Computational Tools for Data Science

Week 7:

Mining social network graphs

Recap: Graphs

- A (**simple** and **undirected**) **graph** is a pair $\boldsymbol{G} = (\boldsymbol{V}(\boldsymbol{G}), \boldsymbol{E}(\boldsymbol{G}))$.

- The set $\boldsymbol{V}(\boldsymbol{G})$ is the **vertex set** of the graph G. Its elements are the **vertices** of G (sometimes they are also called **nodes**).

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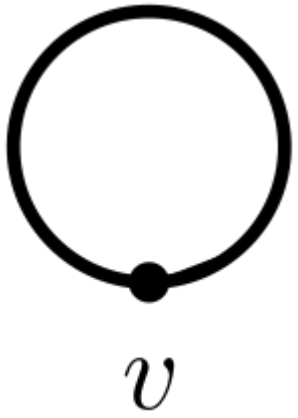
- The set $\boldsymbol{E}(\boldsymbol{G})$ is the **edge set** of G. Its elements are the **edges** of G.
  - An edge $e \in E(G)$ is a **2-element subset** of the vertex set $V(G)$.
    Hence, $e = \{u, v\}$ for some vertices $u, v \in V(G)$.
    We briefly write uv for an edge $\{u, v\}$.

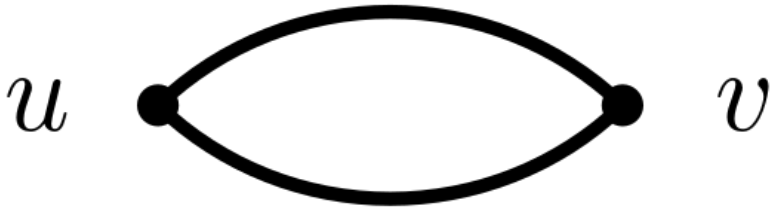
Recap: Graphs

Simple graphs:

1. **No loops:**



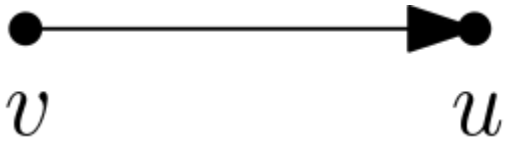
2. **No parallel edges:**



Recap: Graphs

Undirected graphs… what are **directed graphs** (briefly digraphs):

Edges are directed:



Formally, edges are no longer 2-element subsets of $V(G)$.

Model a **directed edge** $\boldsymbol{e}$ (also called **arc**) as a triple $(\boldsymbol{e}, \boldsymbol{v}, \boldsymbol{u})$, meaning that the arc e is directed from vertex v to vertex u.

Graphs as models for networks

Examples:

- Transportation network
- Electric circuits
- Many types of flows: traffic flow, electric flow …
- Phylogenetic networks (more complex than phylogenetic trees)
- Timetables and assignments with priorities (Nobel prize: Shapley)
- Internet

Social networks

Examples:

- Communication networks: telephone networks, email networks
- Financial transactions
- Collaboration networks
- Social media, e.g.:
  - Facebook → **friends relation** corresponds to **undirected edge**
  - Twitter → **follow relation** corresponds to **directed edge**
- (Internet)

Modelling social networks via graphs

1. Vertices correspond to network participants:
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3. **Locality property**

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If A is related to B and B is related to C, then the probability of A and C being related is higher than the average.

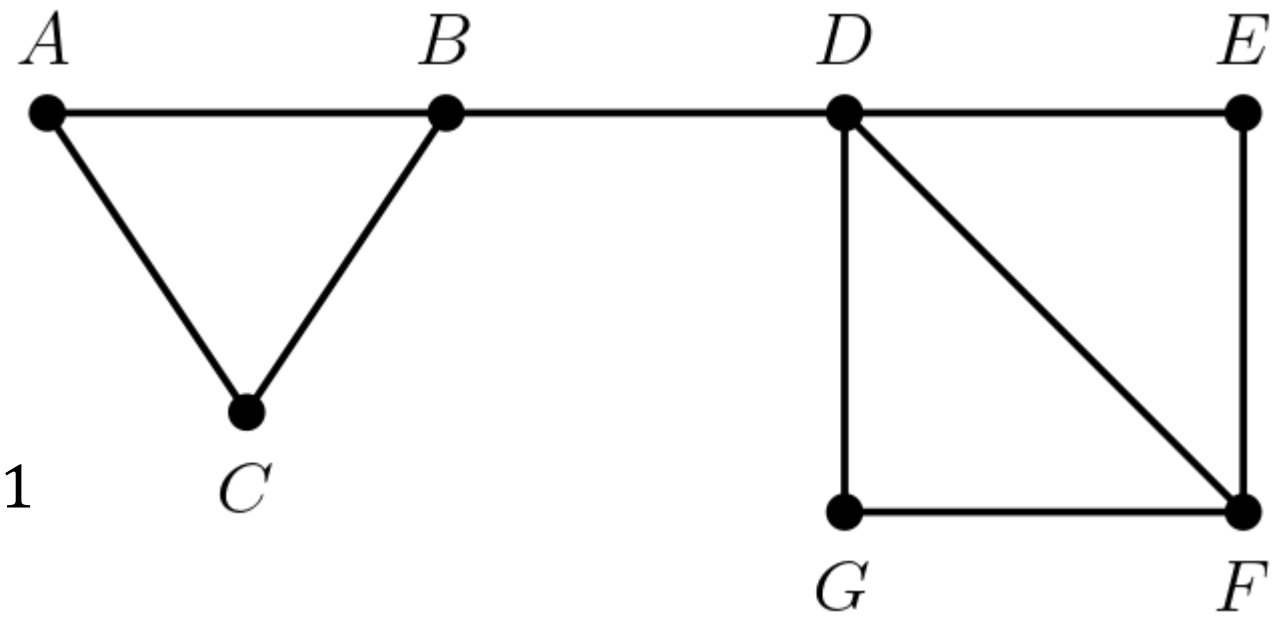
Modelling social networks via graphs

Example

$$|E(G)| = 9$$

$$|V(G)| = 7$$

$$\left|\binom{V(G)}{2}\right| = \binom{7}{2} = 21$$



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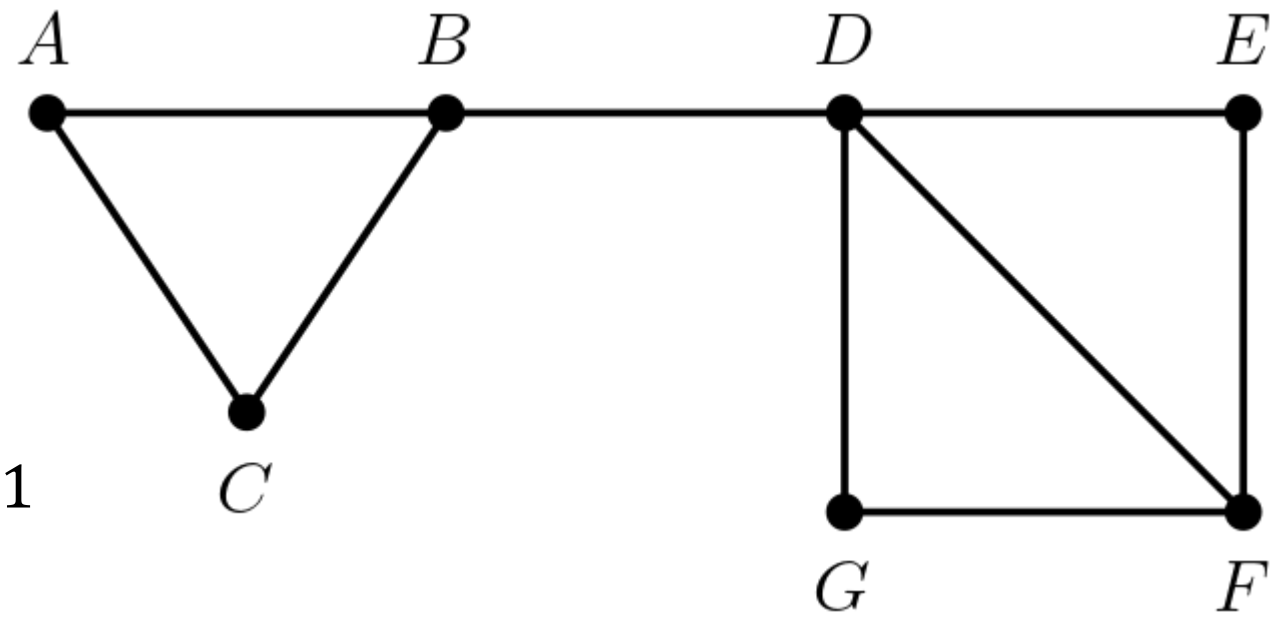

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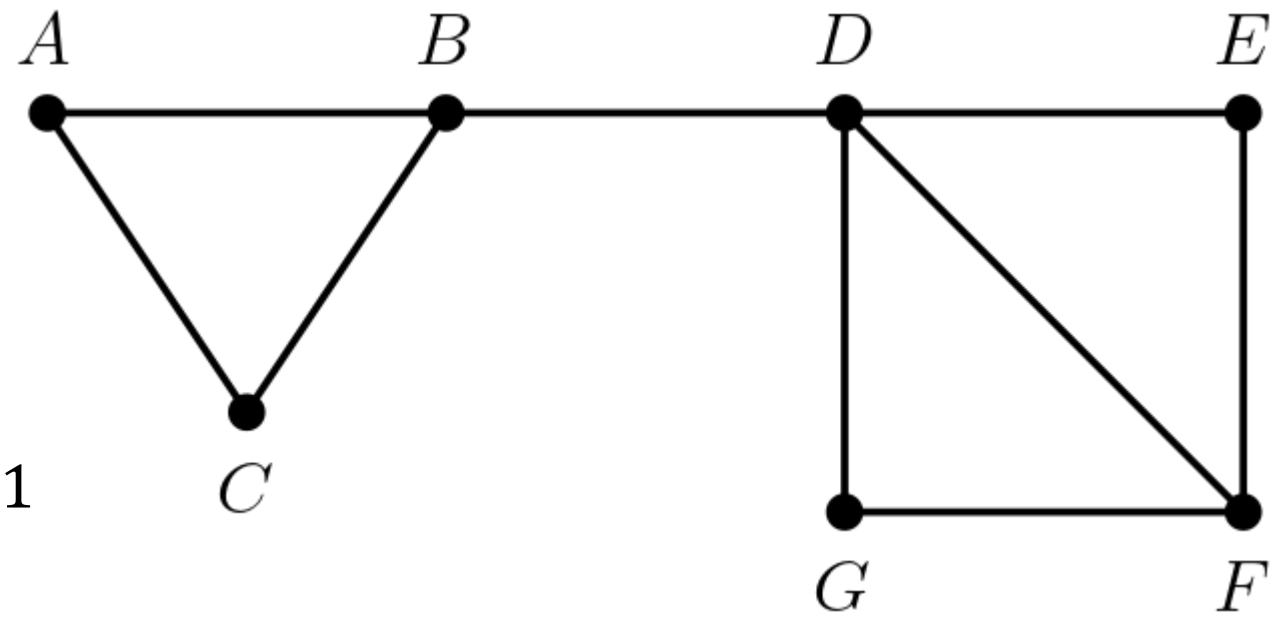

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Random: probability for $\{X, Z\} \in E(G)$: $\frac{|E(G)|-2}{\left|\binom{V(G)}{2}\right|-2} = \frac{7}{19} \approx 0{,}368$

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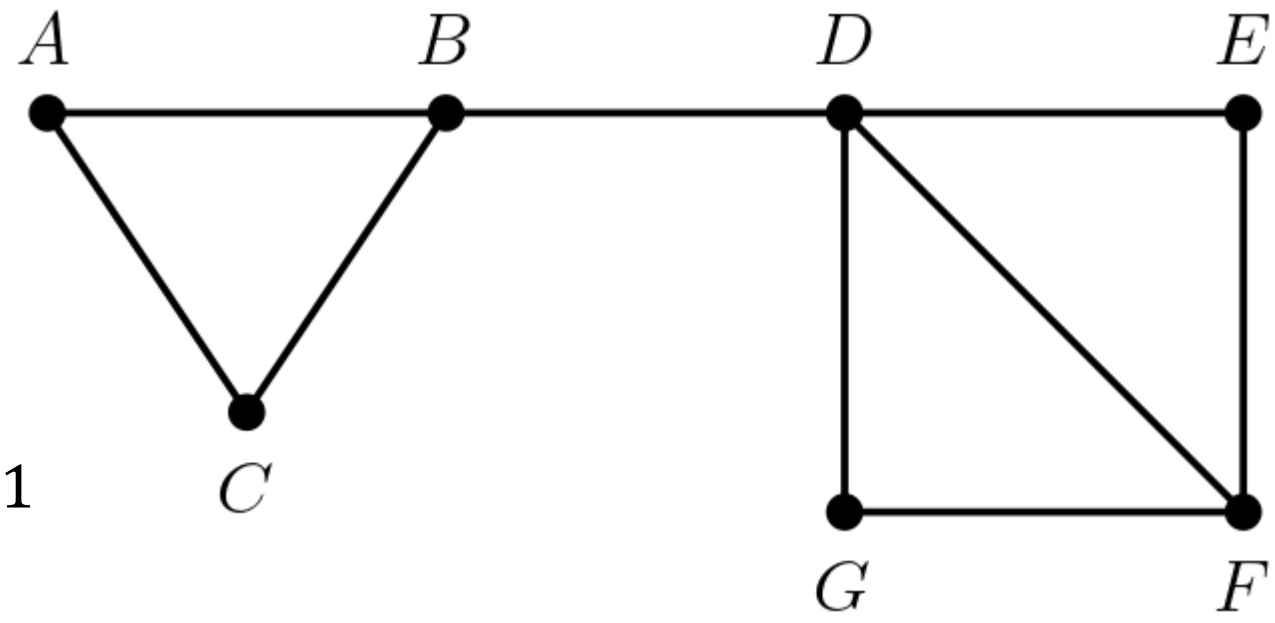

Suppose $\{X, Y\}, \{Y, Z\} \in E(G)$. Check $\{X, Z\}$:

Actually: If $Y = A$, then $\{X, Z\} = \{B, C\}$. Fits locality.

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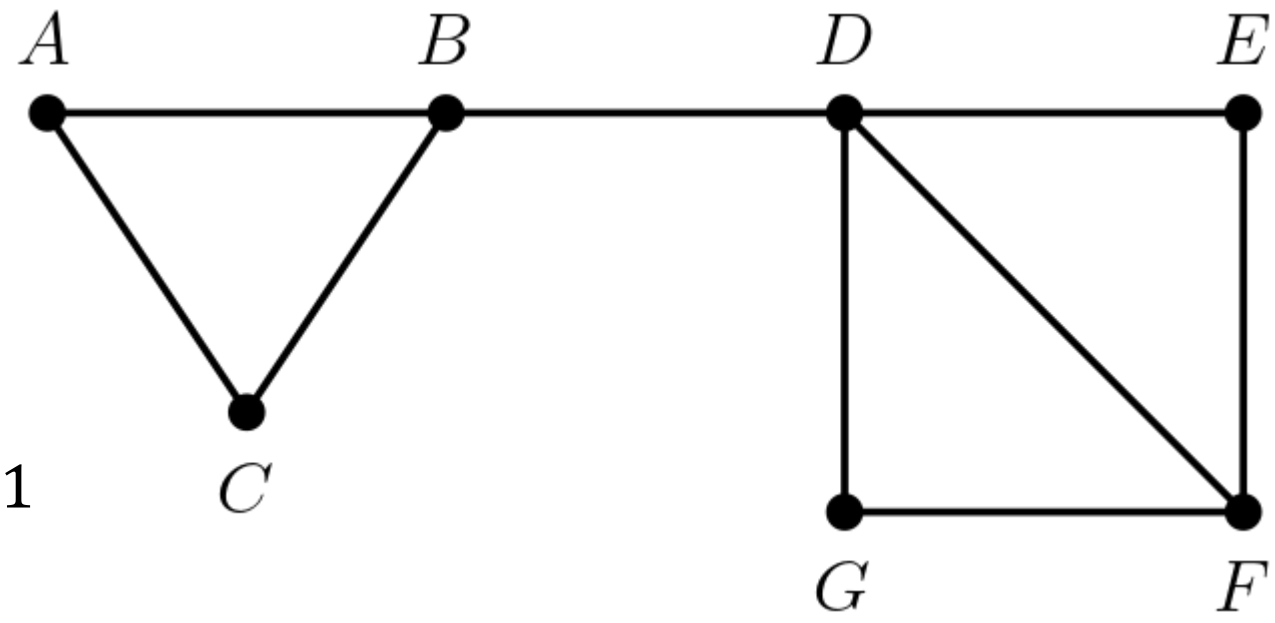

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Actually: Same for $Y = C, G, E$

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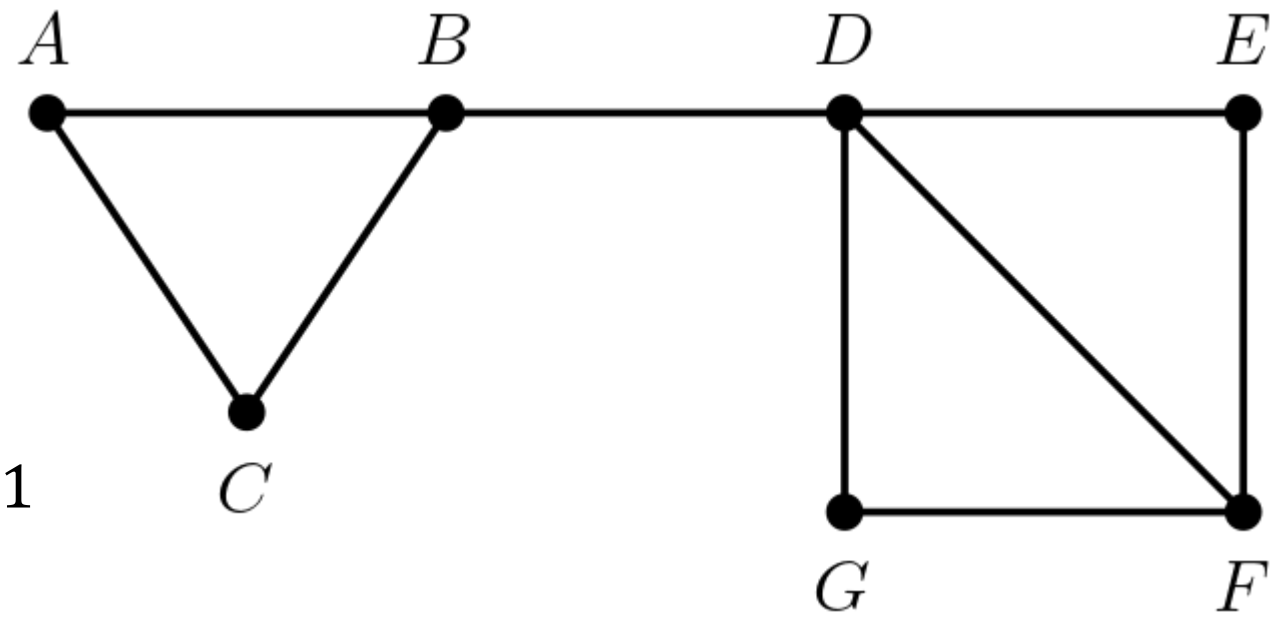

Suppose $\{X, Y\}, \{Y, Z\} \in E(G)$. Check $\{X, Z\}$:

Actually: If $Y = F$, then $\{X, Z\} = \{D, G\}$ and $\{X, Z\} = \{D, E\}$ fit locality.

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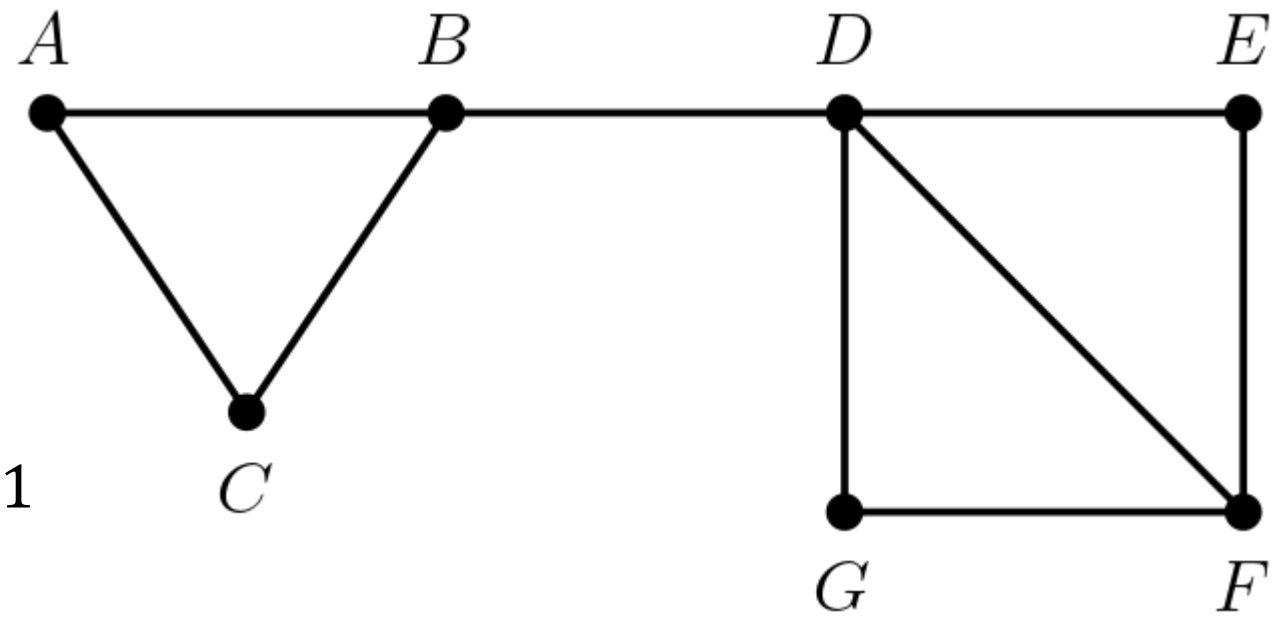

Suppose $\{X, Y\}, \{Y, Z\} \in E(G)$. Check $\{X, Z\}$:

Actually: If $Y = F$, $\{X, Z\} = \{E, G\}$ violates locality.

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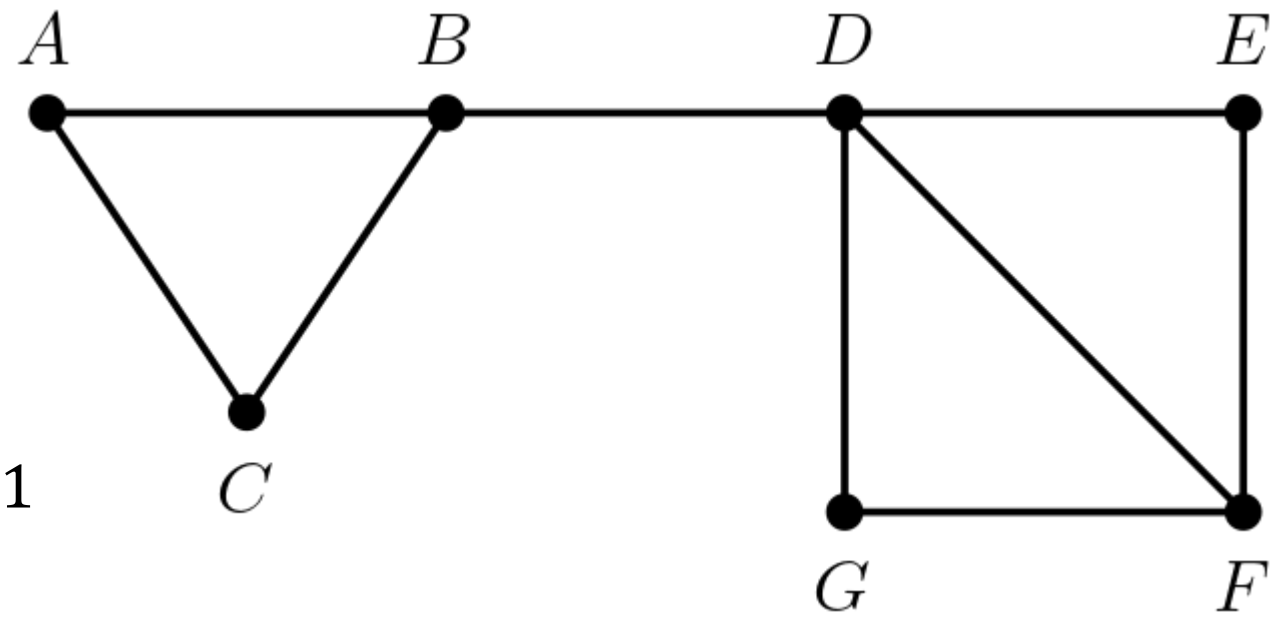

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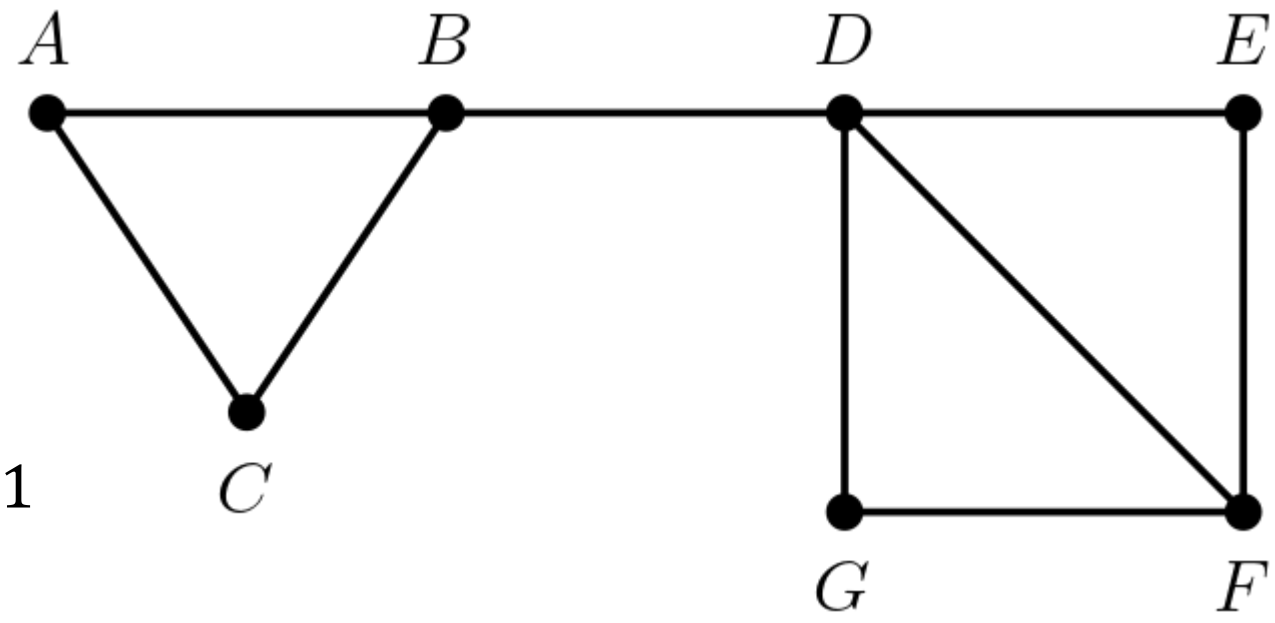

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Suppose $\{X, Y\}, \{Y, Z\} \in E(G)$. Check $\{X, Z\}$:

Actually: If $Y = B$: 3 neighbours, only 2 of them adjacent. **7 vs. 3**

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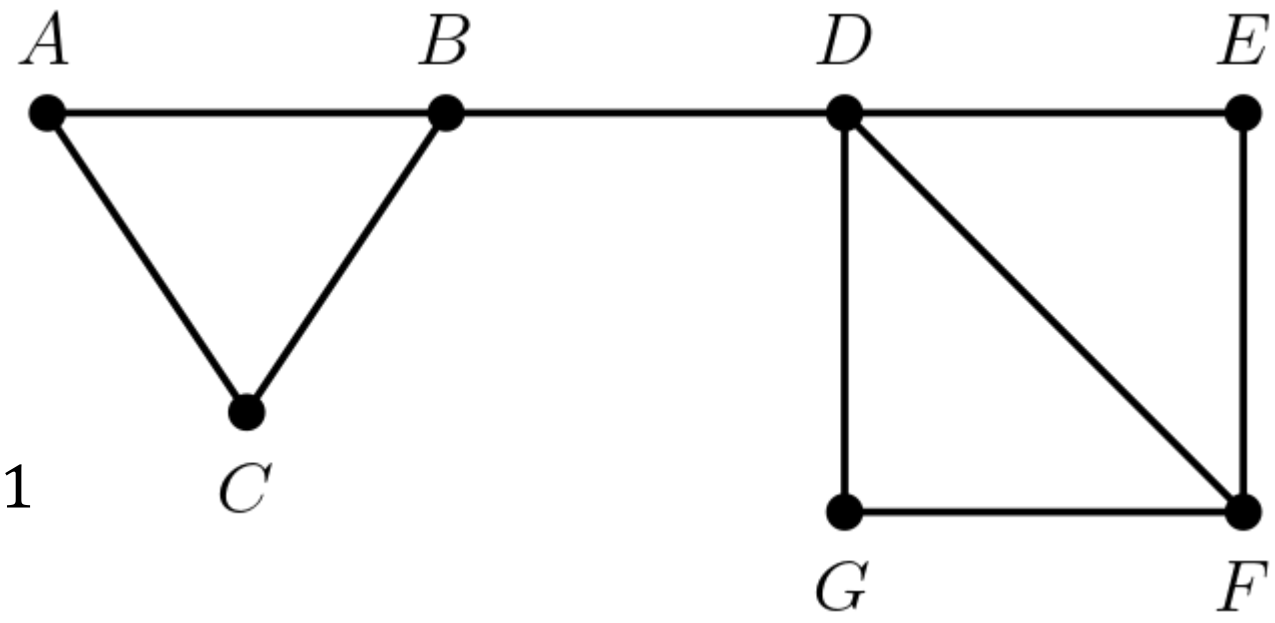

Suppose $\{X, Y\}, \{Y, Z\} \in E(G)$. Check $\{X, Z\}$:

Actually: If $Y = D$: 4 neighbours, 2 pairs of them adjacent. **9 vs. 7**

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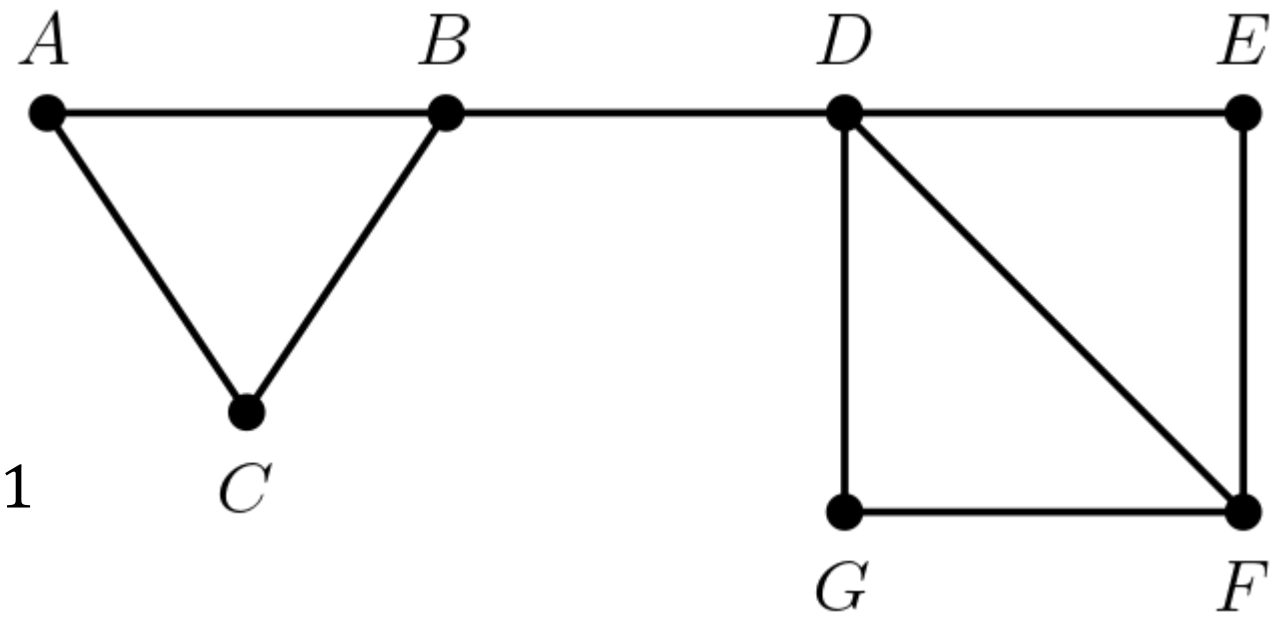

Suppose $\{X, Y\}, \{Y, Z\} \in E(G)$. Check $\{X, Z\}$:

Actually: Fraction the number of times edge $\{X, Z\}$ exists: $\frac{9}{9+7} \approx 0{,}563$

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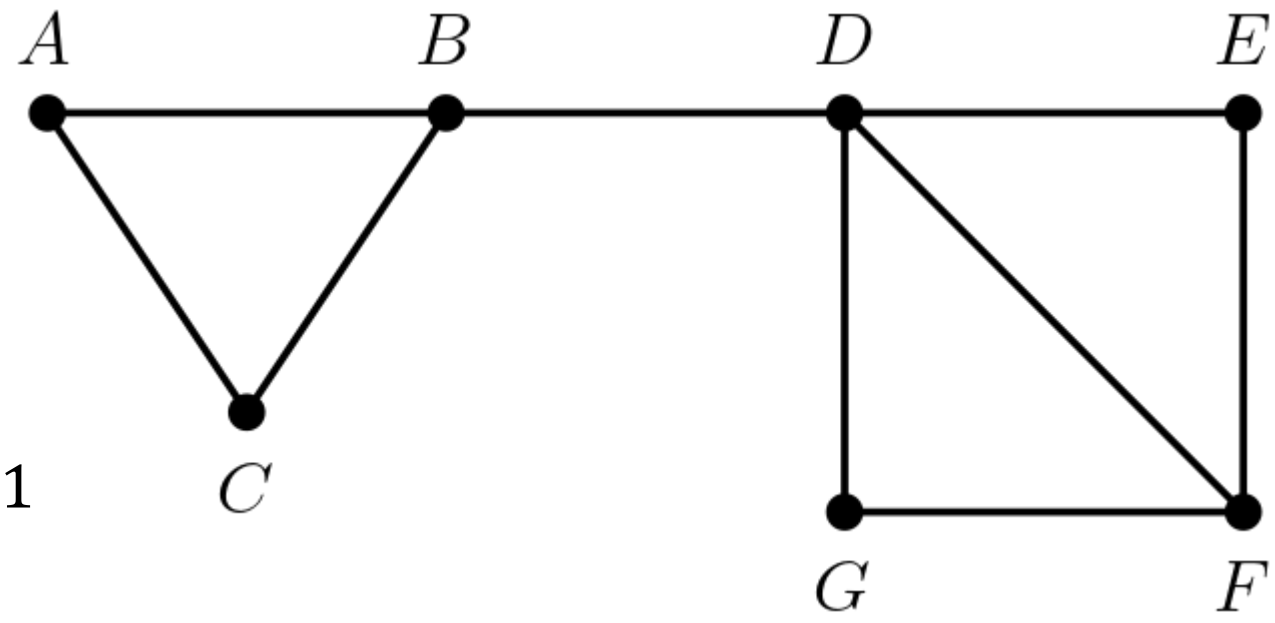

Conclusion: $0{,}563 \gg 0{,}368$. So locality property holds. The graph might be suitable to model a social network.

Clustering (partitioning) social network graphs

Problems with previously introduced clustering tools.

Examples:

1. Agglomerative hierarchical clustering

2. Point assignment tools (e.g. k-means)

Problems with agglomerative clustering

Let $u, v \in V(G)$. The usual **distance** function d on a graph is:

$$d(u,v) = length\ of\ \boldsymbol{shortest\ path}\ between\ u\ and\ v\ in\ G$$

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Hence, we **always** merge two clusters (or vertices) that are directly connected by an edge (yielding shortest possible distance, namely 1).

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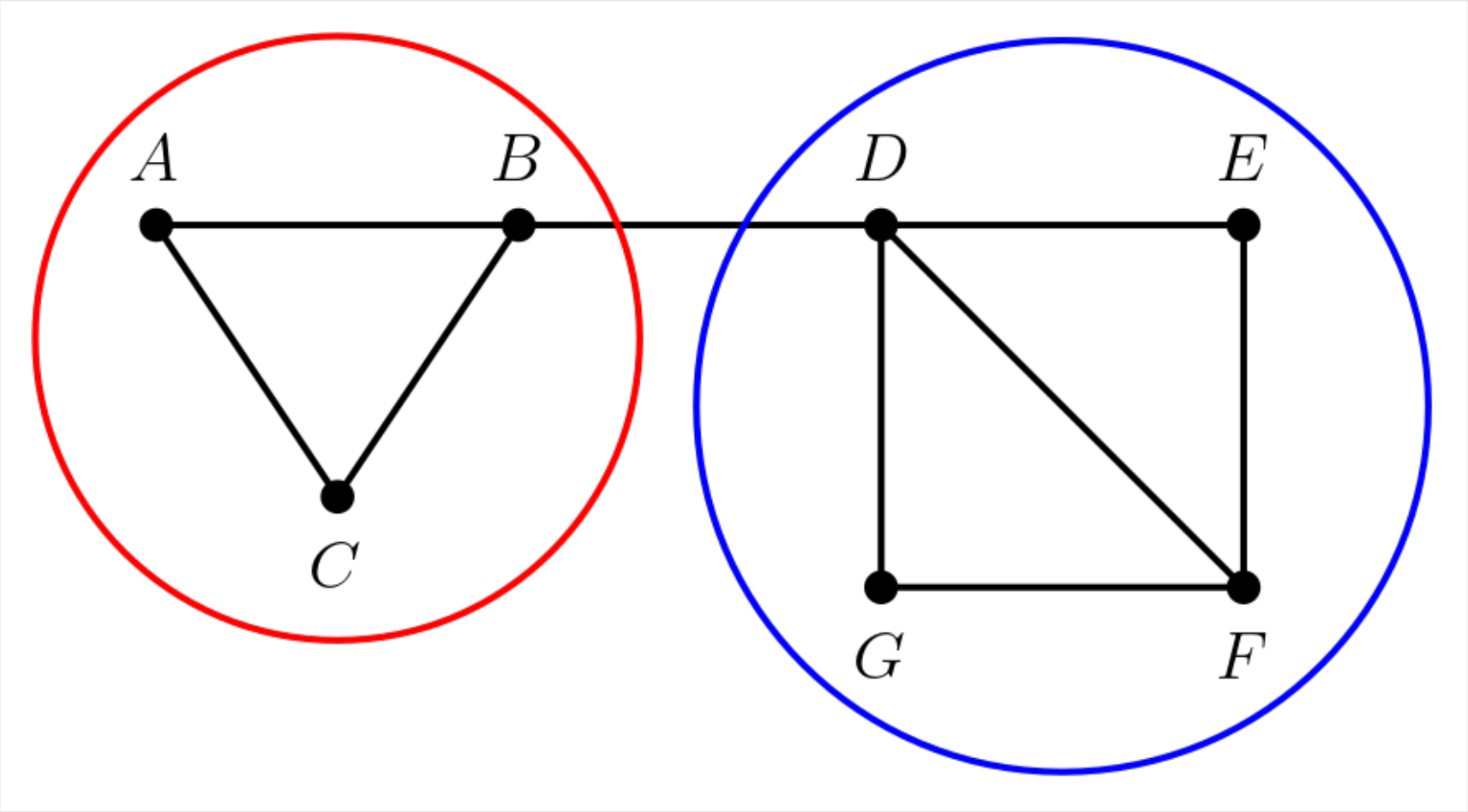

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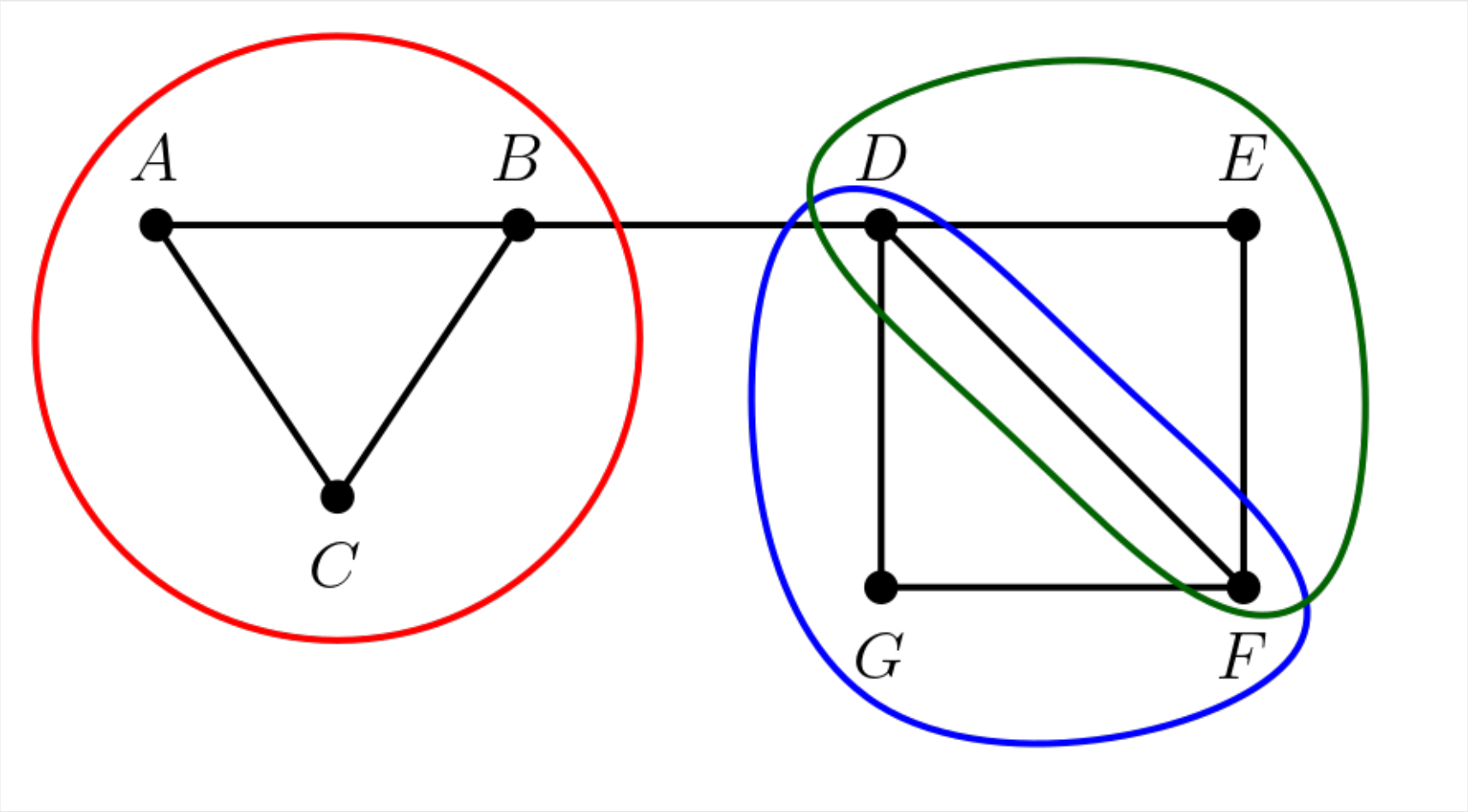

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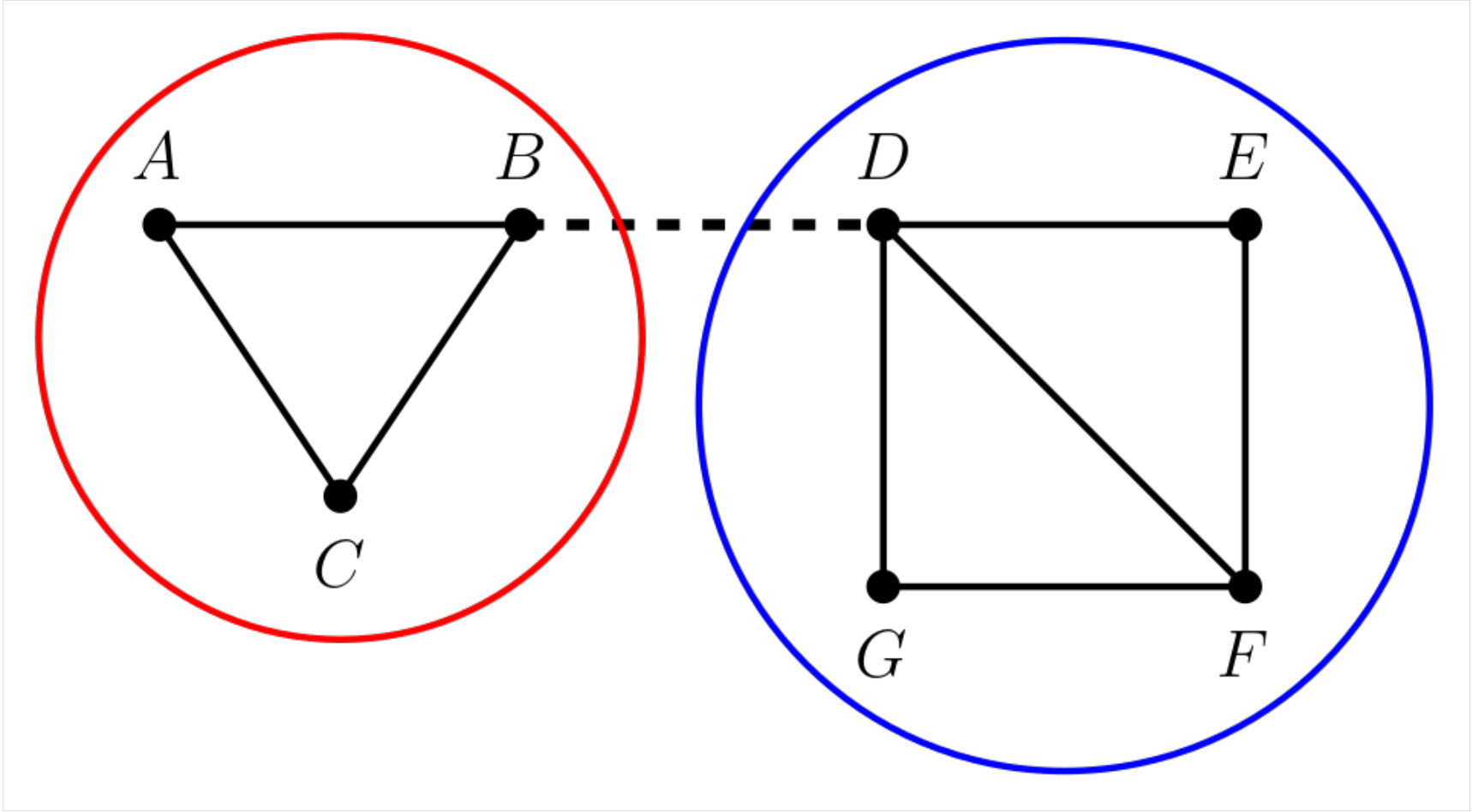

Problems with agglomerative clustering

- Let $e \in E(G)$ whose end vertices lie in different clusters C_1^e, C_2^e. In each merging step, the probability of merging the clusters C_1^e and C_2^e is the same for each such edge e.

- At some point (maybe even initially) it becomes likely that we merge two clusters that should not be combined.

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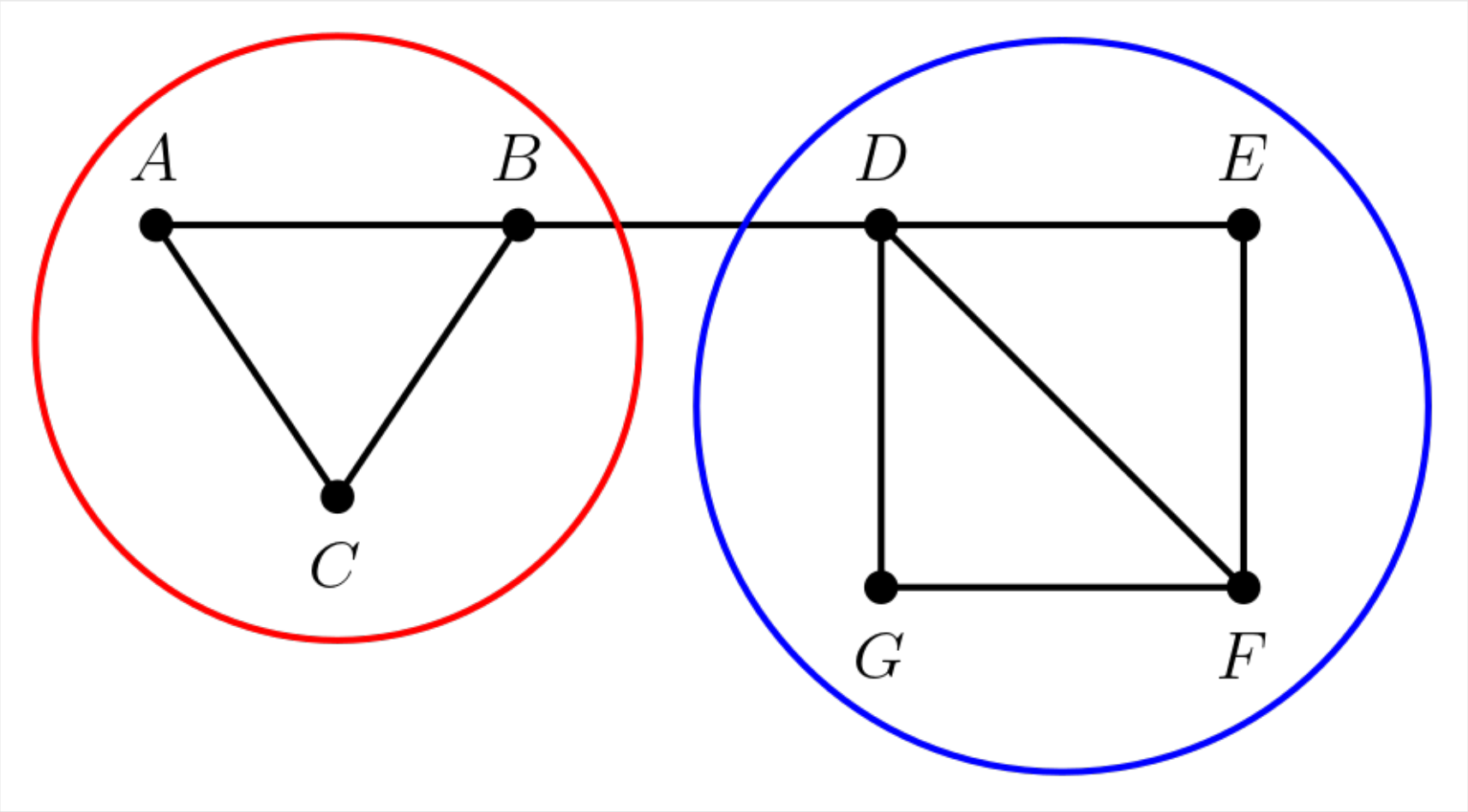
- (We might **prevent this by more sophisticated methods**, e.g. only merge / stop merging when density / cohesion becomes too low, but the **naïve approach is not suitable**.)

Problems with point assignment (e.g. k-means)



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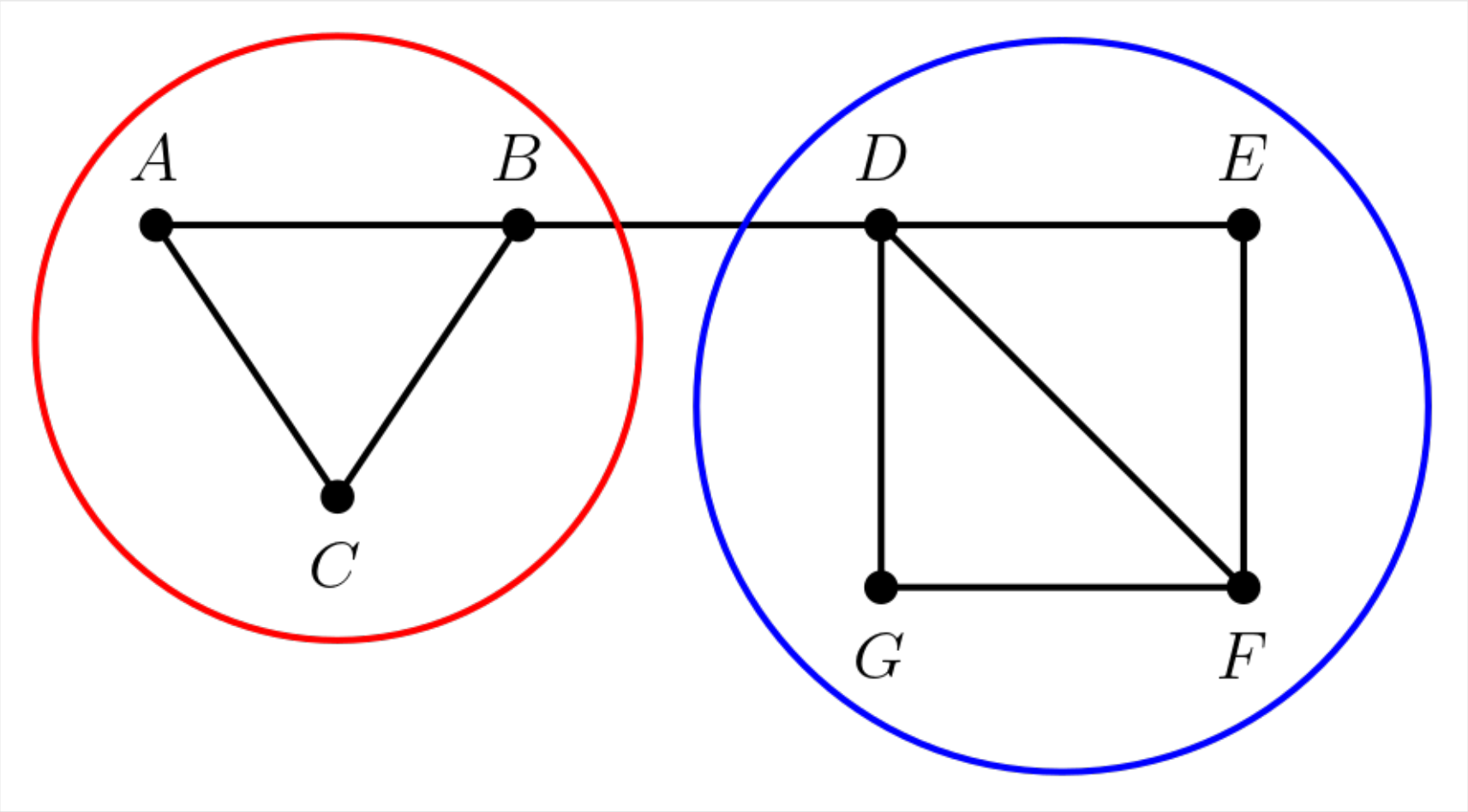

Problems with point assignment (e.g. k-means)

- Say we set $k = 2$ (fitting to our example graph).
- Say our first 2 clustroids are B (at random) and F (far apart from B).
- A and C are assigned to B's cluster.
- E and G are assigned to F's cluster.
- Assigning D to B's or F's cluster is equally reasonable.
  - Hence, with probability 0,5 vertex D ends up in the wrong cluster.

Betweenness

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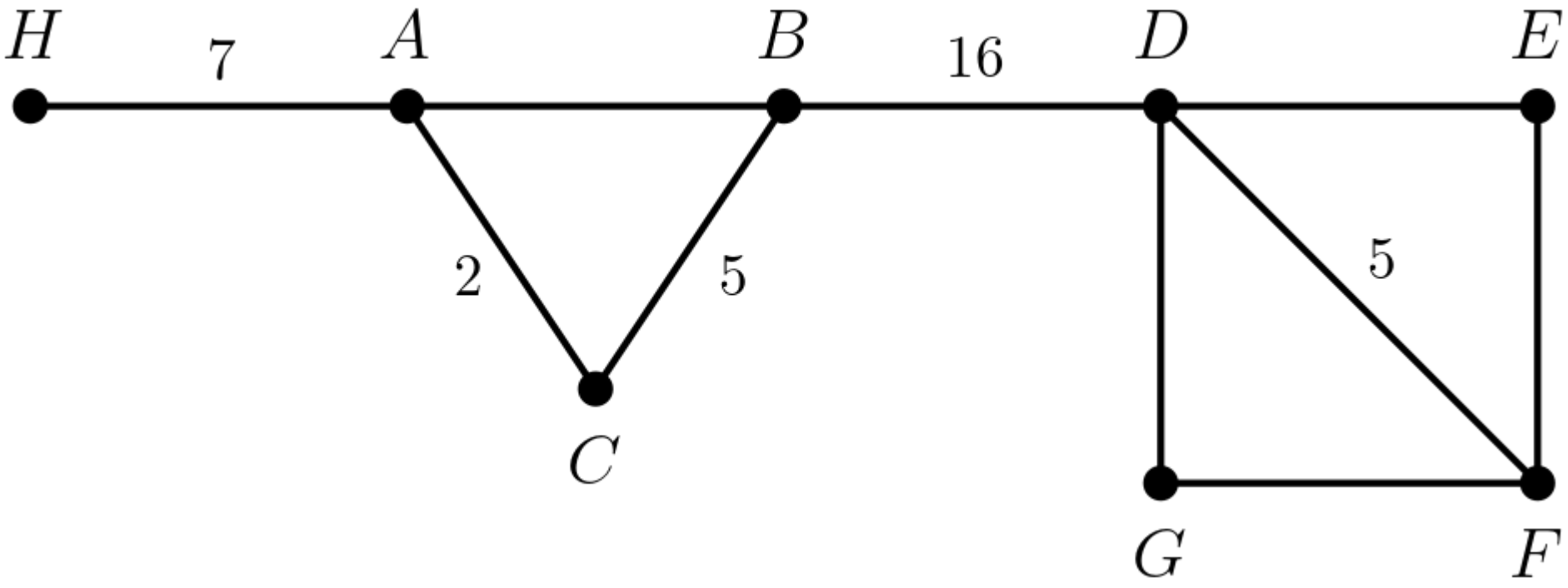
Idea: High betweenness indicates:

1. An edge/vertex of G where many paths must run through (hence, maybe low connectivity).
2. A central position for the edge/vertex, otherwise not many paths.

Betweenness centrality for edges



Divisive hierarchical clustering via betweenness: Girvan-Newman Algorithm

- Start with one cluster (if our initial graph G is **connected**).
- In each step, we consider a subgraph H of G and the clusters correspond to **connected components** of H.

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  - If deletion of the edges does not disconnect a cluster, keep it.

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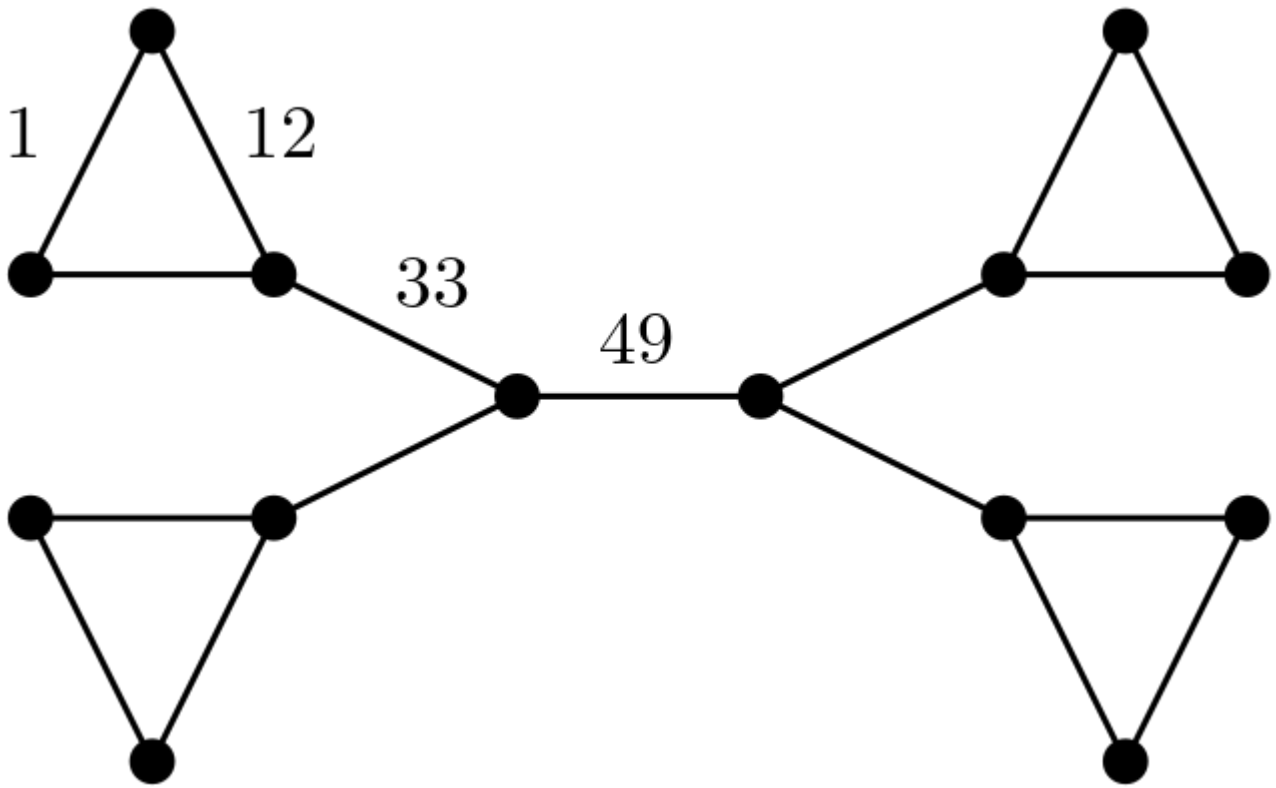

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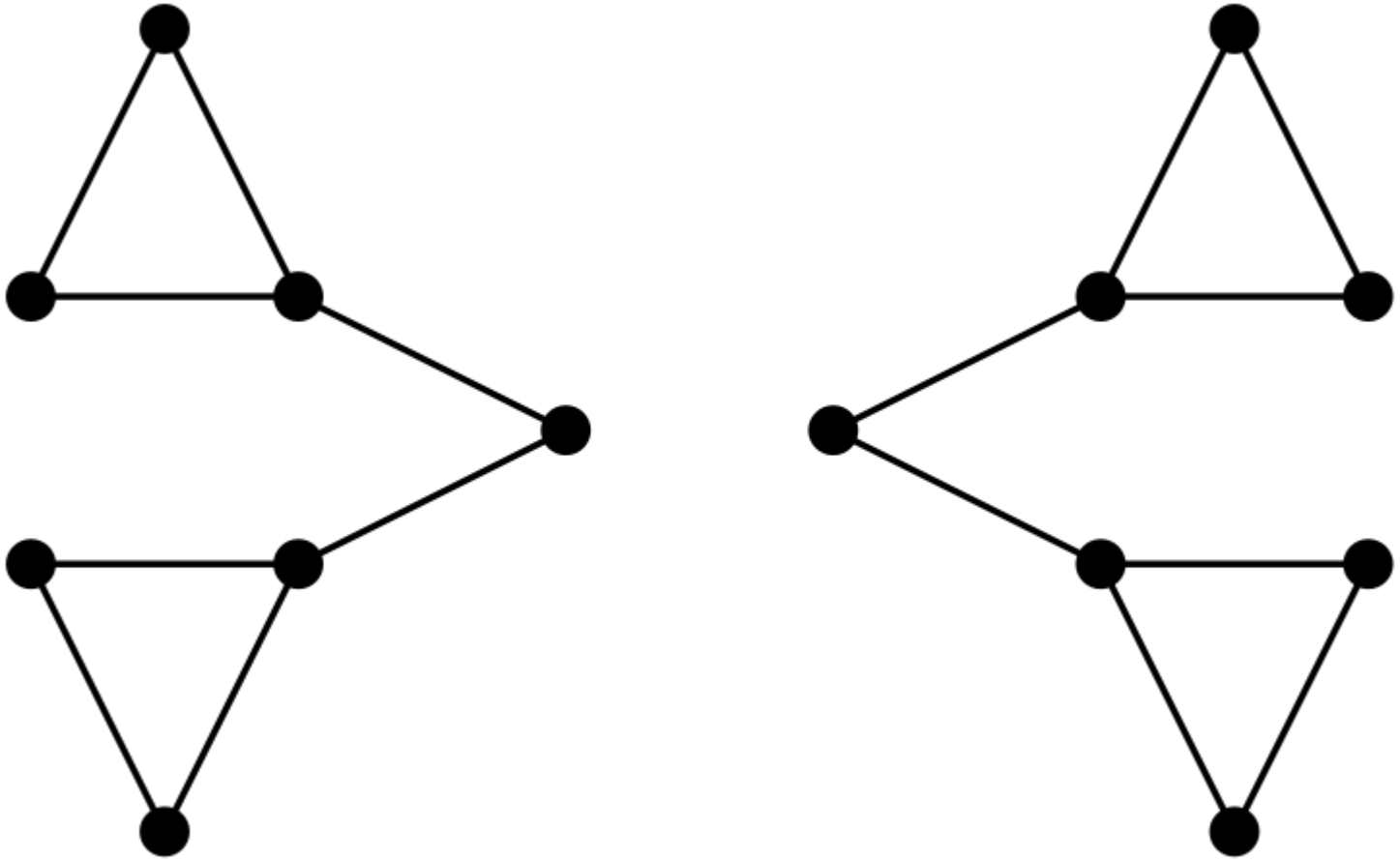

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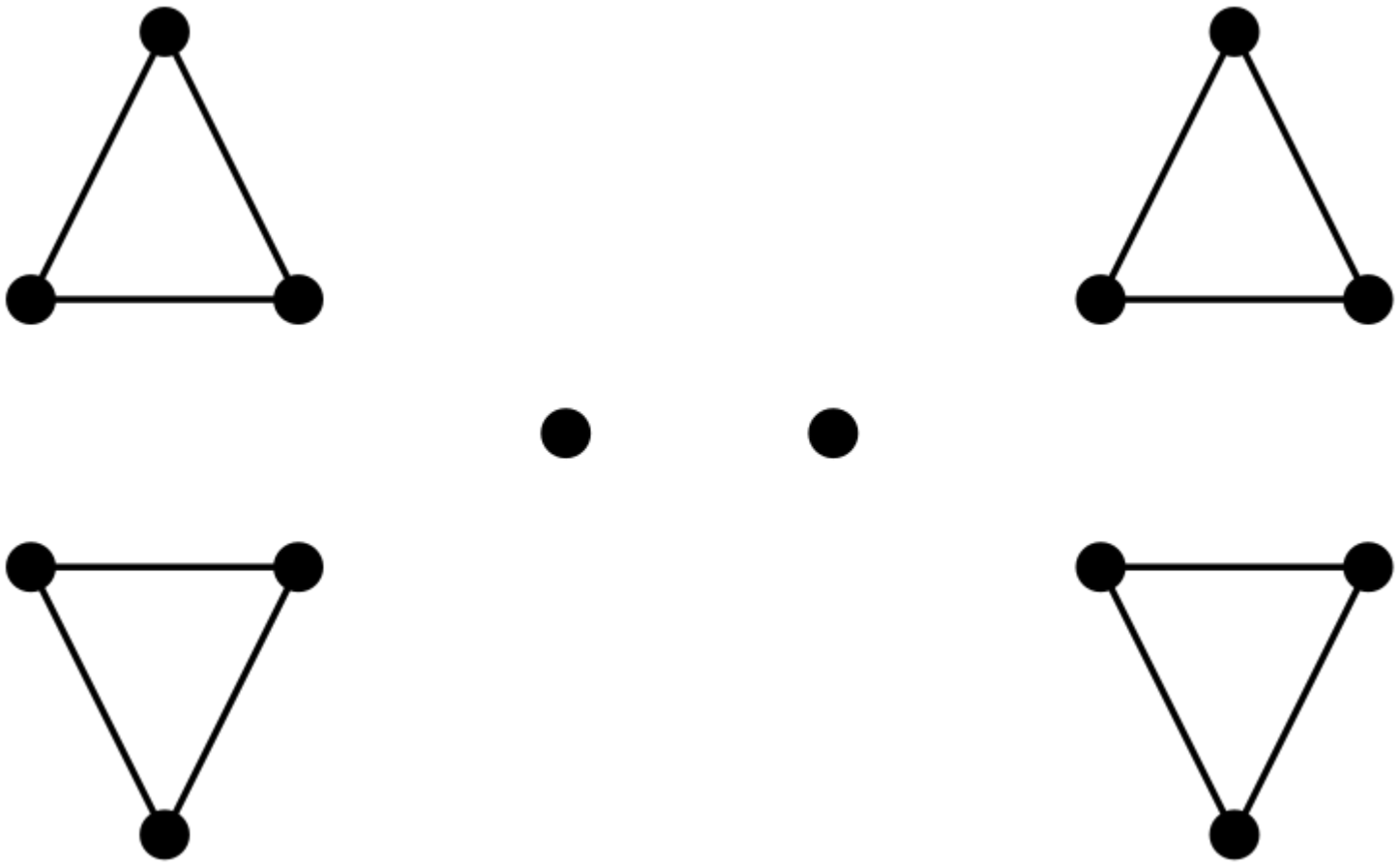

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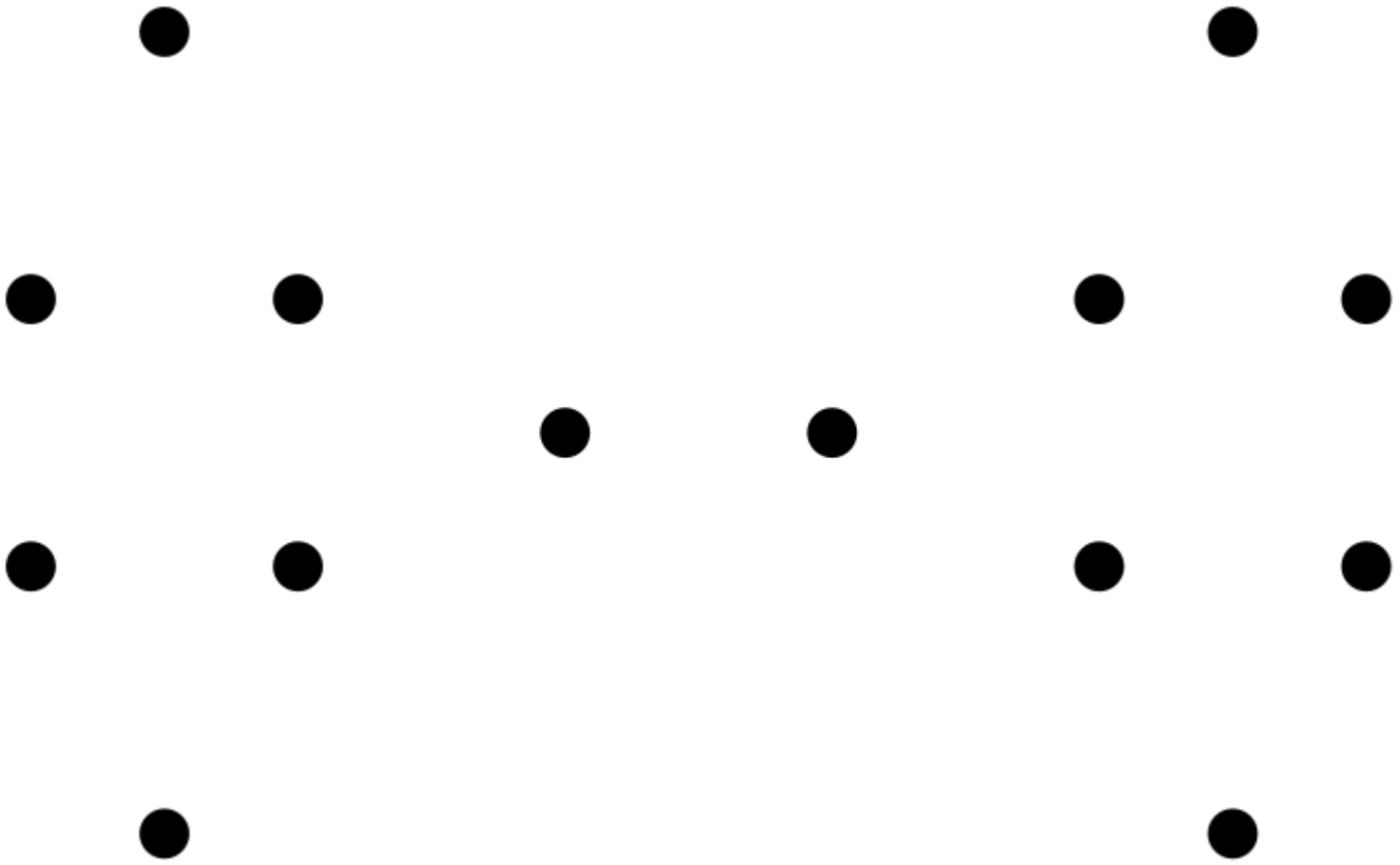

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- **Girvan-Newman Algorithm**
  - Count shortest paths from a given start vertex.
    - This is done in 3 steps.
  - We repeat this for every vertex.
    - Eventually, we will have counted each shortest path twice.

Computing betweenness for edges: Step 1

- Let G be the given graph with $|V(G)| = n$ and $|E(G)| = m$ for some $m, n \in \mathbb{N}$. We **fix a vertex** of G, call it $\boldsymbol{r}$.

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- In other words: we store **no edges** whose end vertices lie in the **same distance class** w.r.t. r, but **all edges** whose end vertices lie in **different distance classes** w.r.t. r.
- The **running time** of BFS is $\boldsymbol{O(m)}$.

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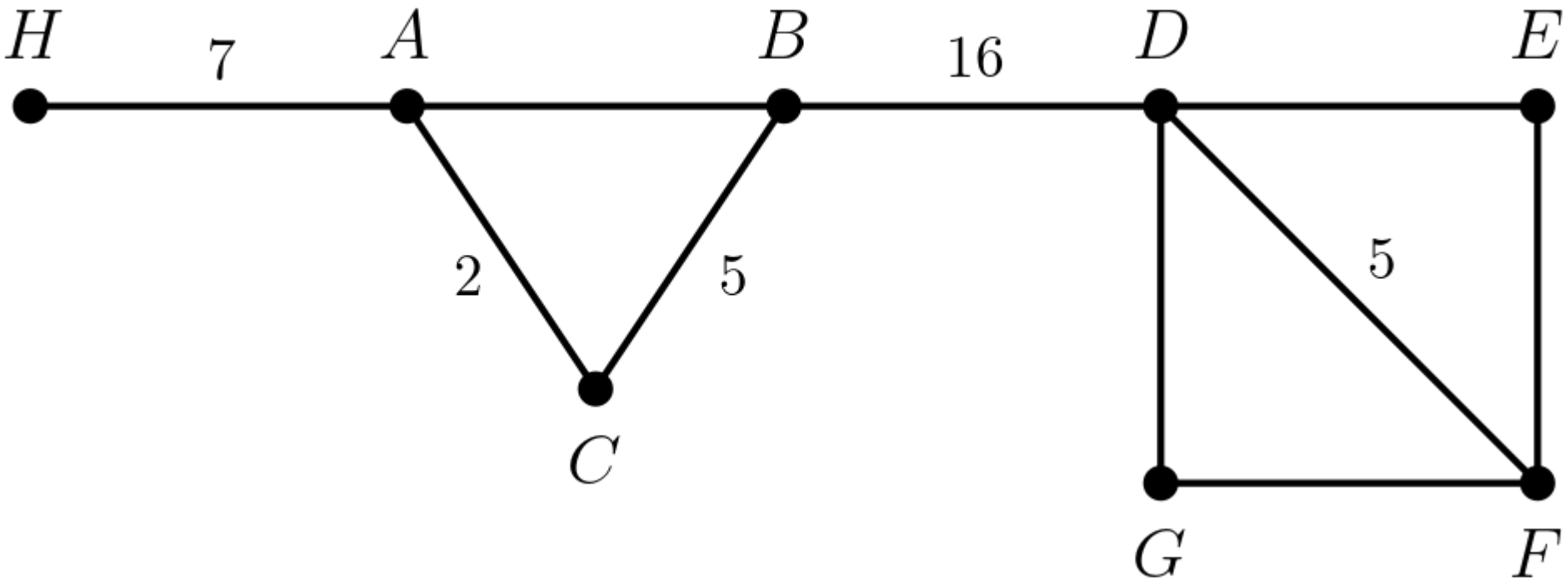

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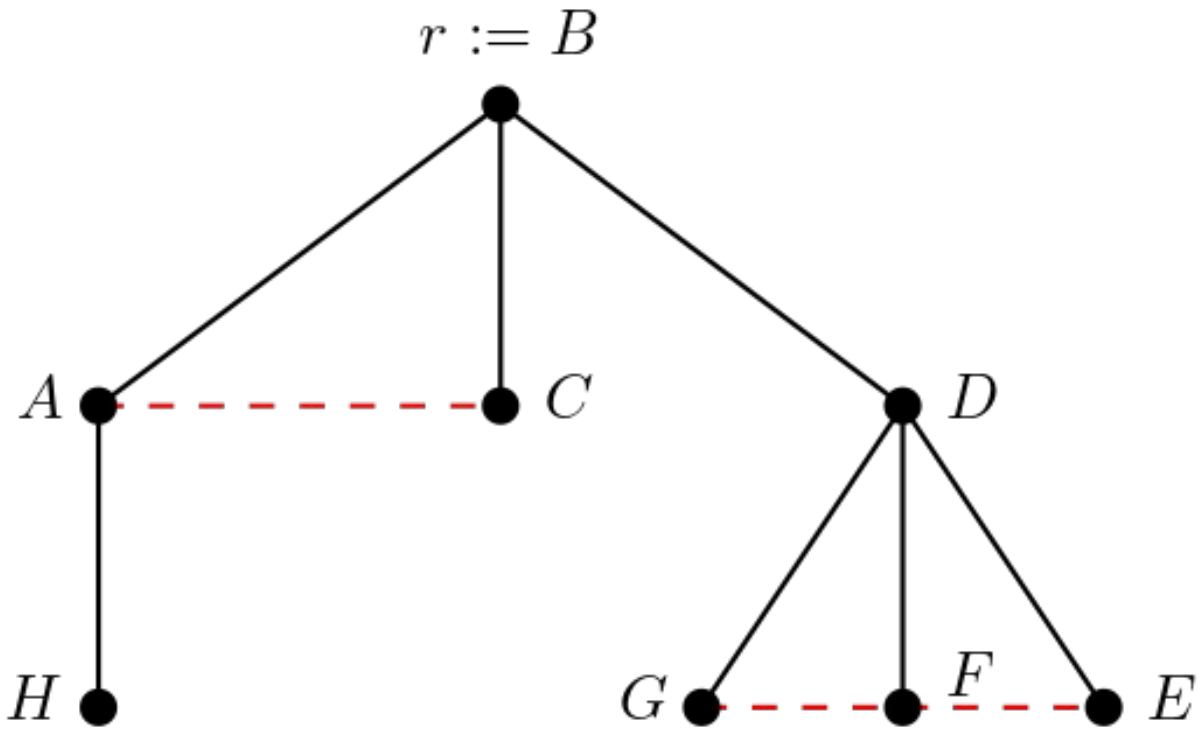

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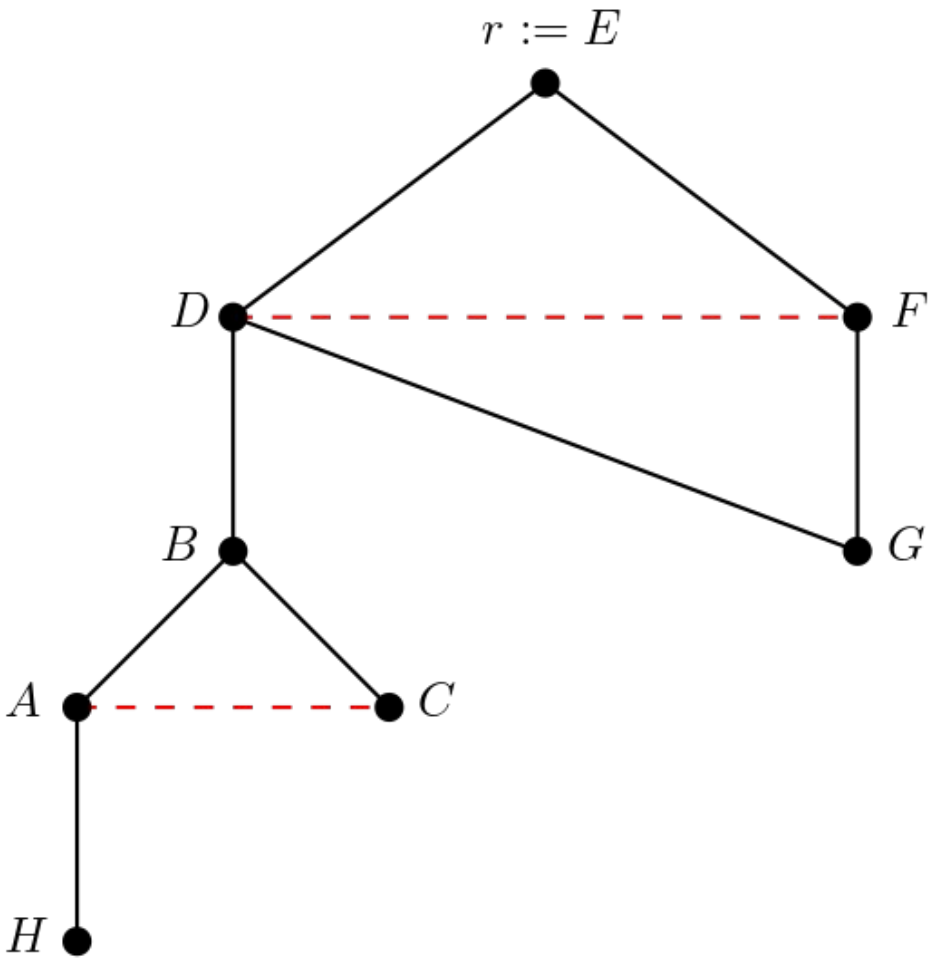

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$$\ell_2(v) := \sum_{\substack{w \in D_{i-1} \\ vw \in E(G)}} \ell_2(w)$$

Hence, we label top (from root r) down along the distance classes.

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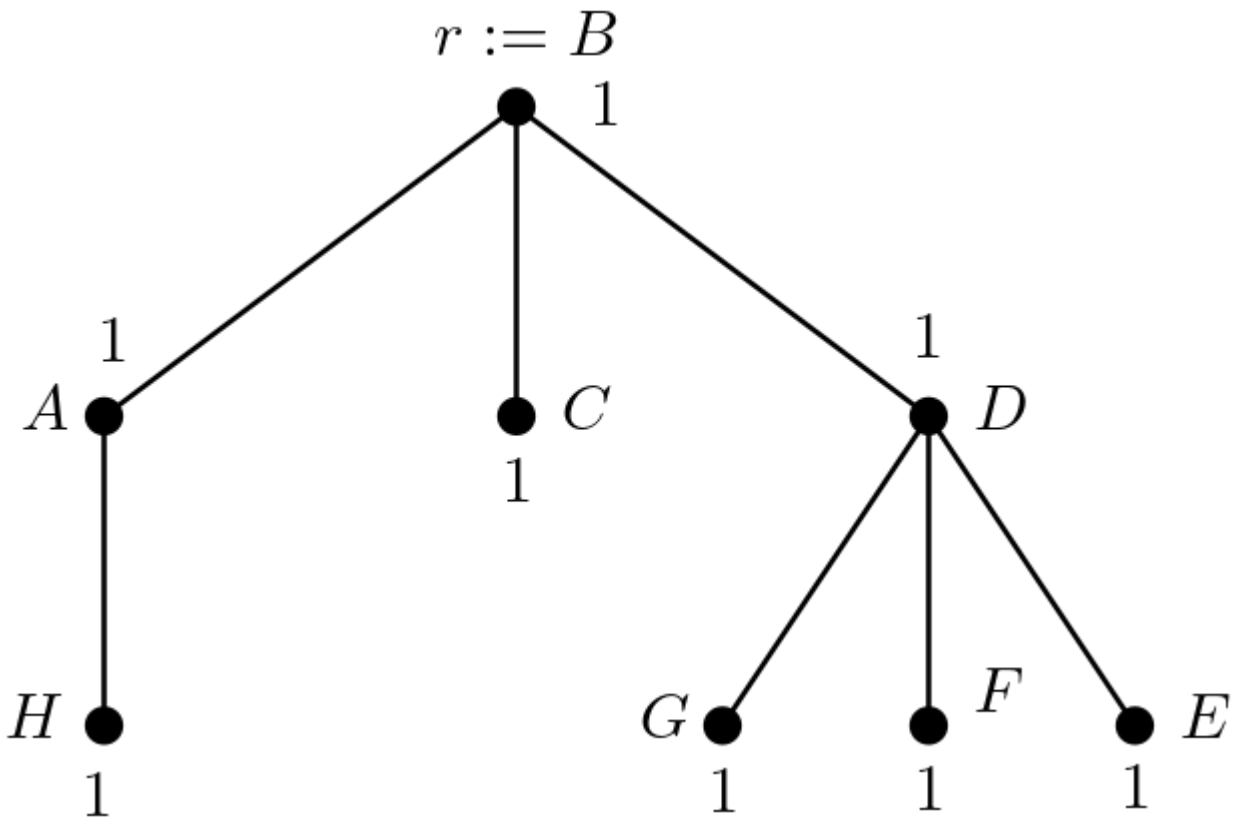

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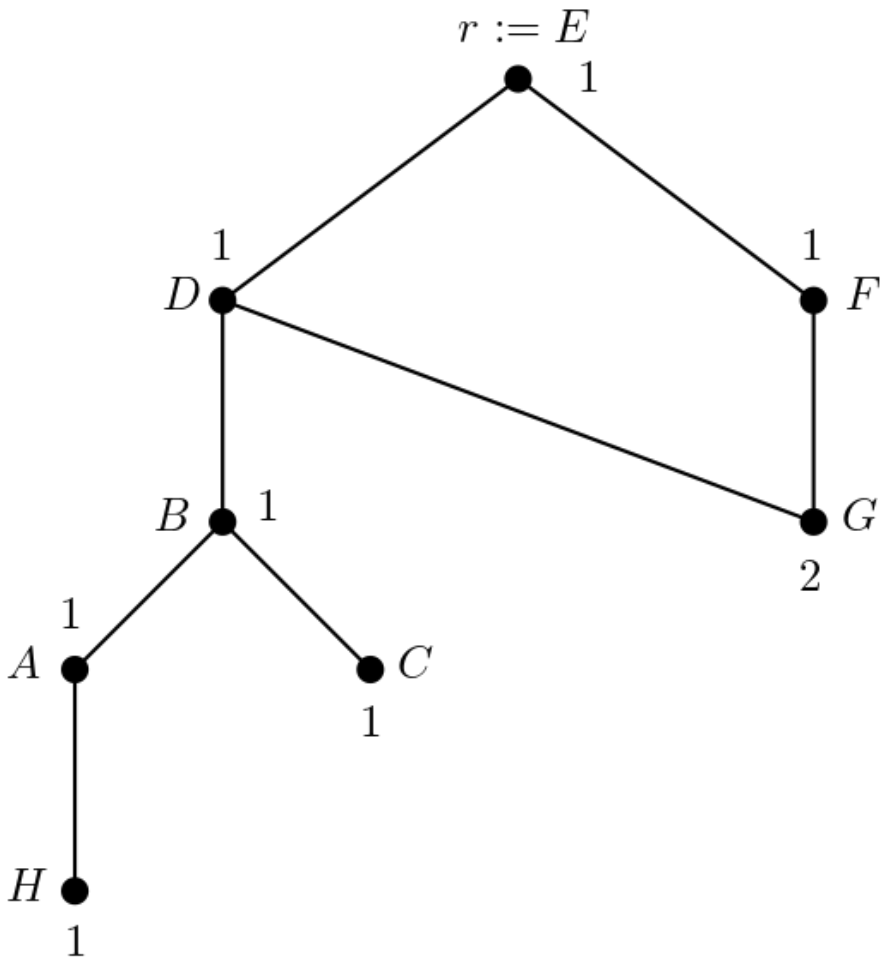

Computing betweenness for edges: Step 3

Label each edge e with the following count $b_r(e)$:

$$b_r(e) = \sum_{y \in V(G)} \frac{\#\ shortest\ r - y\ paths\ that\ use\ e}{\#\ all\ shortest\ r - y\ paths}$$

To label all edges with this count, we use another auxiliary labelling ℓ_3 for the vertices.

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- Think of ℓ_3 and b_r as demand and flow.
- **BUT** instead of Kirchhoff's law, each vertex consumes a flow of 1.

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- How is the total flow (-1) which enters a vertex w split among the edges vw that enter w:
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- Let $w \in D_{i+1}$ and let $v_1, \dots, v_k$ be the neighbours of w in D_i. Let ℓ_2 denote the labelling we have assigned in Step 2. Now label each edge $v_j w$ by

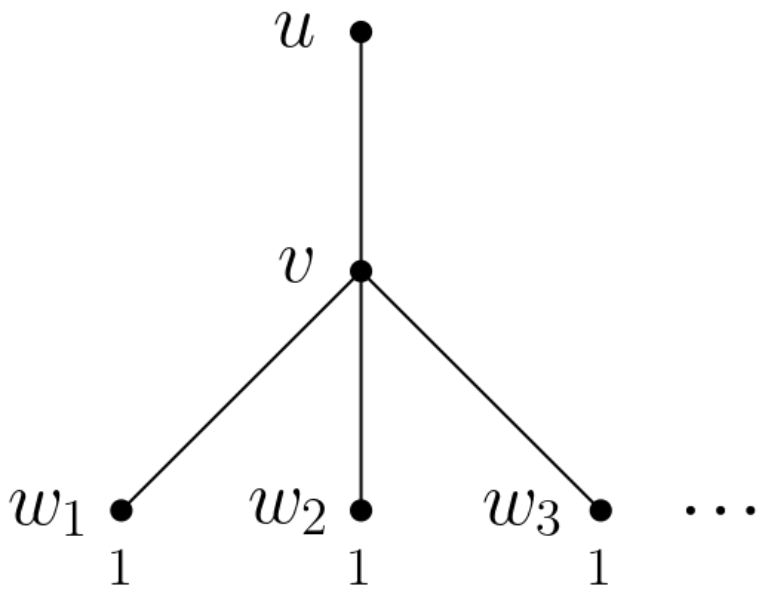
$$b_r(v_j w) := \ell_3(w) \cdot \frac{\ell_2(v_j)}{\sum_{p=1}^{k} \ell_2(v_p)} = \ell_3(w) \cdot \frac{\ell_2(v_j)}{\ell_2(w)}$$

Computing betweenness for edges: Step 3

- Let $\ell_3(w_i) = 1$.

- $b_r(vw_i) = 1 \cdot \frac{\ell_2(v)}{\ell_2(w_i)}$

So $b_r(vw_i)$ really counts the fraction of all r-w_i paths that use the edge vw_i.



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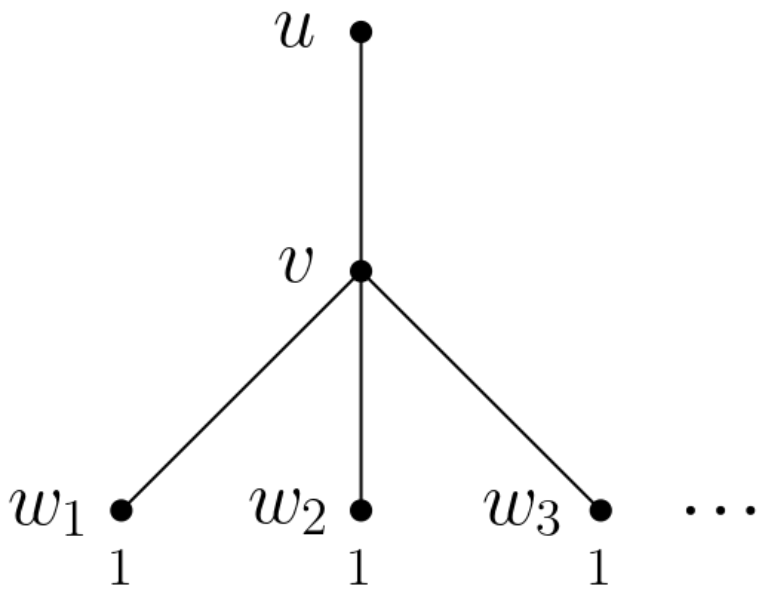

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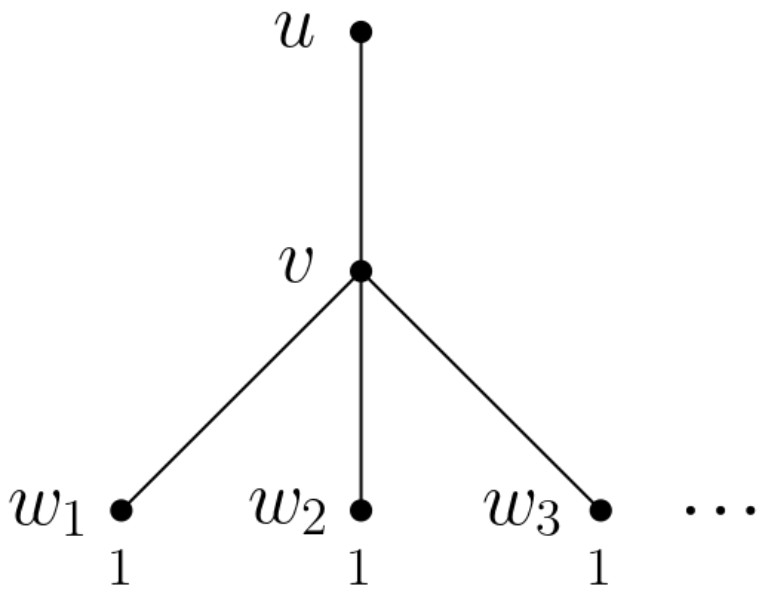

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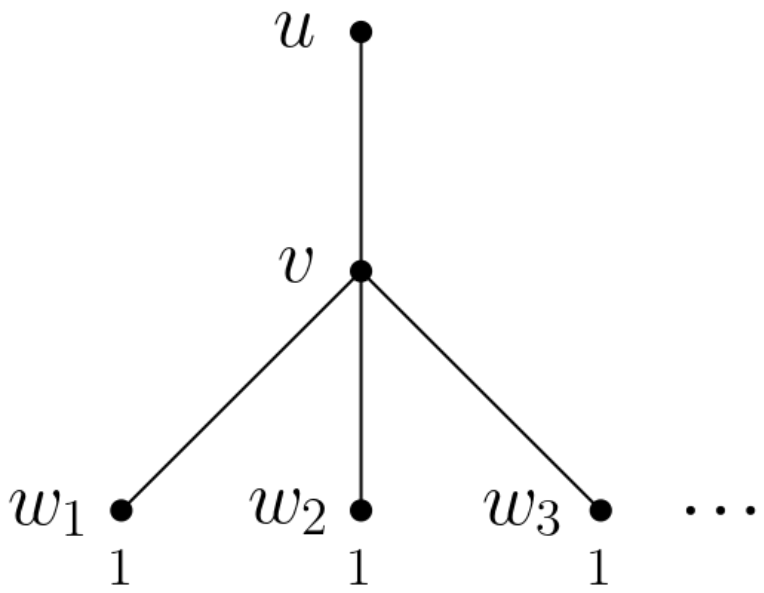

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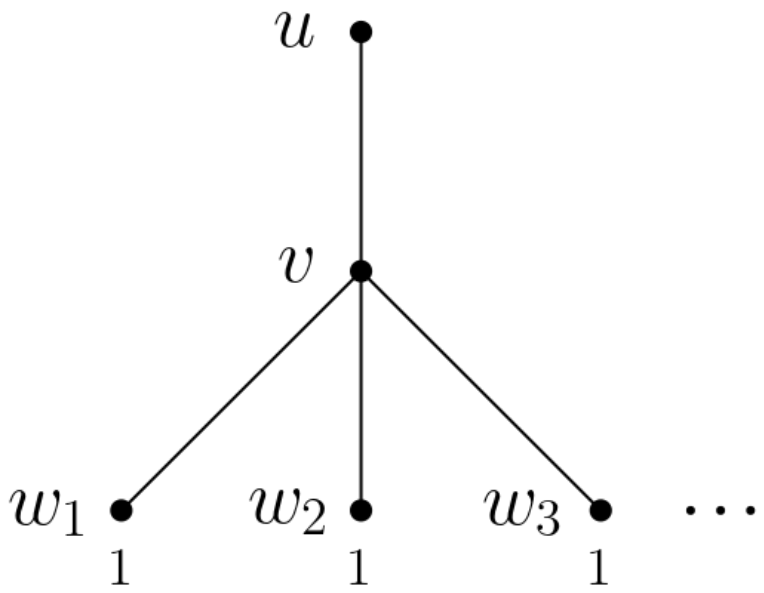

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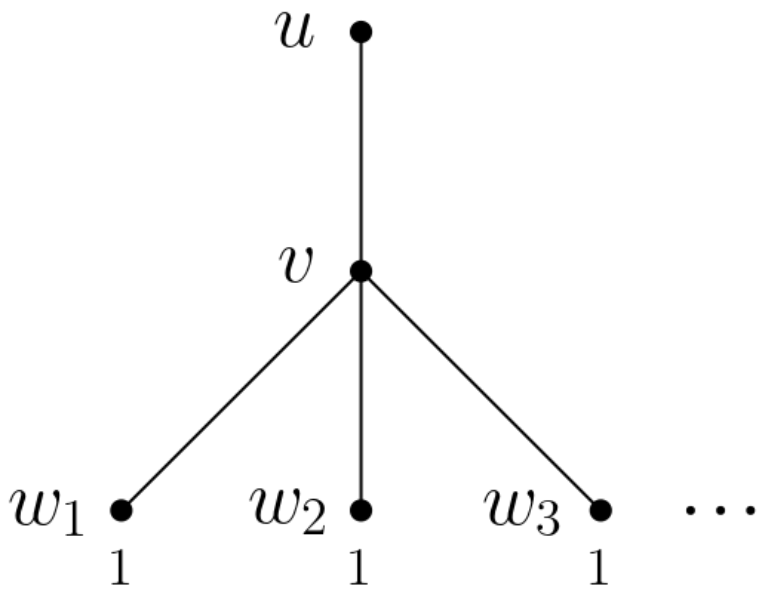

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- For huge data sets: only take random set of vertices for BFS roots.

Modularity

Quality of clusters / communities: Modularity

- Given a graph G and a partitioning (clustering) $\mathcal{C} = (C_1, \dots, C_k)$ of $V(G)$ into communities (clusters) C_i.
- **Rough idea:** Define ***modularity*** $Q(G, \mathcal{C})$ as a measure via:

$$\sum_{C_i \in \mathcal{C}} [\, (\#\ of\ edges\ within\ C_i) - (\boldsymbol{expected}\ \#\ of\ edges\ within\ C_i)\,]$$

- We need a model for an average / random graph on our cluster C_i.

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- Idea of building $\mathcal{R}_d(G)$: Cut the edges at every vertex and rewire them randomly, allowing multiple edges and loops.

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- Expected # of edges between v and w in $\mathcal{R}_d(G)$:

$$d_G(v) \cdot \frac{d_G(w)}{2m-1} \approx \frac{d_G(v) \cdot d_G(w)}{2m}$$

Quality of clusters / communities: Modularity

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- Define **modularity** $Q(G, C)$ as:

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- Usually: $Q(G, \mathcal{C}) > 0{,}3$ is an indicator for good community structure.

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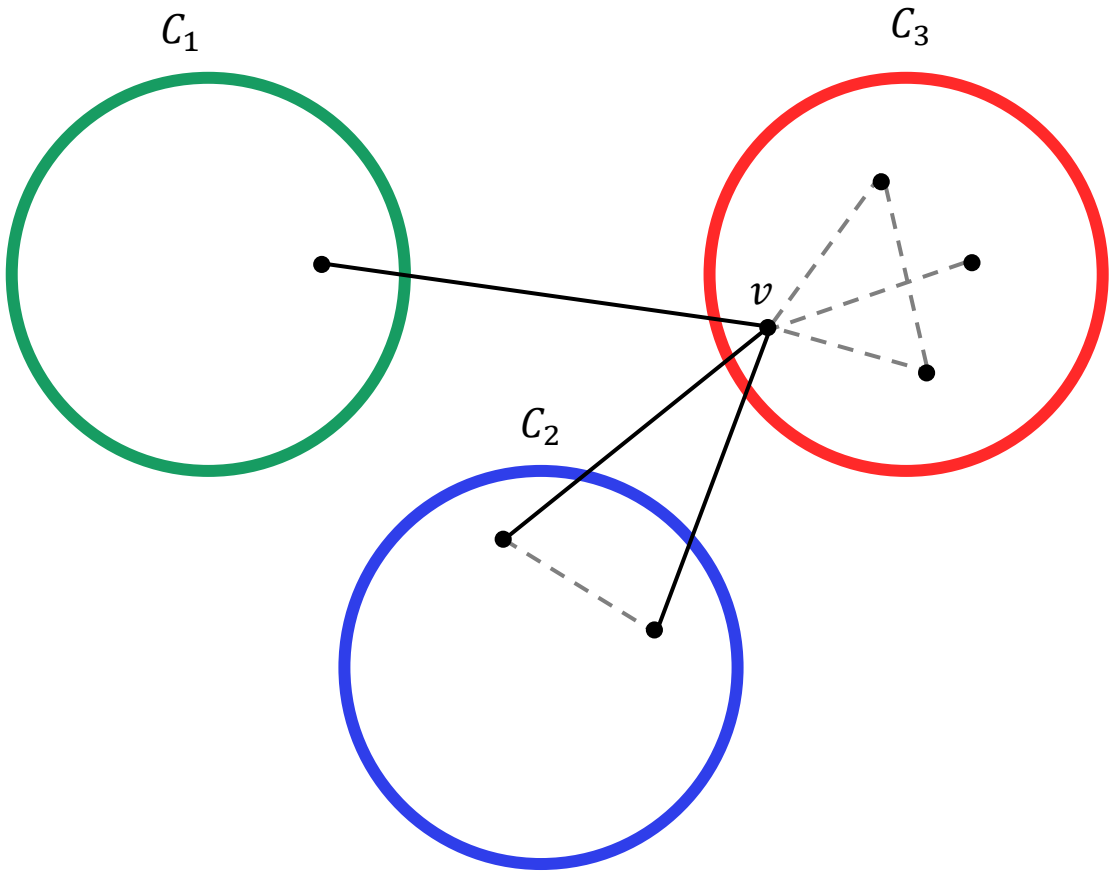
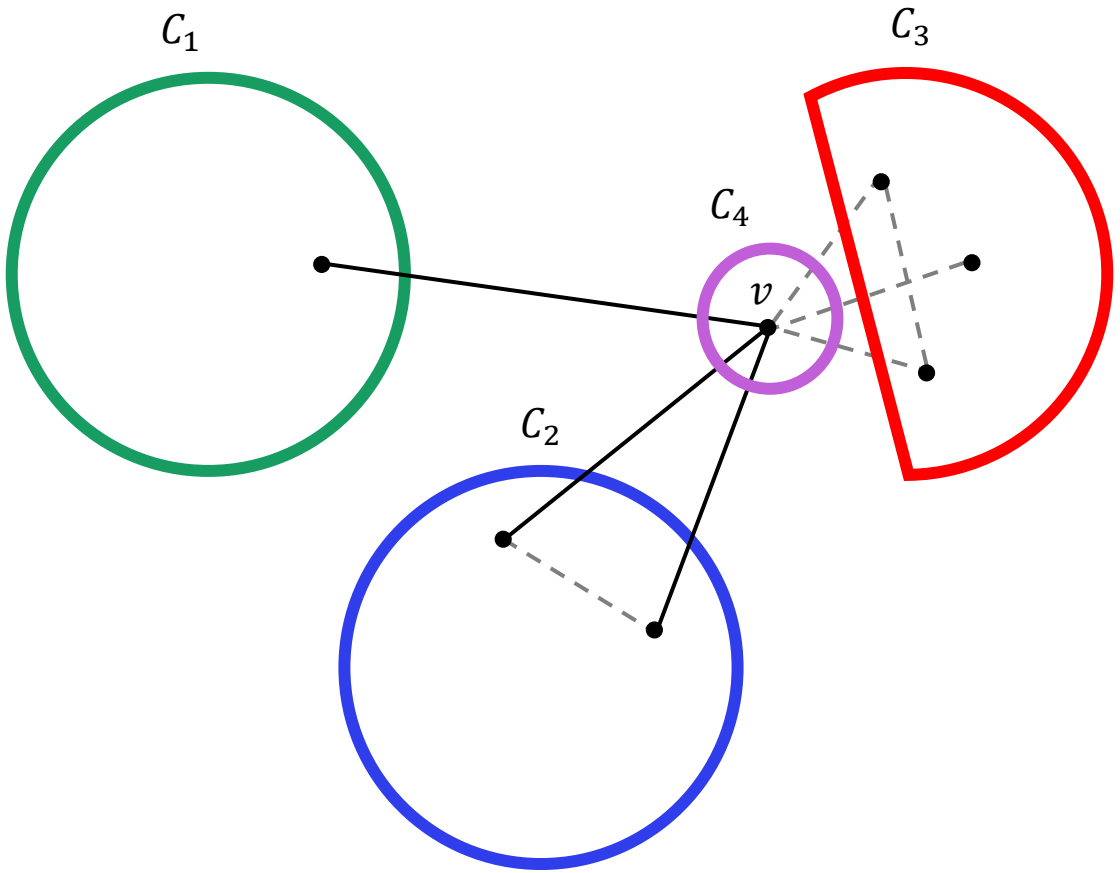
- The algorithm can be split into 2 steps, which are iterated.

Louvain algorithm: the main idea



Louvain algorithm: the main idea

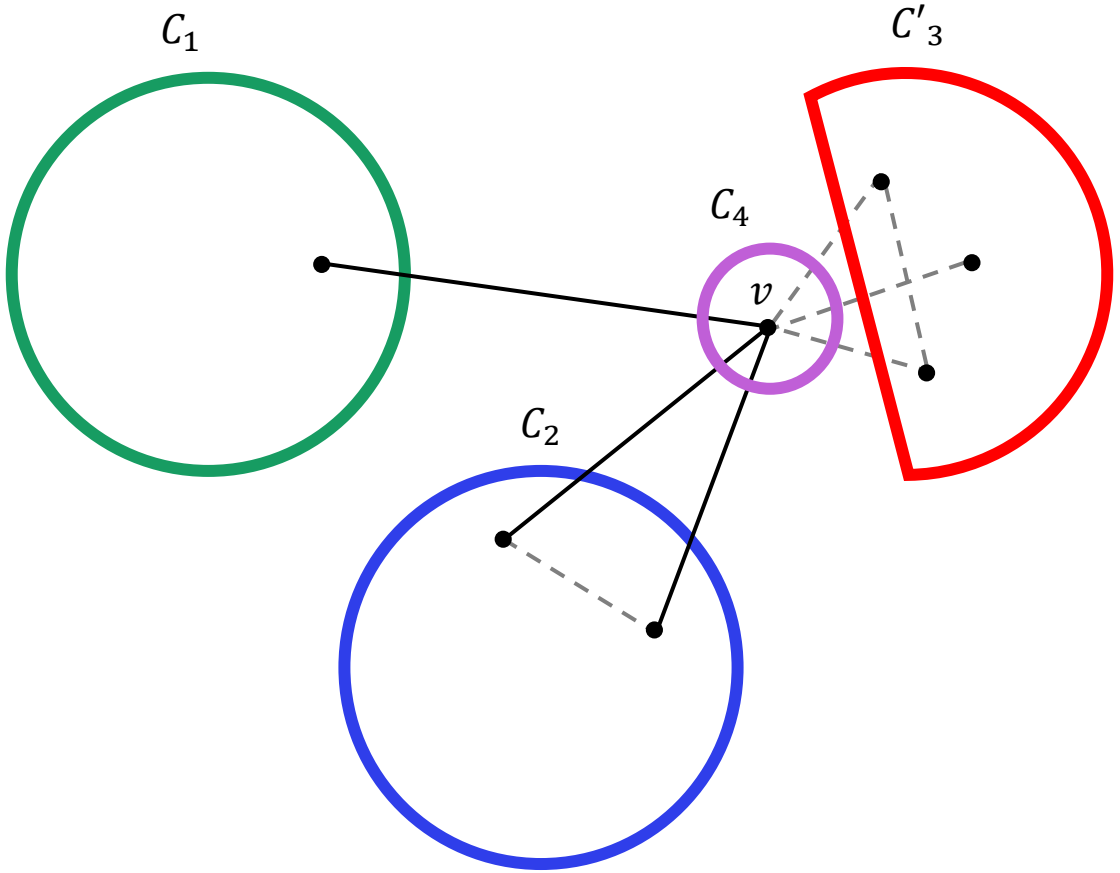
- Remove a vertex v from its community (here C_3). → Modularity change
- Put v into its own community (here C_4). → Modularity change



Louvain algorithm: the main idea

- Modularity change when switching to this refined clustering:

$$\Delta Q_{remove} := Q(G, C_1, C_2, C'_3, C_4) - Q(G, C_1, C_2, C_3)$$



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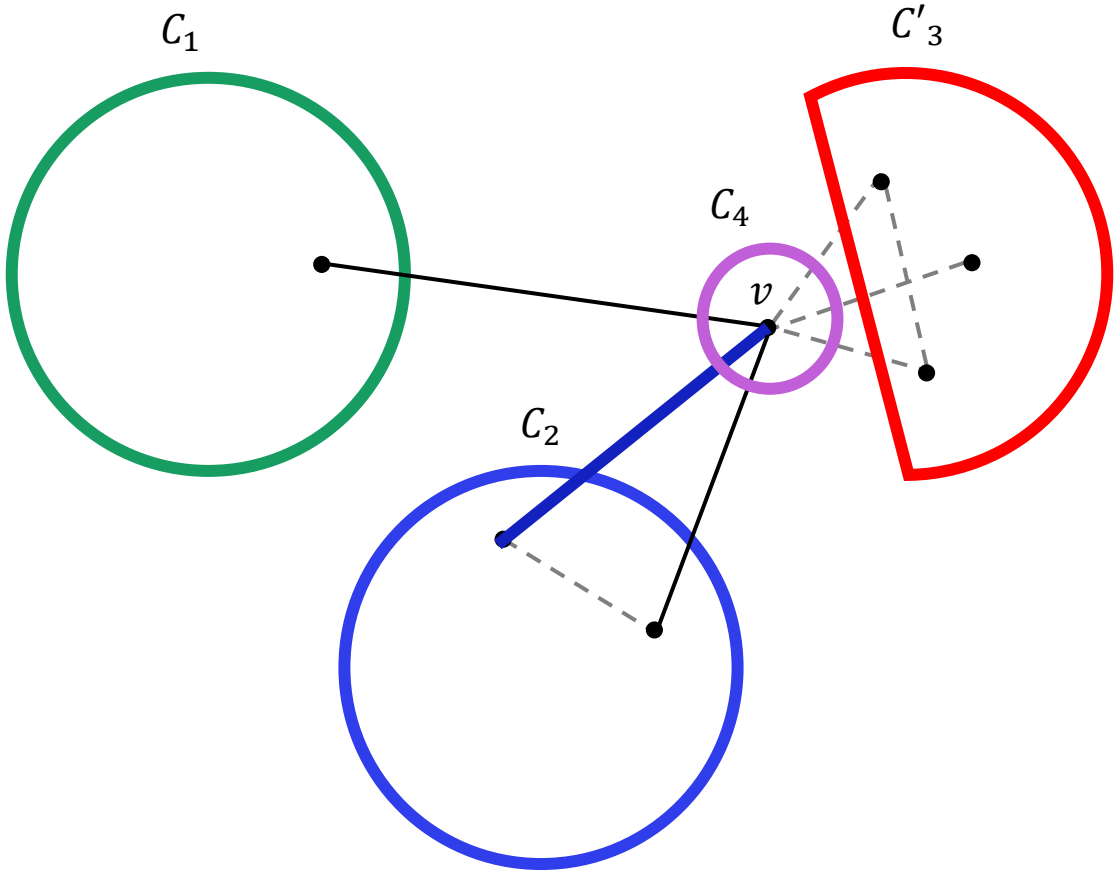
- Now move v to a community that contains a neighbour of v.



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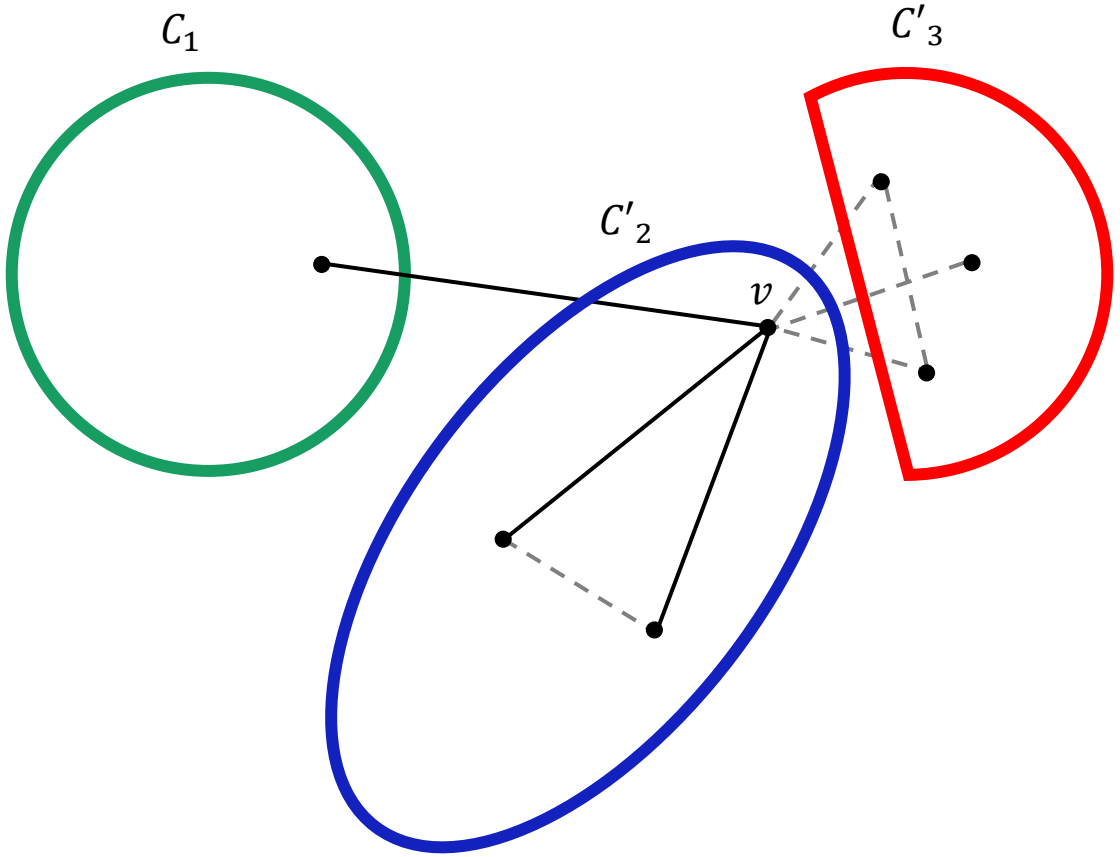

Louvain algorithm: the main idea

- Modularity change when switching to this clustering:

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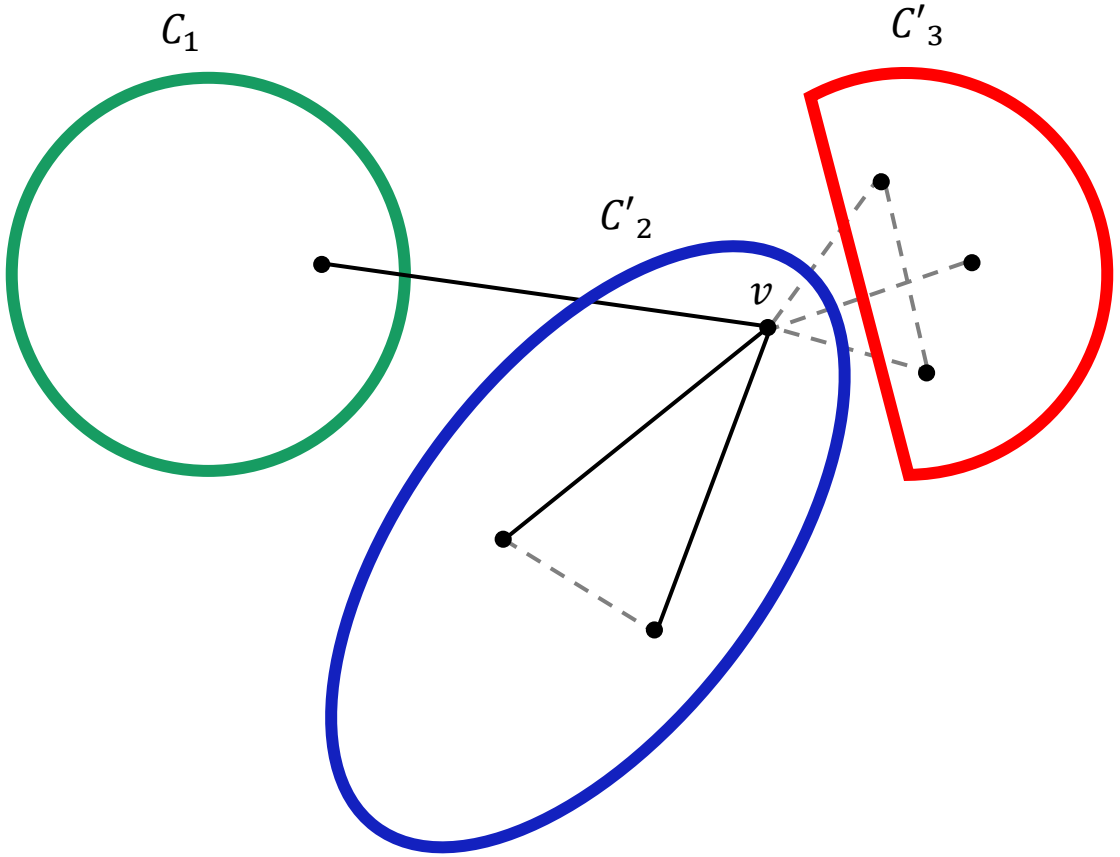

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- ΔQ_{remove} and ΔQ_{insert} can be computed locally by only considering those communities that are affected by the change.
  - (See e.g. Stanford lecture notes from 2021 on Machine Learning with Graphs by Leskovec)

Louvain algorithm: the full picture of step 1

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- Order the vertices arbitrarily: $v_1, v_2, \ldots, v_n$.
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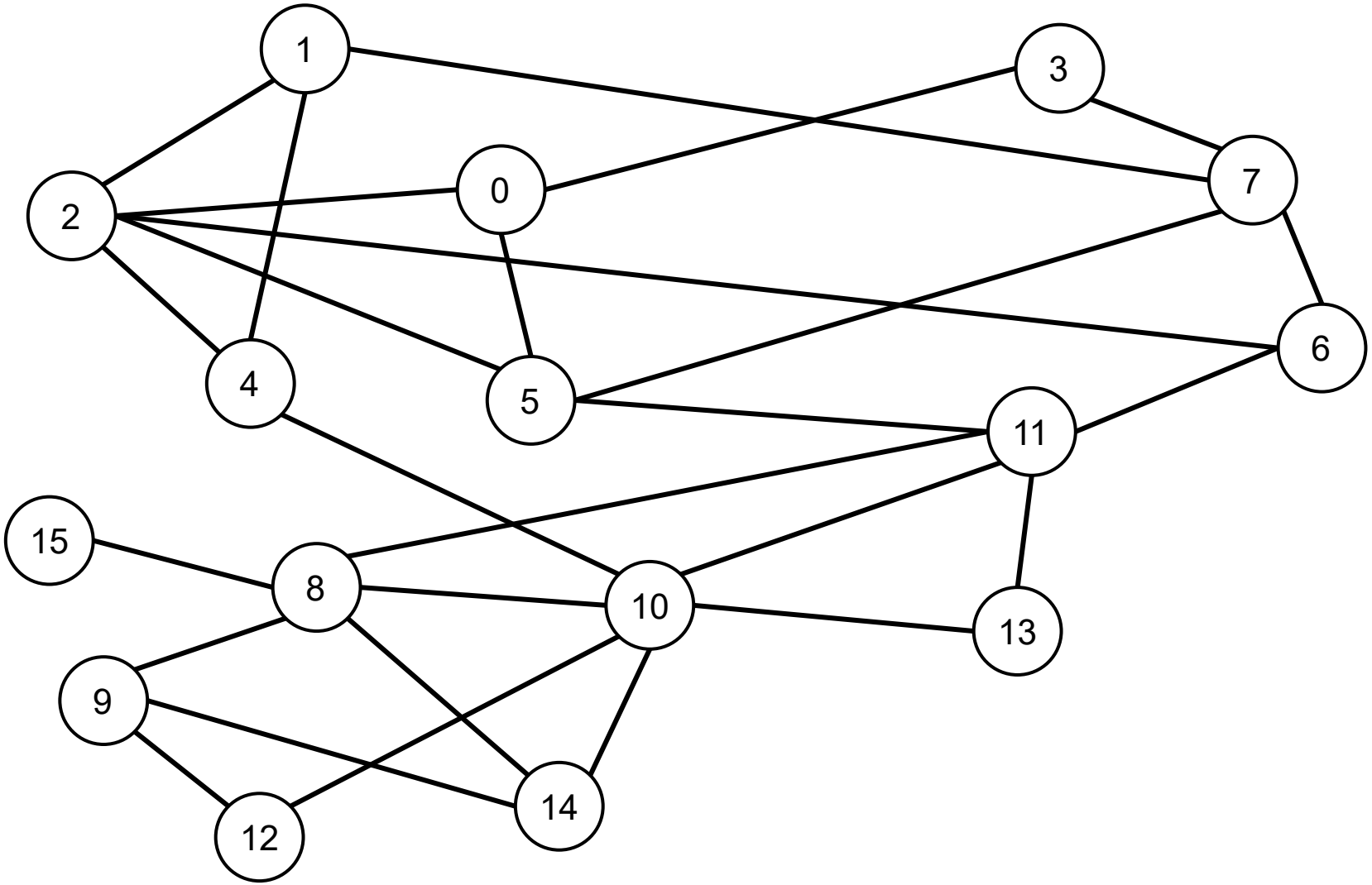
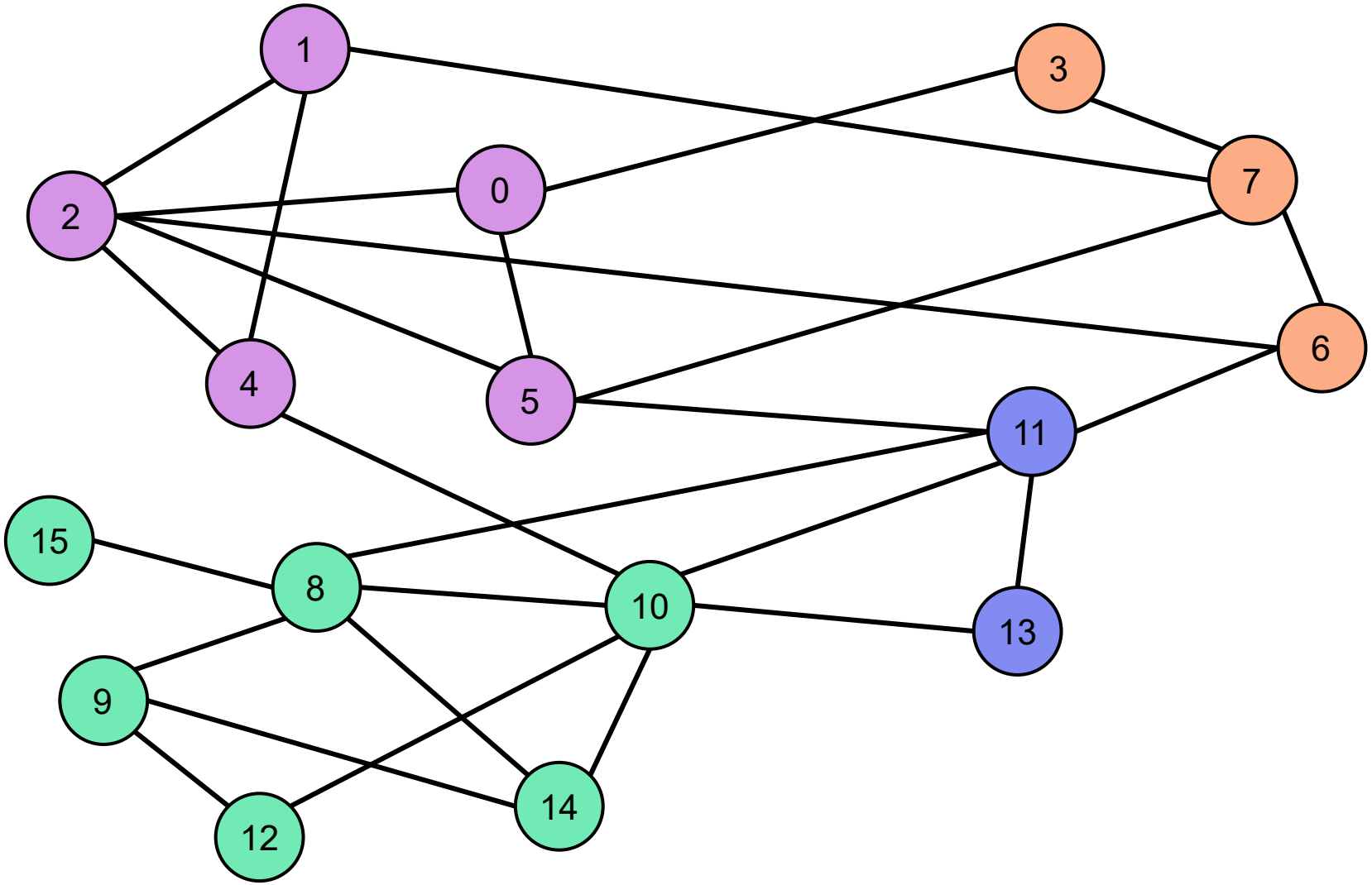
- Stop if all vertices have been processed.

Louvain algorithm: illustration



Louvain algorithm: end of step 1



Louvain algorithm: step 2

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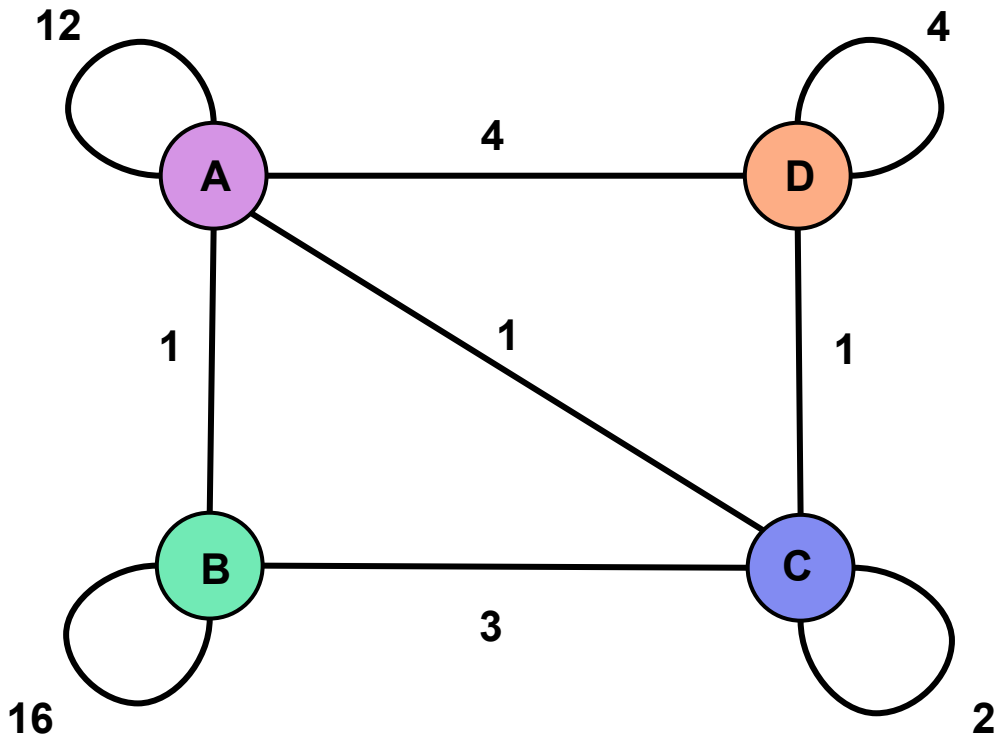
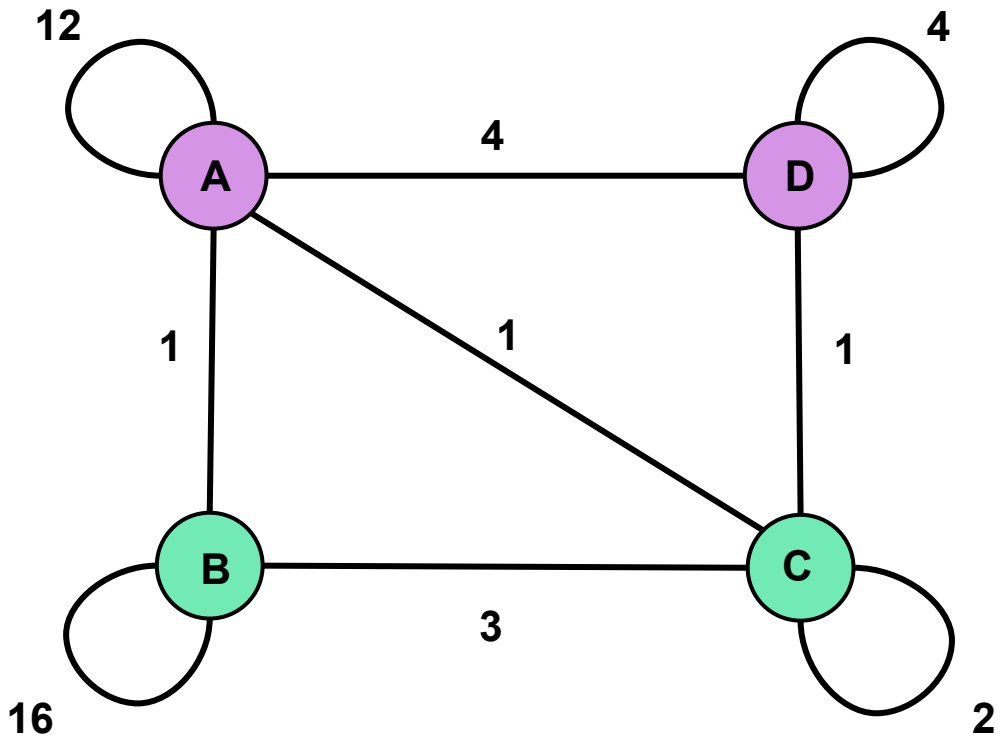
- Replace all edges between two former communities by one edge weighted by the sum of all (weights of) removed edges.

Louvain algorithm: step 2



Louvain algorithm: second pass of step 1



Louvain algorithm: weighted modularity involved

- Recall: Definition of modularity:

$$Q(G,\mathcal{C}) = \frac{1}{2m} \cdot \sum_{C_i \in \mathcal{C}} \sum_{\substack{v,w \in V(C_i) \\ v \neq w}} \left[A_{vw} - \frac{d_G(v) \cdot d_G(w)}{2m} \right]$$

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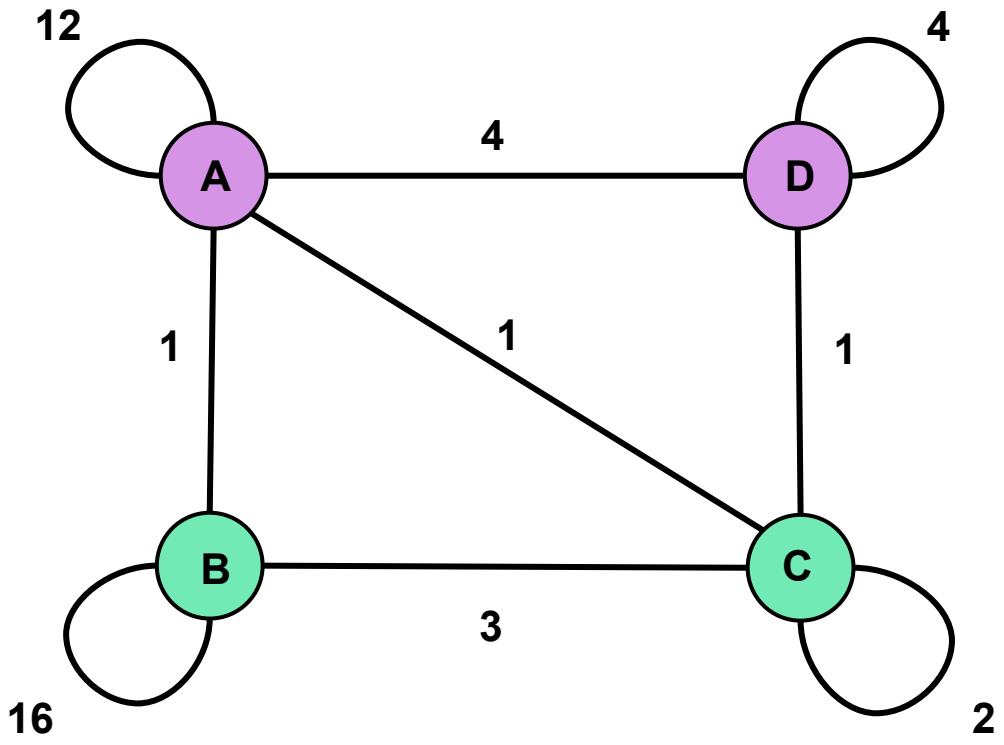
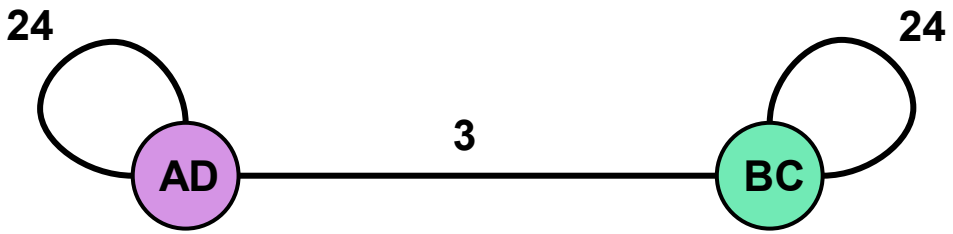
now: indicate weighted degrees

Louvain algorithm: second pass of step 1



Louvain algorithm: second pass of step 2



Spectral clustering

Remarks about spectral clustering

- Spectral clustering can be applied to several data sets, but you need to **turn** the **data into a graph** (there are several ways).

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- For spectral clustering the **data** set does **not have** to be of a **special shape** (e.g. not ‘sperical’ as for k-means). The algorithm adapts to the shape of the data.
- Spectral clustering yields very good results.
- **Computing all eigenvalues** is **expensive** for **dense matrices**.
  – But there are quite efficient algorithms for computing only the first few smallest eigenvalues and their eigenvectors.

Spectral clustering

- Let G be a simple undirected graph.
- **Task: Partition $V(G)$ into two classes** (clusters) such that:
  1. we maximise the # of edges within the clusters, and
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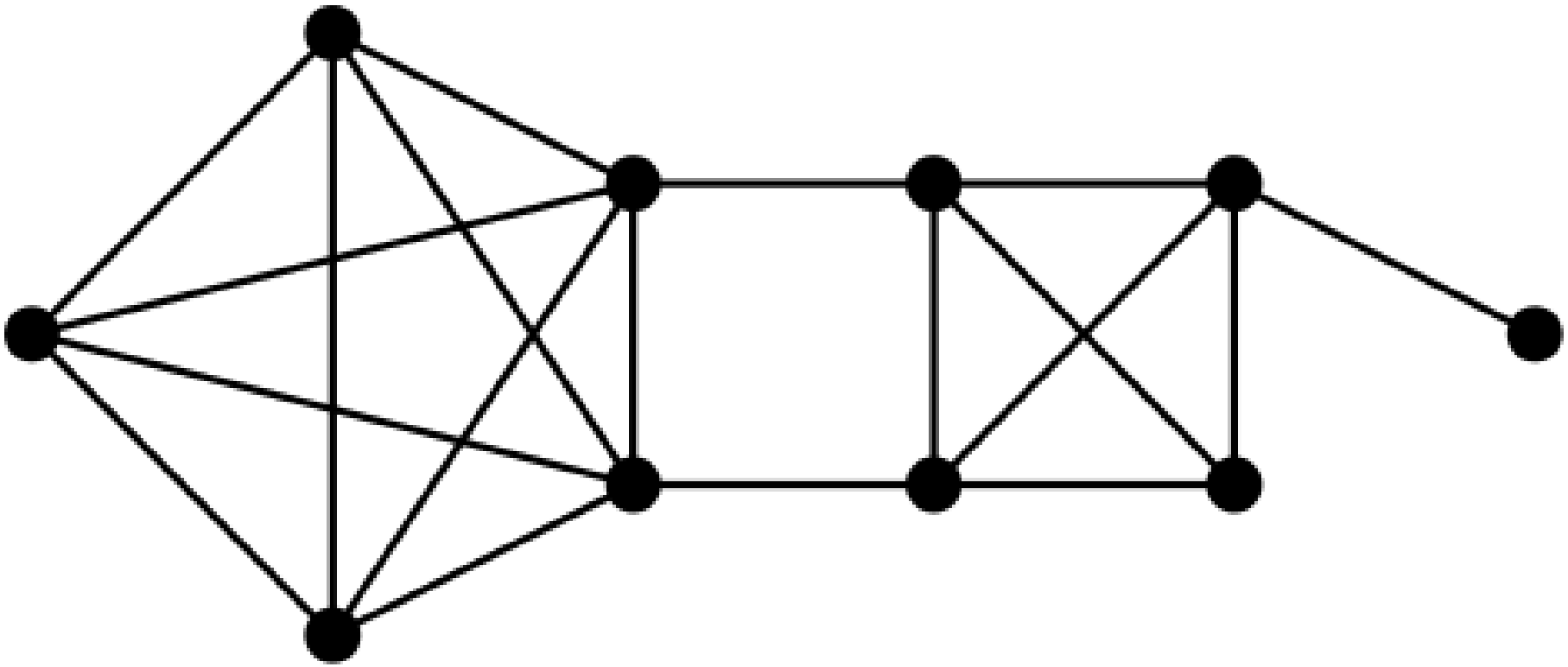
- For two vertex sets $A, B \subseteq V(G)$ let $\boldsymbol{E(A,B)}$ denote the set of edges that have one end vertex in A and the other in B.
- If $A \subseteq V(G)$ and $B = V(G) \setminus A$ (the complement of A within $V(G)$), then $E(A,B)$ is called a **cut of $\boldsymbol{G}$**.
  (Sometimes we also refer to the partition (A,B) as the cut.)

Spectral clustering: “good” cut

- **Idea:** Find the smallest cut $E(A, B)$ within G.
- **Pro:** Can be done (rather) efficiently (Ford-Fulkerson, Karger).
- **Con:** Only focusses on minimising edges between the 2 clusters.
  - What about maximising edges within clusters?

Spectral clustering: “good” cut



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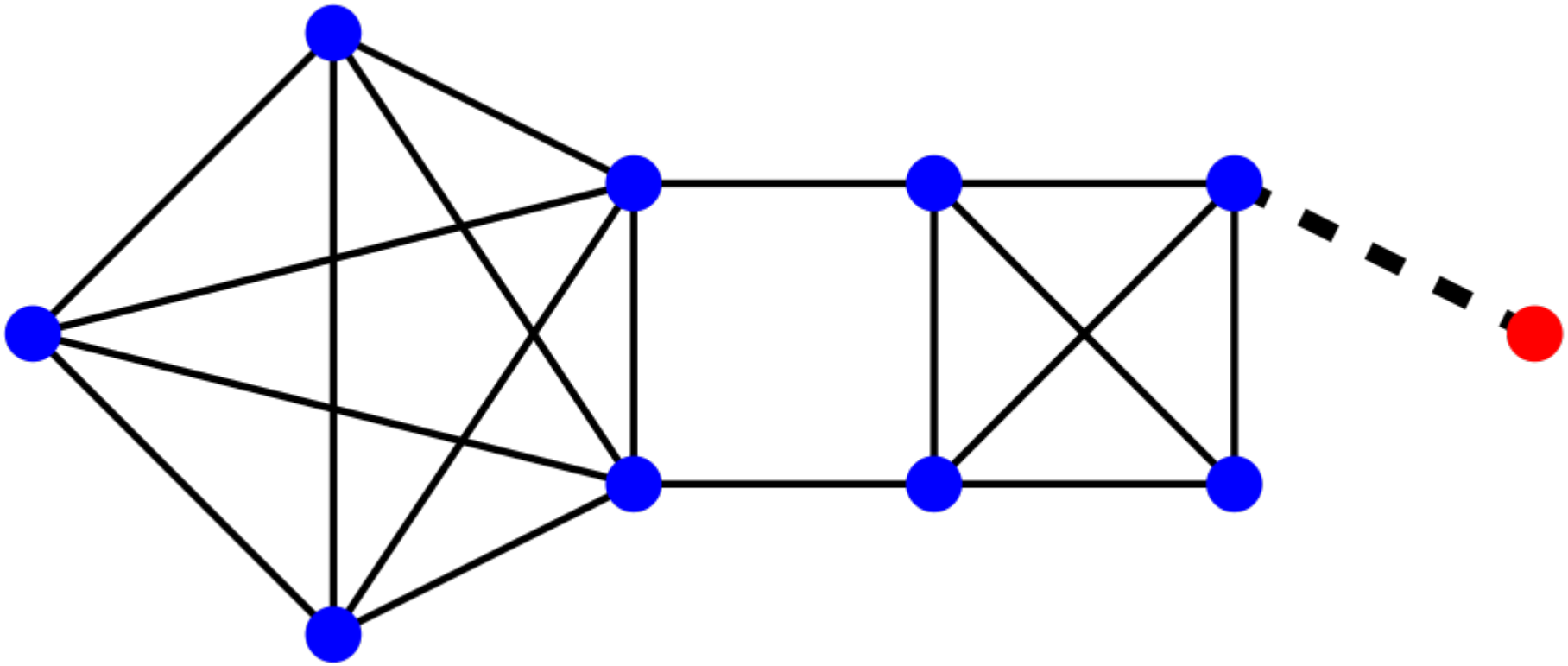

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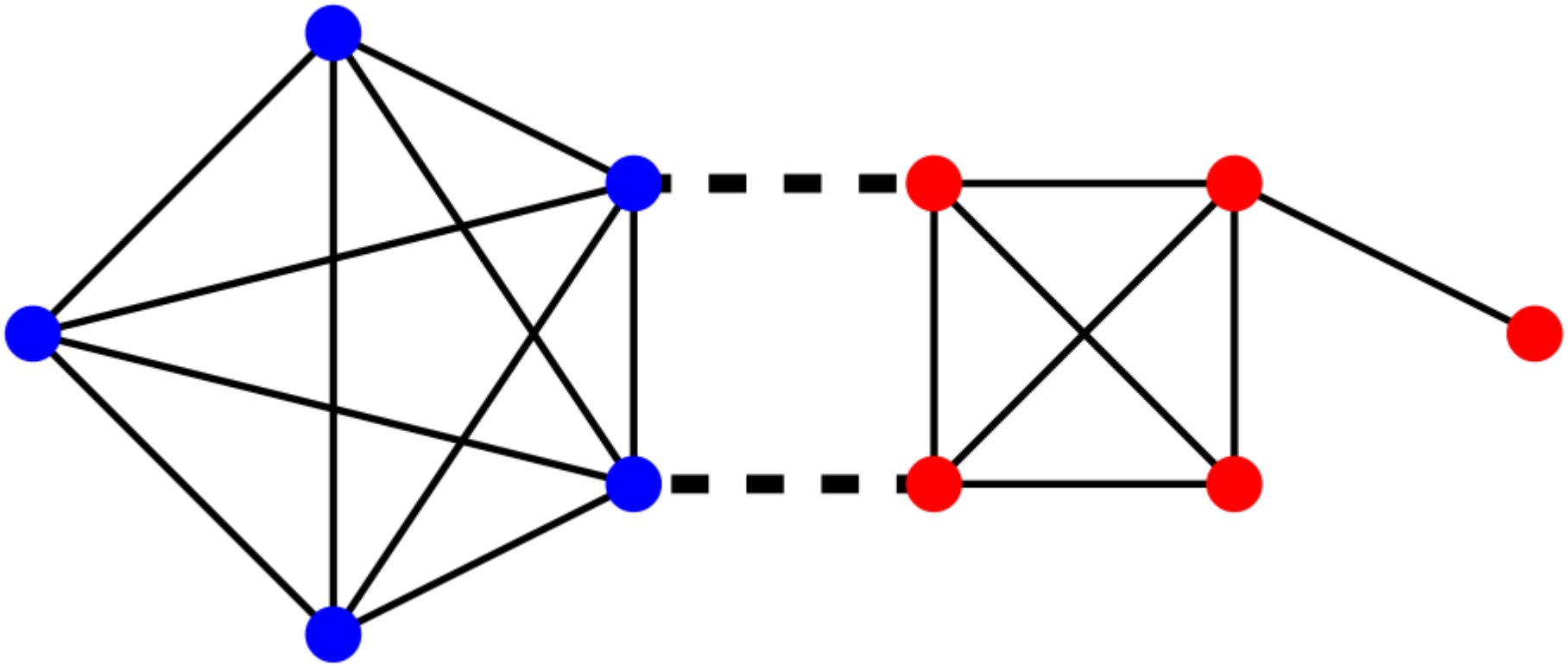

Spectral clustering: “good” cut

- **Better:** Consider ***normalised cuts*** and **minimise**.
- Let $E(A,B)$ be a cut of G. Then the ***normalised cut value*** is:

$$ncut(A,B) := \frac{|E(A,B)|}{vol(A)} + \frac{|E(A,B)|}{vol(B)}$$

Here $\boldsymbol{vol(A)} := \sum_{v \in A} d(v)$.

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- This way we produce more balanced bipartitions, still inducing a small cut.
- However, finding a cut with minimised $ncut$-value is NP-hard!

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- **Or consider: RatioCut**

$$RatioCut(A,B) := \frac{|E(A,B)|}{|A|} + \frac{|E(A,B)|}{|B|}$$

RECAP: Adjacency matrix of a graph

- Let G be a simple undirected graph with $|V(G)| = n$.
  Enumerate the vertices of G by $v_1, \dots, v_n$.

- Define ***Adjacency Matrix*** $A = A(G) \in \mathbb{R}^{n \times n}$ of G as follows:

  Let a_{ij} be the entry of A in row i and column j.

  Set $a_{ij} = 1$ iff $v_i v_j \in E(G)$, otherwise set $a_{ij} = 0$.

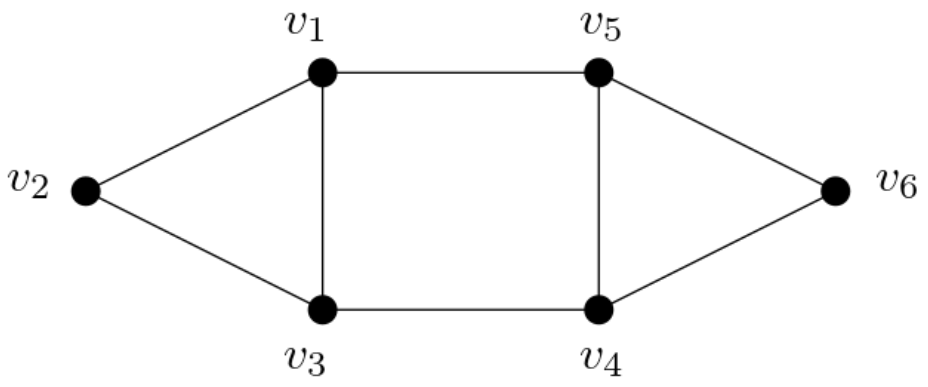
- If $Ax = y$, then the following holds for the i-th component y_i of y:

$$y_i = \sum_{j=1}^{n} a_{ij}\, x_j = \sum_{v_i v_j \in E(G)} x_j$$

RECAP: Adjacency matrix of a graph

Example:

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



Spectral Graph Theory

- Analysing the ***spectrum*** of a graph G, i.e. of its adjacency matrix A to obtain insight about the structure of G.

- The **spectrum** of A is the set $\boldsymbol{\Lambda} = \{\lambda_1, \dots, \lambda_n\} \subseteq \mathbb{R}$ of its **eigenvalues**. Usually we sort Λ by $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$.

- **Recap** (**eigenvalue** λ and one **eigenvector** x of it):

$$Ax = \lambda \cdot x$$

RECAP: symmetric matrices

- $\boldsymbol{A}(\boldsymbol{G}) = \boldsymbol{A}$ is a **symmetric real matrix**. Hence:
  1. A is diagonalisable.
  2. There is an orthogonal basis of eigenvectors.
  3. A has only real eigenvalues.

- Also: $A(G) = A$ is ***positive semidefinite*** (i.e. all eigenvalues ≥ 0).

- Fact: A is positive semidefinite iff $x^T A x \geq 0$ for all $x \neq 0$.

Some intuition: d-regular graphs

- As special case: Let G be a **connected** graph where each vertex has the same degree $d \in \mathbb{N}$ (the latter property is called $\boldsymbol{d}$**-regular**).

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$$A \cdot (1, 1, \dots, 1)^T = d \cdot (1, 1, \dots, 1)^T$$

- Why? Because for each vertex, we sum over all its d neighbours.

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Actually:

1. d is the largest eigenvalue of A.
2. d has multiplicity 1. So there is only one eigenvector for it.

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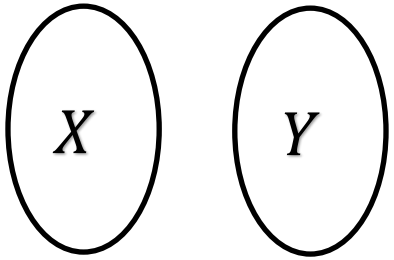
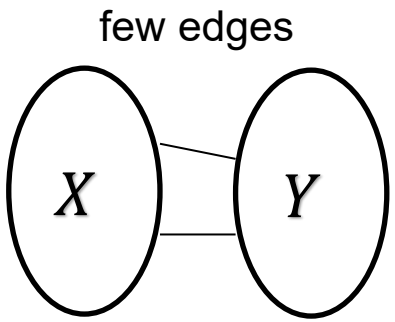
- Now: $\lambda_n = \lambda_{n-1} = d$.
- **Intuition:**



$\lambda_n - \lambda_{n-1} = 0$



$\lambda_n - \lambda_{n-1} \approx 0$

General case

- Let G be a simple undirected connected graph.
- Define ***Degree Matrix D*** $= D(G) \in \mathbb{R}^{n \times n}$ of G as follows:

  Let d_{ij} be the entry of D in row i and column j.

  Set $d_{ij} = 0$ for all $i \neq j$ and $d_{ii} = d(v_i)$ for all i.
- Define the **Laplacian Matrix** $\boldsymbol{L} = L(G) \in \mathbb{R}^{n \times n}$ of G as $A - D$.

Facts about L:

- L is symmetric
- L is diagonalisable.
- There is an orthogonal basis of eigenvectors.
- L has only real eigenvalues and $\lambda_1 = 0$ witnessed by $(1, \dots, 1)^T$.
- L is positive semidefinite, hence $x^T L x \geq 0$ for all $x \neq 0$..

General case

- **Fact:** If $\boldsymbol{x}$ is **orthogonal to** the **eigenvector of** $\boldsymbol{\lambda_1}$ (so: $\sum_i x_i = 0$) and x is **normalised**, i.e. $x^T x = 1$, then the following holds (by Rayleigh):

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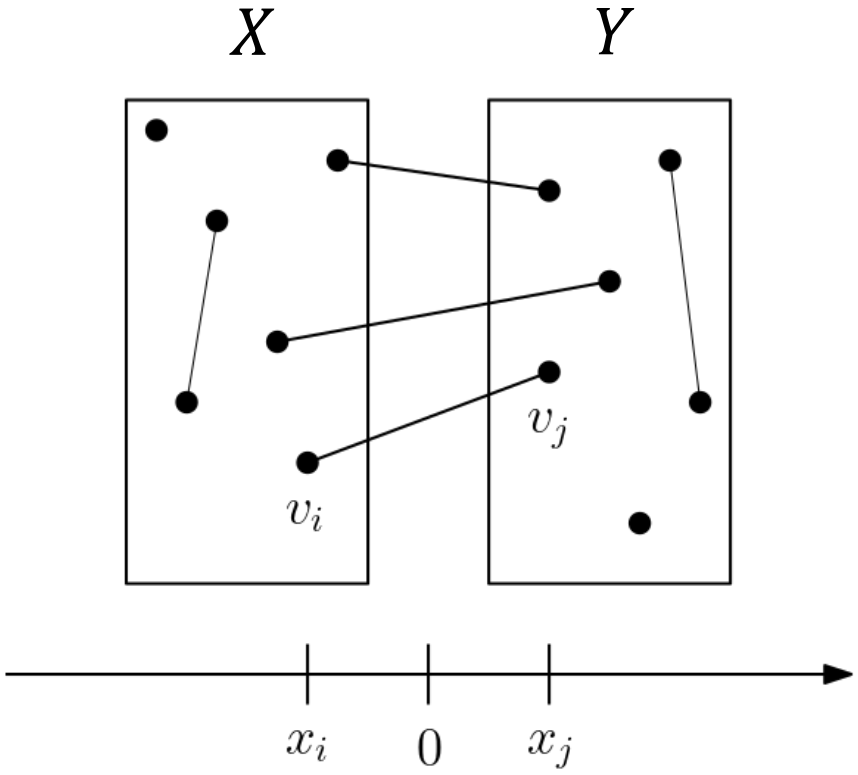
- **CLUSTERING:** Put all v_i with $x_i < 0$ into set X, the rest into set Y. This yields bipartition of $V(G)$.

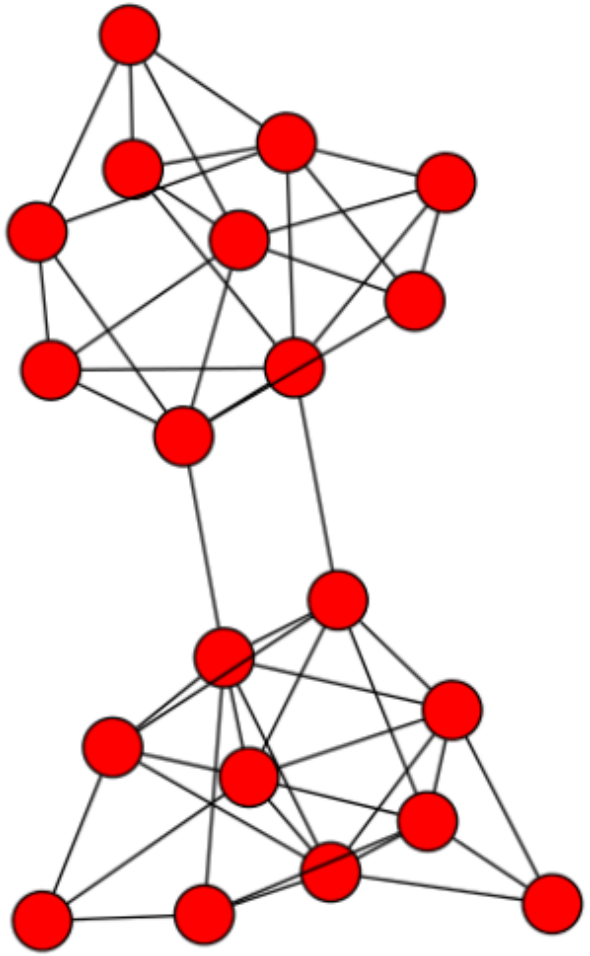
General case

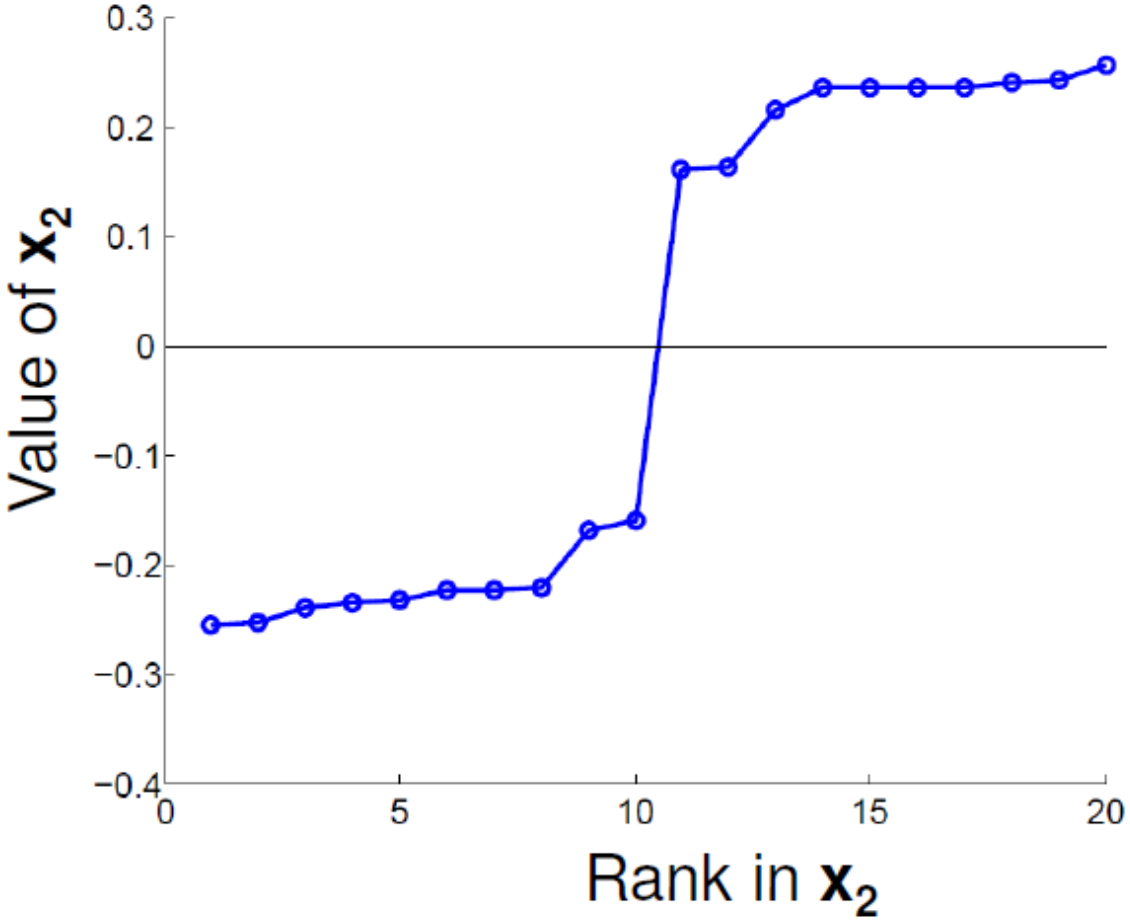
$$\lambda_2 = \min_{\substack{x \\ \sum_i x_i = 0}} x^T L x = \sum_{v_i v_j \in E(G)} \left(x_i - x_j\right)^2$$

- If $v_i v_j \in E(G)$, ideally $x_i \approx x_j$.
- Indication for $|X| \approx |Y|$.
- But some x_i are > 0 and some < 0, since $x \neq 0$ and $\sum_i x_i = 0$.



Example 1




0.3
0.2
0.1
0
−0.1
−0.2
−0.3
−0.4
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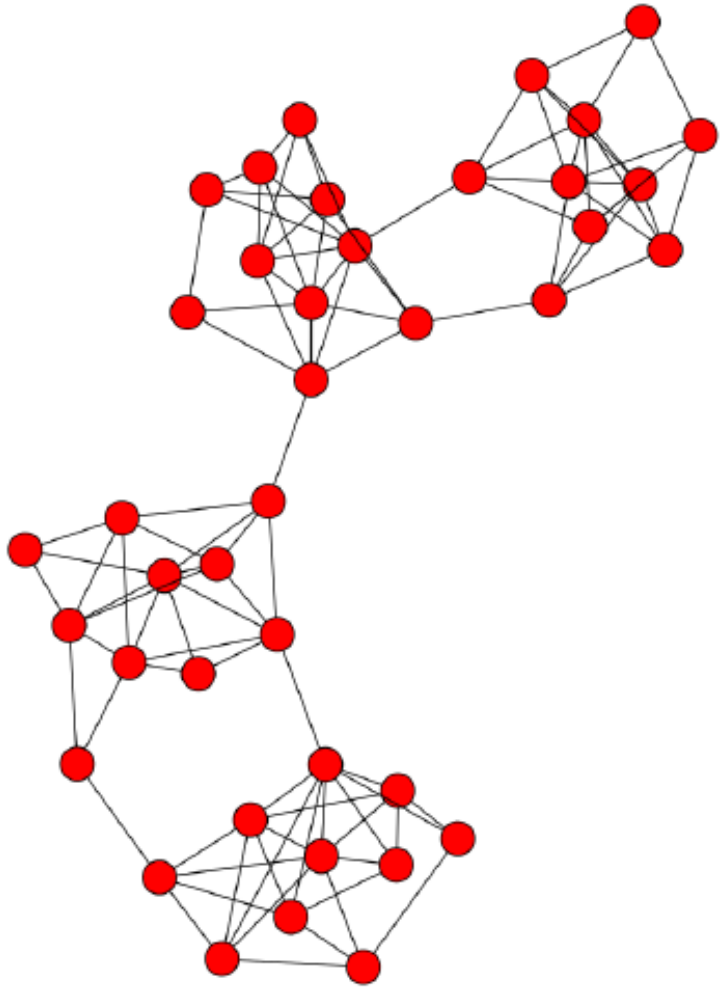
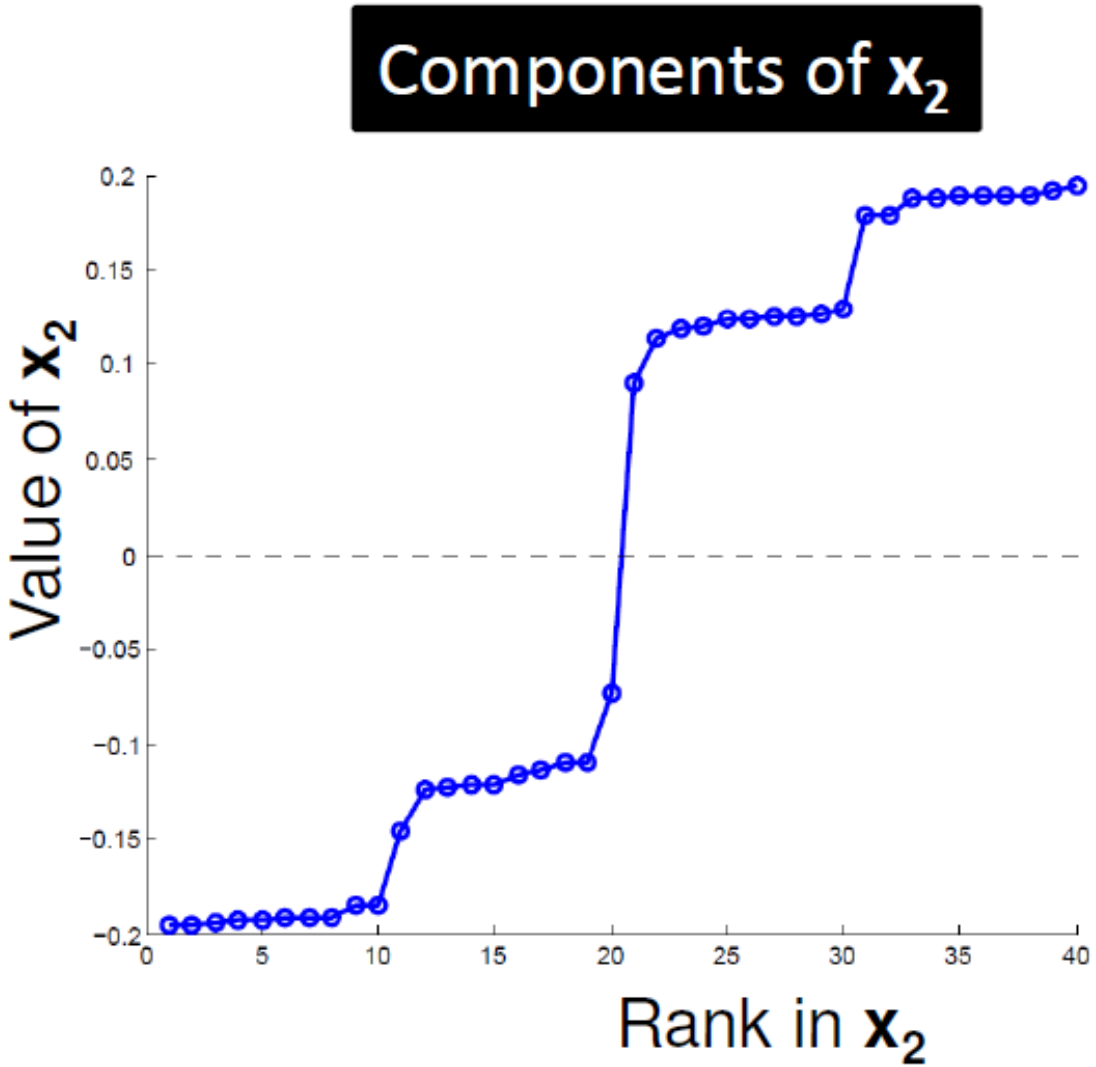
5
10
15
20
Value of $\mathbf{x}_2$
Rank in $\mathbf{x}_2$

Example 2




Components of $\mathbf{x}_2$
Value of $\mathbf{x}_2$
Rank in $\mathbf{x}_2$
0.2
0.15
0.1
0.05
0
−0.05
−0.1
−0.15
−0.2
0
5
10
15
20
25
30
35
40

Indication for good balanced partition

- Let $E(X,Y)$ be a cut of G. Then define:

$$\alpha = \alpha(X,Y) = \frac{|E(X,Y)|}{min\{|X|,|Y|\}}$$

- Let $\boldsymbol{\Delta(G)}$ denote the **maximum degree** of G.
  Then the following (Cheeger inequality) holds:

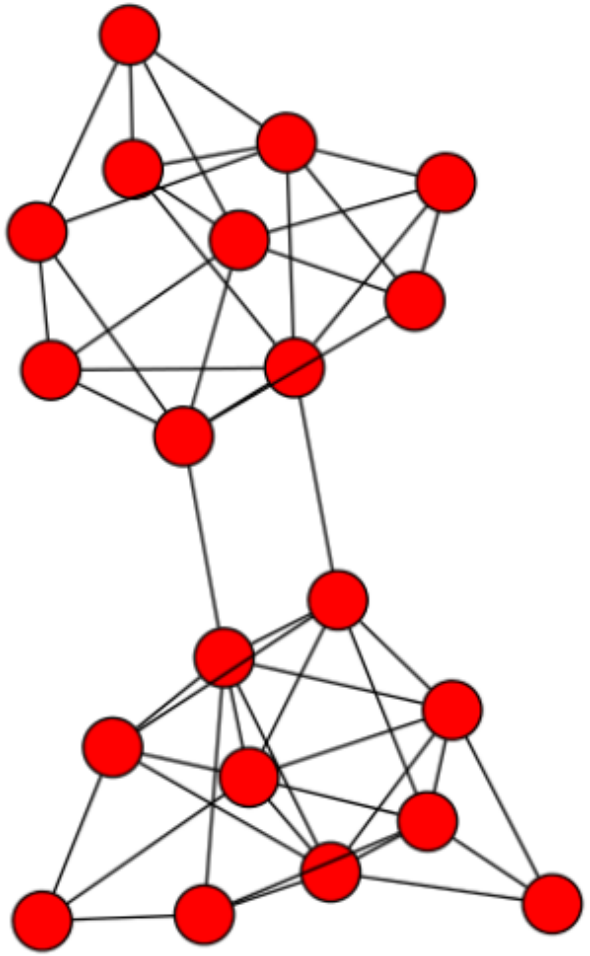
$$\frac{\alpha^2}{2\Delta(G)} \leq \lambda_2 \leq 2\alpha$$

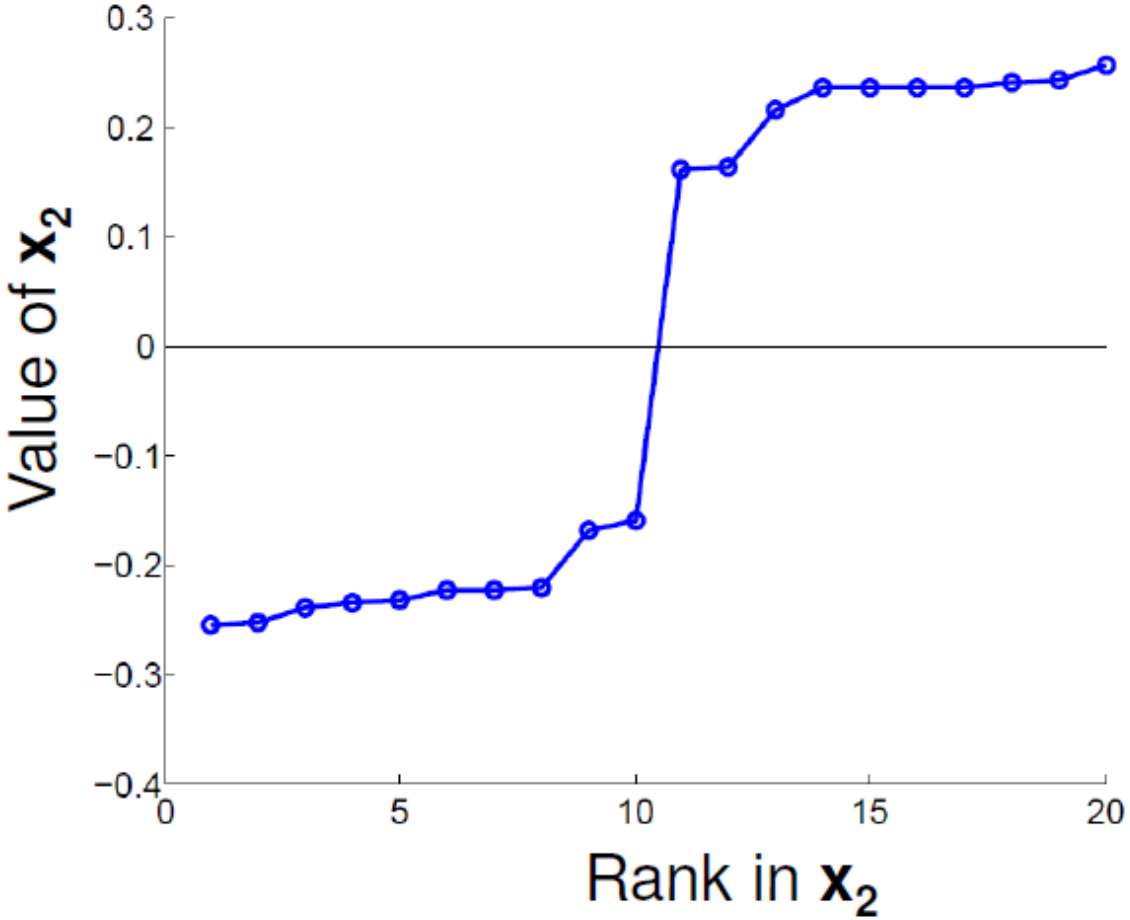
- Hence, we approximately (at most factor 2) find some balanced (w.r.t. α) cut $E(X,Y)$ via an eigenvector of L corresponding to λ_2.

Spectral clustering mixed with k-means

- Often: building the bipartition (X, Y) for $V(G)$ from the components of the eigenvector x_2 of λ_2 by checking the sign is not ideal.
  - Some other threshold than 0 might be better (especially if we partition into more than 2 clusters).
- **Idea:** Perform k-means algorithm on the entries of x_2, e.g. just in $\mathbb{R}^1$.
  - A similar approach works for partitioning into k clusters. There we consider entries of several eigenvectors (w.r.t. further eigenvalues) as vectors of $\mathbb{R}^{k-1}$.

Example 1

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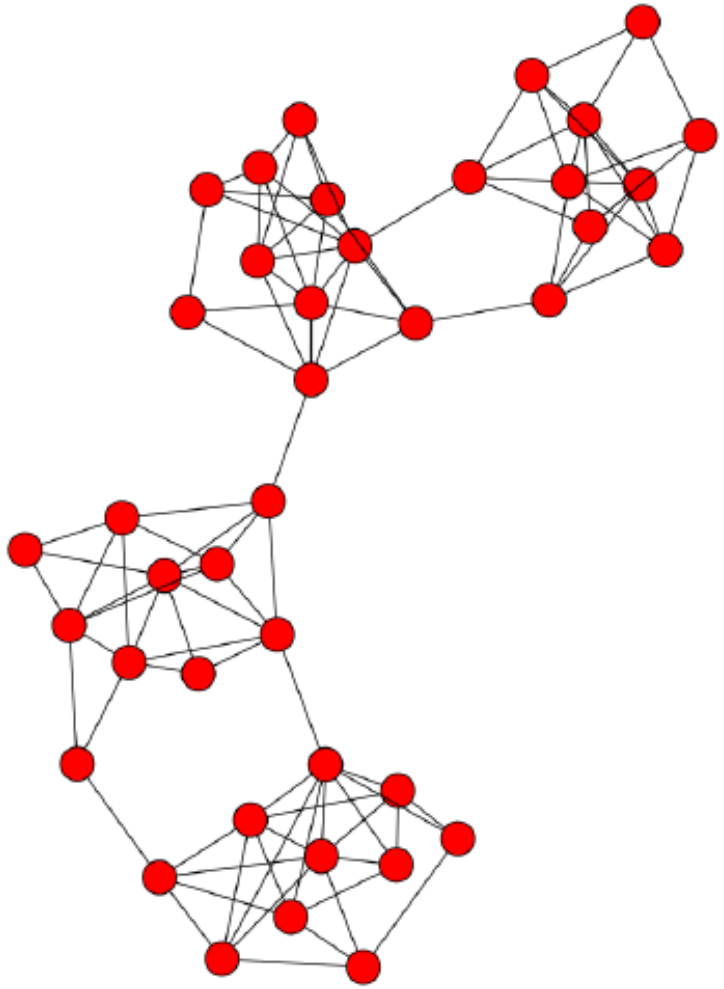

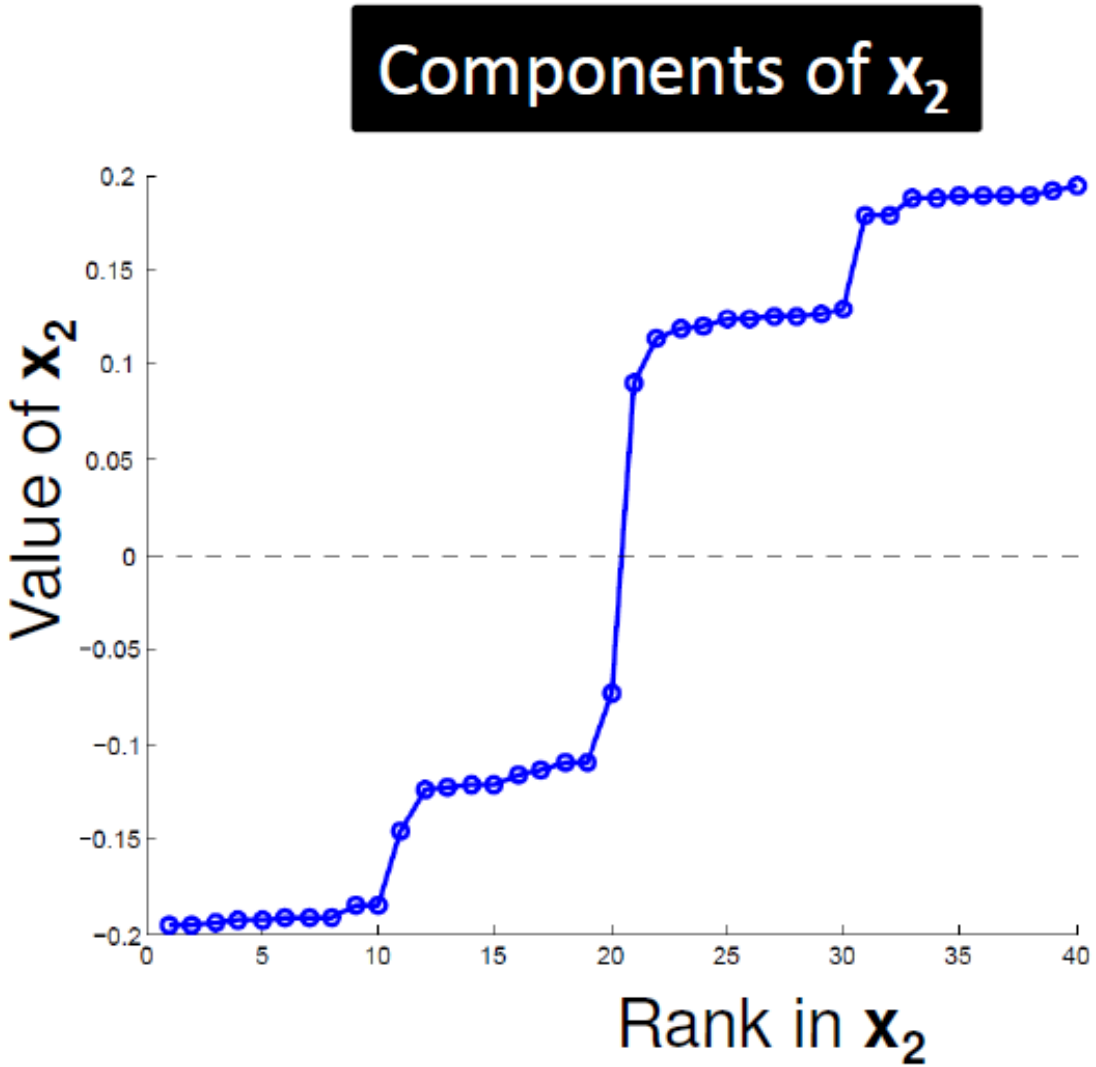
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30
35
40

Spectral clustering with k clusters

- **Idea 1 (naive):** Recursively apply bipartitioning algorithm in a divisive hierarchical manner.
  - **Con:** Not very efficient.
- **Idea 2 (better):** Use more eigenvectors, also for bigger eigenvalues. Can be done similarly, but with a normalised Laplacian.
  - Preferable and commonly used.
- Efficient approximation algorithms (up to a constant factor) for k clusters w.r.t similar normalised cut conditions do not exist.