More general, consider weighted edges.

2-way Spectral Graph Partitioning

- Weighted adjacency matrix **W**
  - $w_{i,j}$: the weight between two vertices *i* and *j*

- (Cluster) Membership vector **q**

$$q_i = \begin{cases} 1 & i \in Cluster\ A \\ -1 & i \in Cluster\ B \end{cases}$$



$$\mathbf{q} = \underset{\mathbf{q} \in [-1,\ 1]^n}{\operatorname{argmin}}\ CutSize\,,$$

$$CutSize = \mathrm{J} = \frac{1}{4} \sum_{i,j} (q_i - q_j)^2 w_{i,j}$$

Solving the Optimization Problem

$$\mathbf{q} = \underset{\mathbf{q}\in[-1,\ \ 1]^n}{\operatorname{argmin}} \frac{1}{4}\sum_{i,j}(q_i - q_j)^2 w_{i,j}\ ,$$

- Directly solving the above problem requires combinatorial search → exponential complexity
- How to reduce the computational complexity?

Relaxation Approach

- Key difficulty: q_i has to be either -1,1.
  - Relax q_i to be any real number.
  - Impose Constraint: $\sum_{i=1}^{n} q_i^2 = n$

$$J = \frac{1}{4}\sum_{i,j}(q_i - q_j)^2 w_{i,j} = \frac{1}{4}\sum_{i,j}(q_i^2 - 2q_i q_j + q_j^2) w_{i,j}$$

$$= \frac{1}{4}\sum_i 2q_i^2\left(\sum_j w_{i,j}\right) - \frac{1}{4}\sum_{i,j} 2q_i q_j w_{i,j}$$

$$= \frac{1}{2}\sum_i q_i^2 d_i - \frac{1}{2}\sum_{i,j} q_i (d_i \delta_{i,j} - w_{i,j}) q_j$$

where $d_i = \sum_j w_{i,j}$ and $D \equiv [d_i \delta_{i,j}]$

$$\Rightarrow \; J = \frac{1}{2}\mathbf{q}^T(\mathbf{D} - \mathbf{W})\mathbf{q}$$

Relaxation Approach (cont'd)

- The final problem formulation:

$$\mathbf{q} = \underset{\mathbf{q}}{\operatorname{argmin}}\ J = \underset{\mathbf{q}}{\operatorname{argmin}}\, \mathbf{q}^T(\mathbf{D} - \mathbf{W})\mathbf{q} \ ,$$

subject to $\sum_{i=1}^{n} q_i^2 = n$

- Solution: the second minimum eigenvector for **D-W**

$$(\mathbf{D} - \mathbf{W})\mathbf{q} = \lambda_2\ \mathbf{q}$$

Graph Laplacian

- $\mathbf{L} = \mathbf{D} - \mathbf{W}$
- $\mathbf{L}$ is semi-positive definitive matrix.
  - For any $\mathbf{x}$, we have $\mathbf{x}^T\mathbf{L}\mathbf{x} \geq 0$. (Why?)
- Minimum eigenvalue $\lambda_1 = 0$ (what is the eigenvector?)

$$0 = \lambda_1 < \lambda_2 < \lambda_3 \ldots < \lambda_k$$

- The eigenvector that corresponds to the second minimum eigenvalue λ_2 gives the best bipartite graph partition.

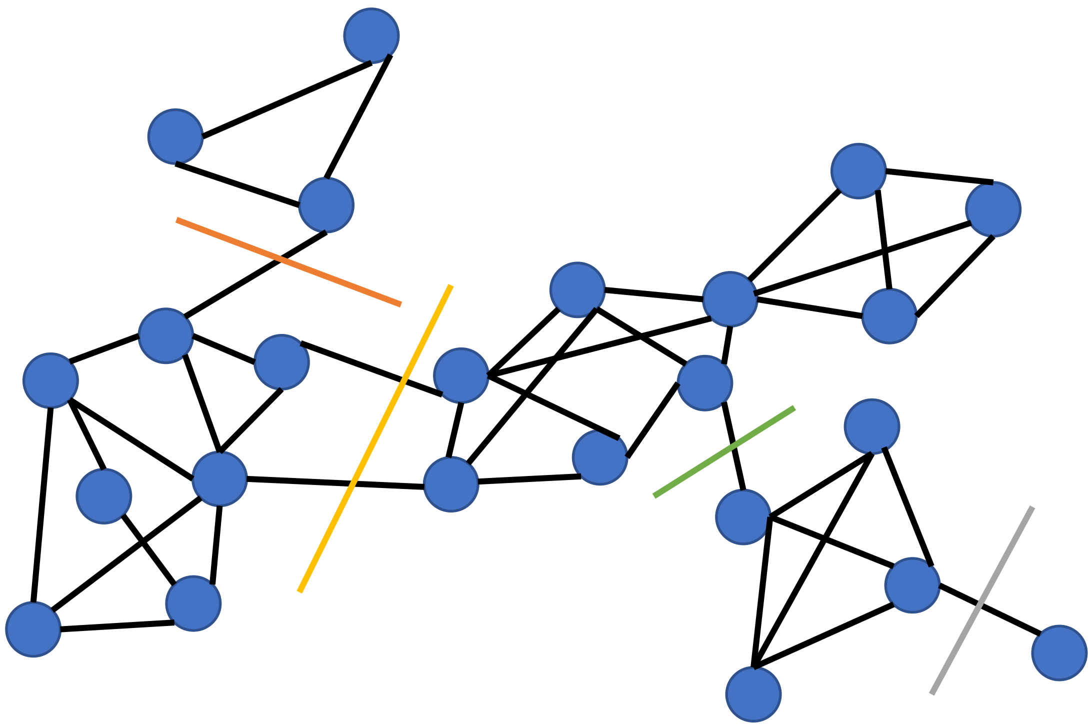
Recovering the Partitions

- Due to the relaxation, **q** can be any number (not just -1 and 1)
- How to construct the partition based on the eigenvector?
- A simple strategy :

$$A = \{i | q_i < 0\}, \qquad B = \{i | q_i \geq 0\}$$

One Obvious Drawback

- Minimum cut does not balance the size of bipartite graphs.



- How should we consider other factors like the sizes of the partitions?