

# **Computational Tools for Data Science**

# **Week 7:**

# Mining social network graphs

#### **Recap: Graphs**

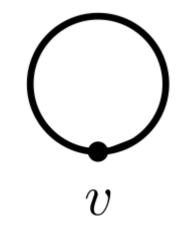
- A (simple and undirected) graph is a pair G = (V(G), E(G)).
- The set *V*(*G*) is the vertex set of the graph *G*. Its elements are the vertices of *G* (sometimes they are also called **nodes**).
- The set E(G) is the edge set of G. Its elements are the edges of G.
  - An edge  $e \in E(G)$  is a **2-element 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):



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

Model a **directed edge** e (also called **arc**) as a triple (e, v, 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)

- 1. Vertices correspond to network participants: people, addresses, websites, accounts
- Edges correspond to relationship between two participants: friends or no friends (undirected edge) following (directed edge) flow of transactions (weighted edge) different types of relationship (coloured edge)

#### 3. Locality property

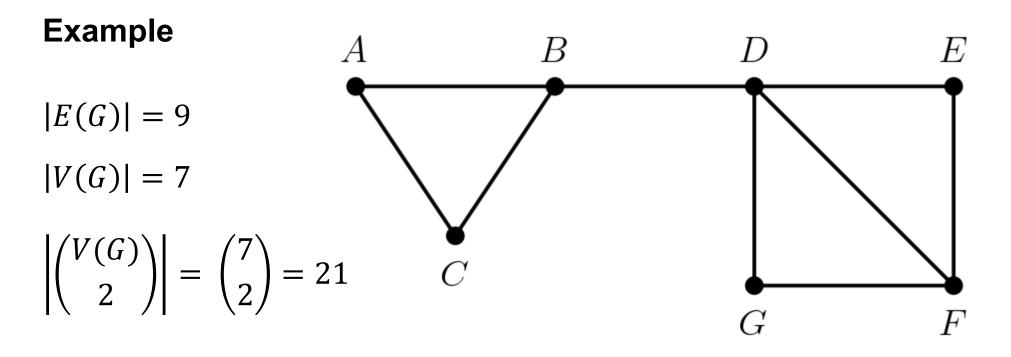
#### 3. Locality property

We assume the network is not random.

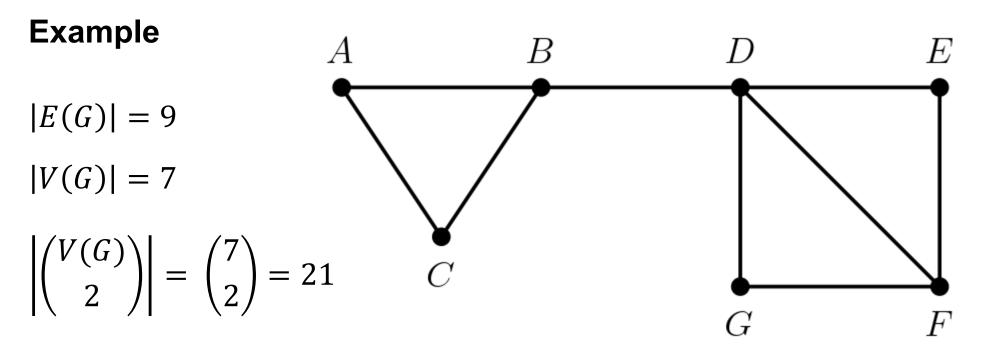
Relations within the network tend to cluster in communities.

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.

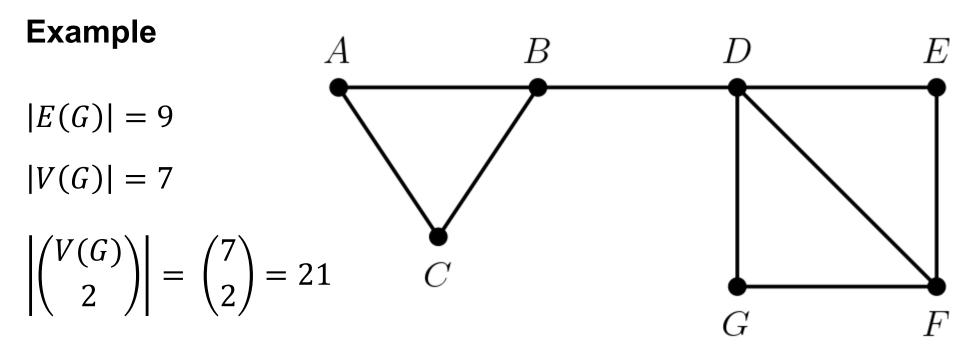






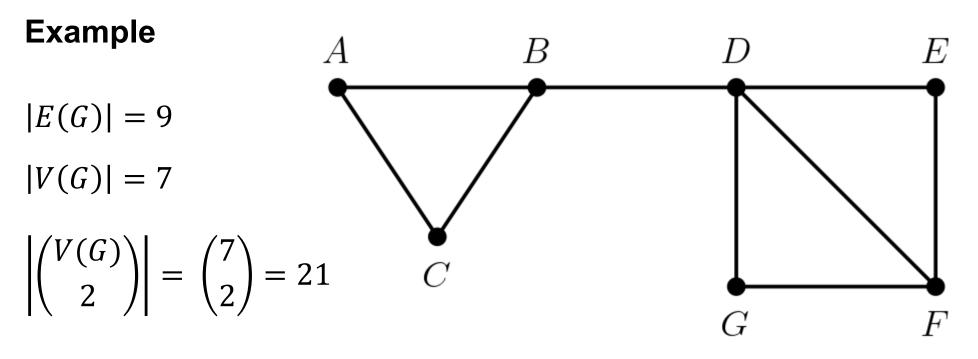


Suppose  $\{X, Y\}, \{Y, Z\} \in E(G)$ . Check  $\{X, Z\}$ :



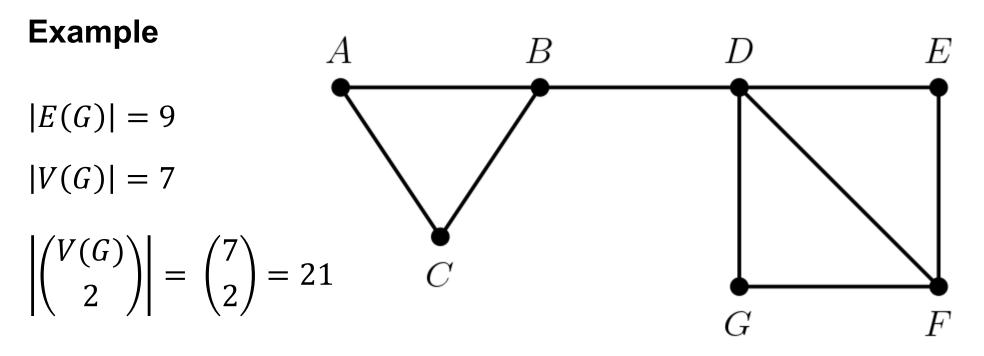
Suppose  $\{X, Y\}, \{Y, Z\} \in E(G)$ . Check  $\{X, Z\}$ :

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



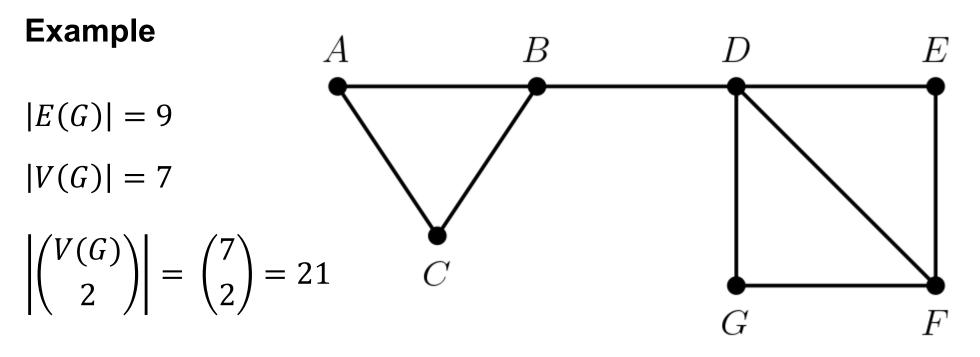
Suppose  $\{X, Y\}, \{Y, Z\} \in E(G)$ . Check  $\{X, Z\}$ :

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



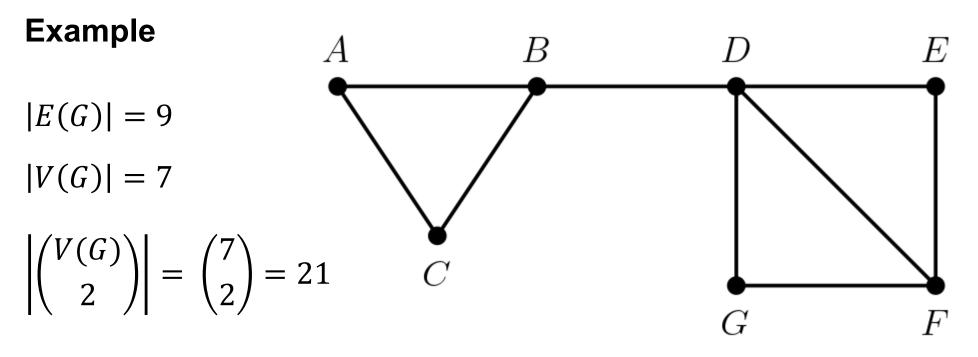
Suppose  $\{X, Y\}, \{Y, Z\} \in E(G)$ . Check  $\{X, Z\}$ :

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



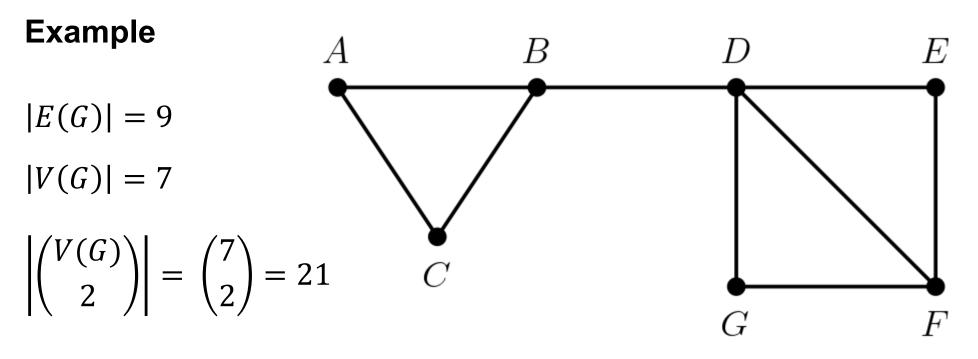
Suppose  $\{X, Y\}, \{Y, Z\} \in E(G)$ . Check  $\{X, Z\}$ :

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



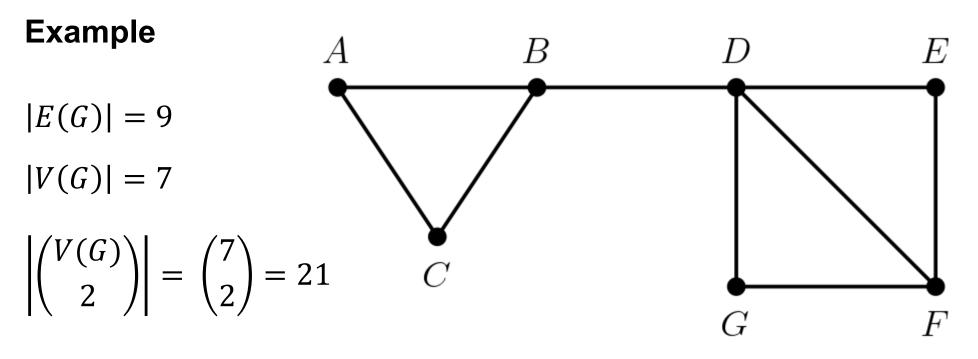
Suppose  $\{X, Y\}, \{Y, Z\} \in E(G)$ . Check  $\{X, Z\}$ :

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



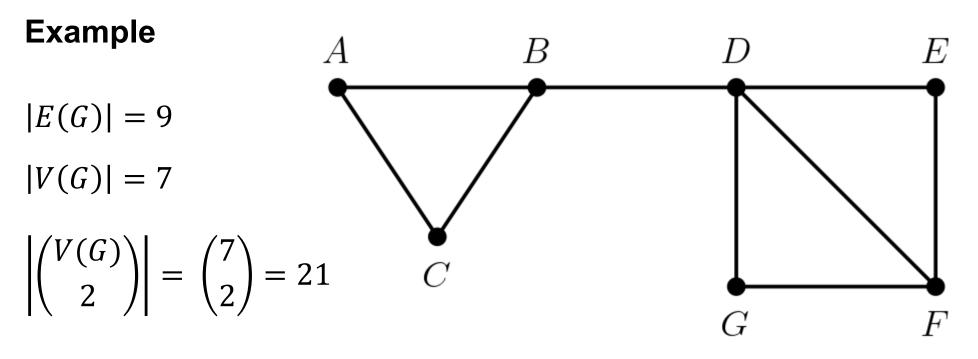
Suppose  $\{X, Y\}, \{Y, Z\} \in E(G)$ . Check  $\{X, Z\}$ :

Actually: If Y = F,  $\{X, Z\} = \{E, G\}$  violates locality. So far: 6 vs. 1.



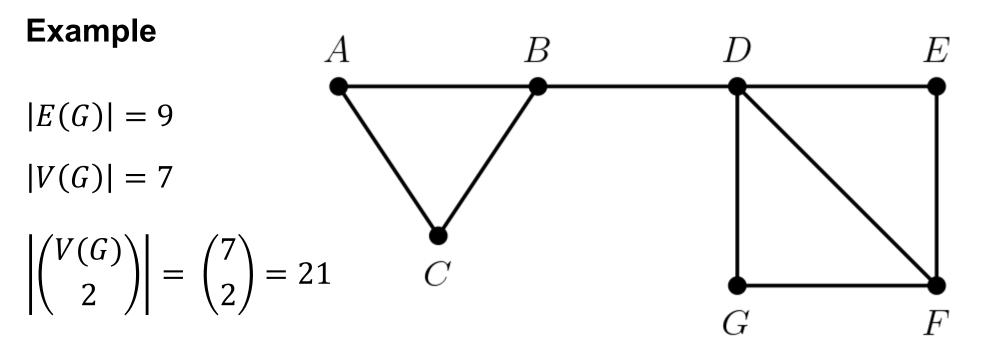
Suppose  $\{X, Y\}, \{Y, Z\} \in E(G)$ . Check  $\{X, Z\}$ :

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



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

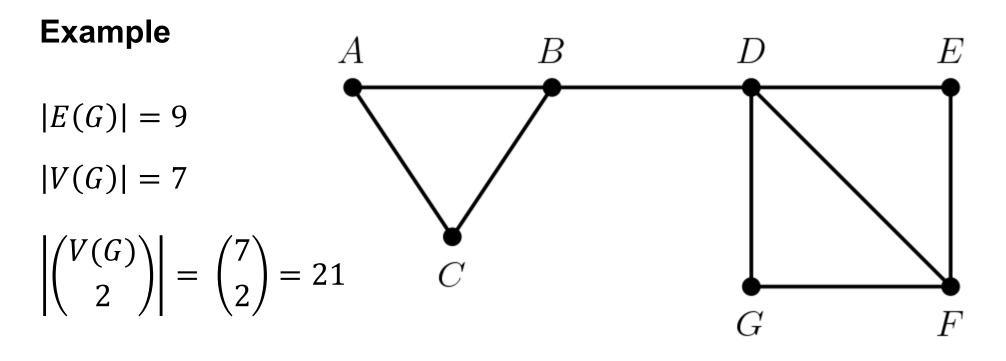
Actually: If Y = D: 4 neighbours, 2 pairs of them adjacent. 9 vs. 7



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

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





**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)

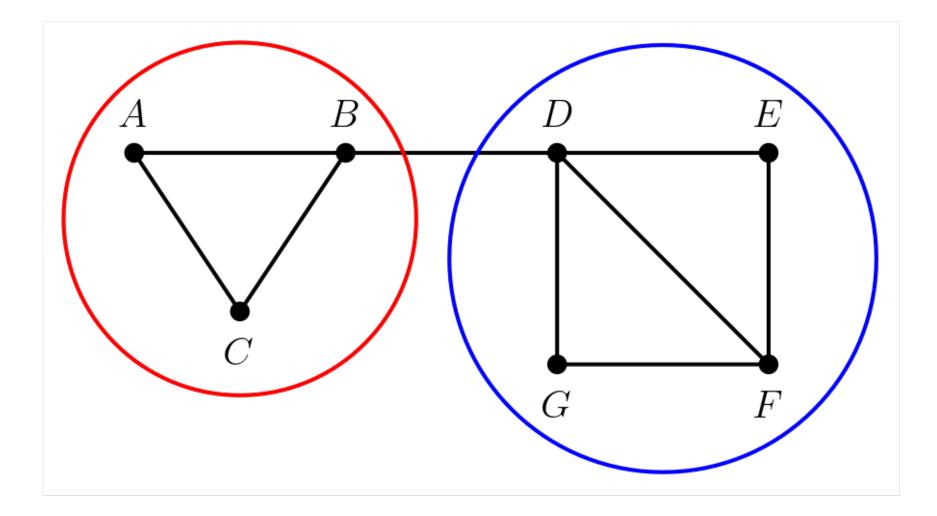
Let  $u, v \in V(G)$ . The usual **distance** function d on a graph is:

d(u, v) = length of shortest path between u and v in G

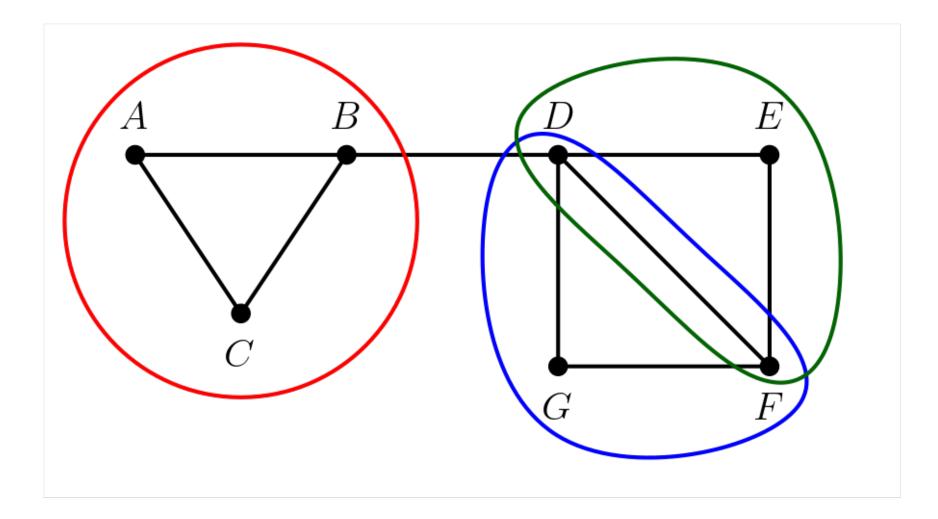
Say we measure **distance between two clusters**  $C_1$  and  $C_2$  via shortest distance between two members, one from each cluster.

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

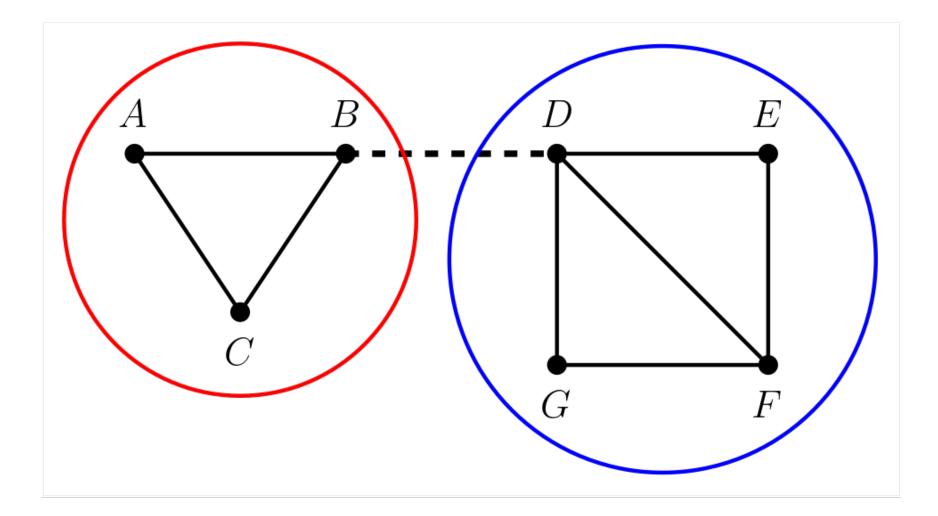








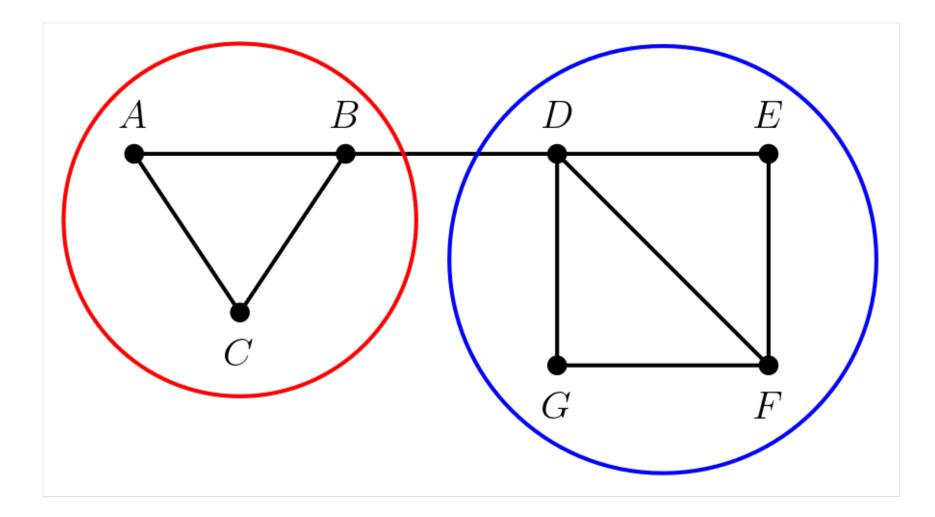






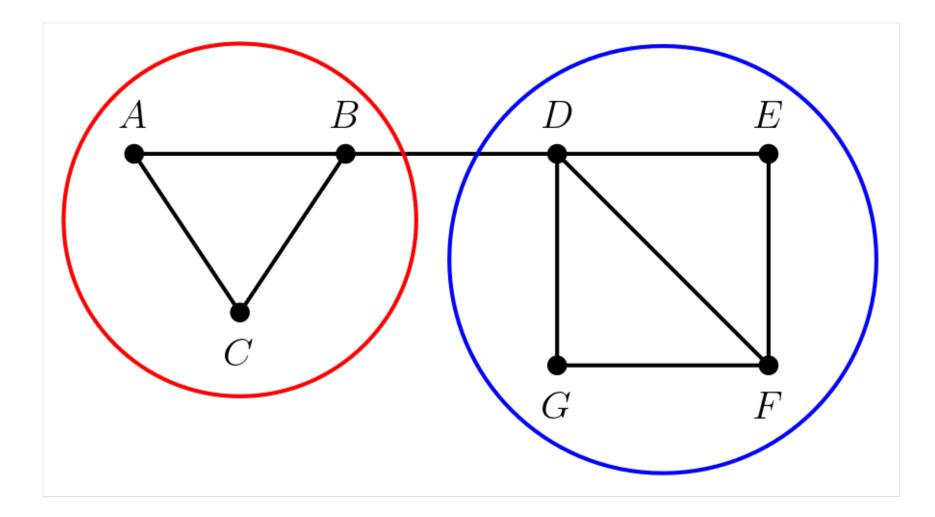
- Let  $e \in E(G)$  whose end vertices lie in different clusters  $C_1^e$ ,  $C_2^e$ . In each merging step, the probability of merging the clusters  $C_1^e$  and  $C_2^e$  is the same for each such edge e.
- At some point (maybe even initially) it becomes likely that we merge two clusters that should not be combined.
- (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.)





- 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).





# 

- 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

#### **Betweenness centrality**

Label each edge  $e = \{u, v\} \in E(G)$  with a score b(e). Define:

$$b(e) = \sum_{\substack{x,y \in V(G) \\ x \neq y}} \frac{\# \text{ shortest } x - y \text{ paths that use } e}{\# \text{ all shortest } x - y \text{ paths}}$$

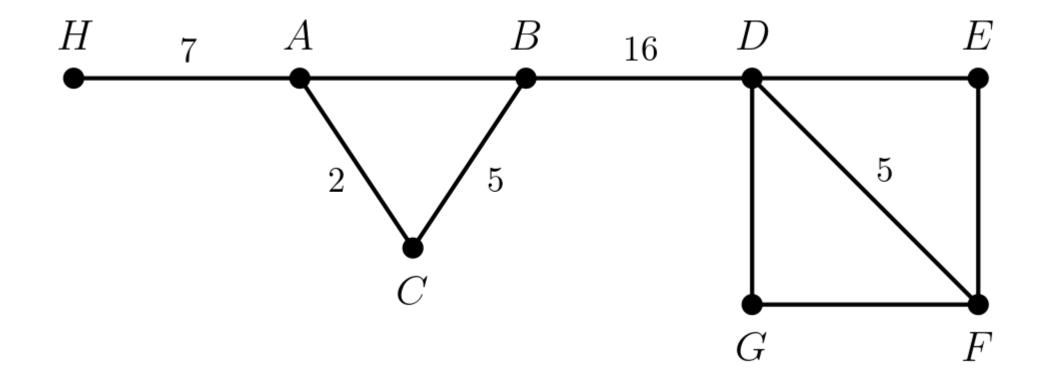
This labelling is called the **betweenness centrality** (sometimes also just called betweenness) **of the edge** *e*. The betweenness (centrality) for vertices is defined analogously.

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**



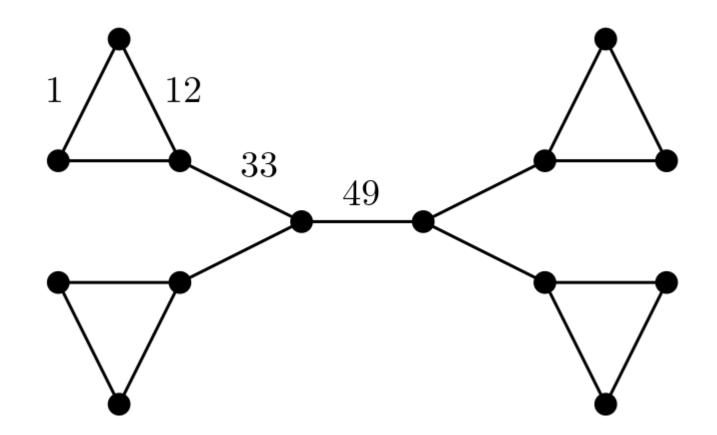
# 

#### 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*.
- Per step: delete the edges of highest betweenness.
  - If some connected component / cluster decomposes into new ones (2 or maybe more), replace cluster by the new connected components (2 or maybe more).
  - If deletion of the edges does not disconnect a cluster, keep it.

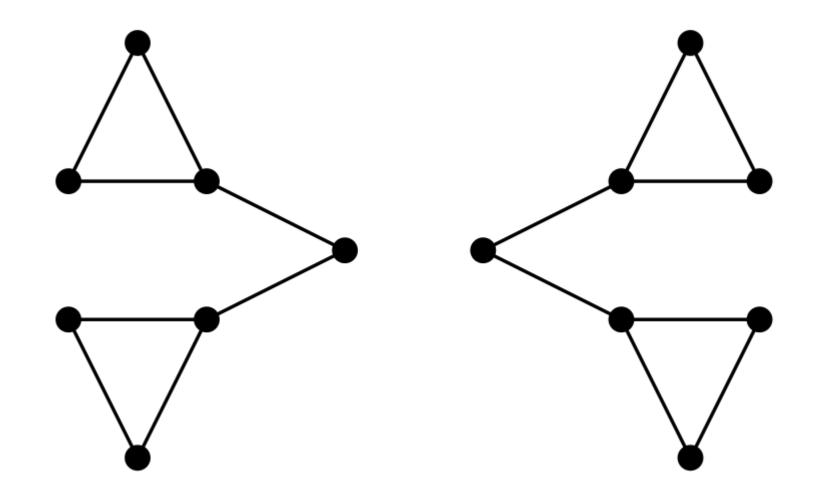


#### Divisive hierarchical clustering via betweenness: Girvan-Newman Algorithm



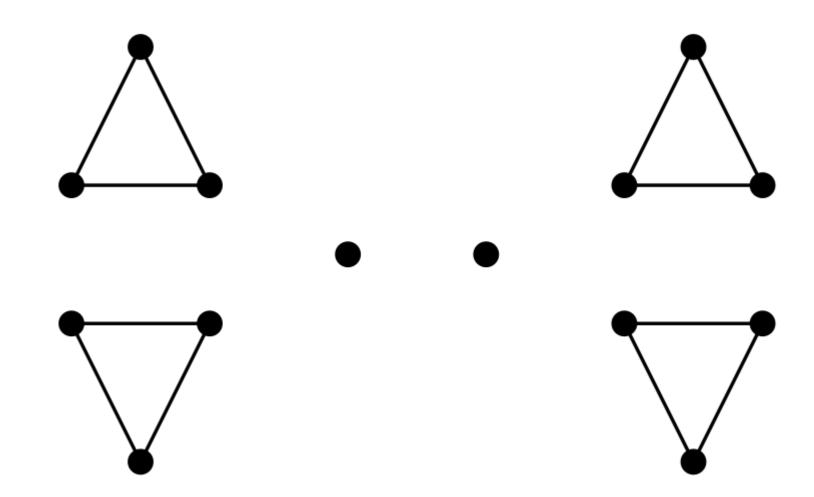


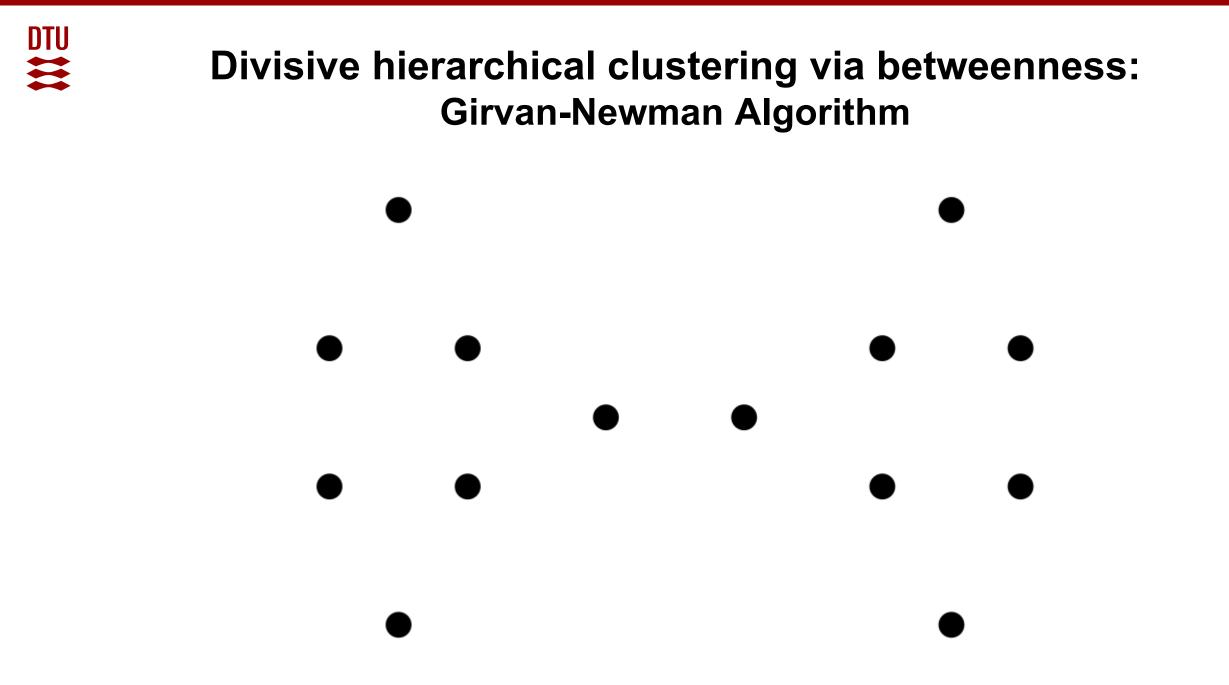
#### Divisive hierarchical clustering via betweenness: Girvan-Newman Algorithm





#### Divisive hierarchical clustering via betweenness: Girvan-Newman Algorithm



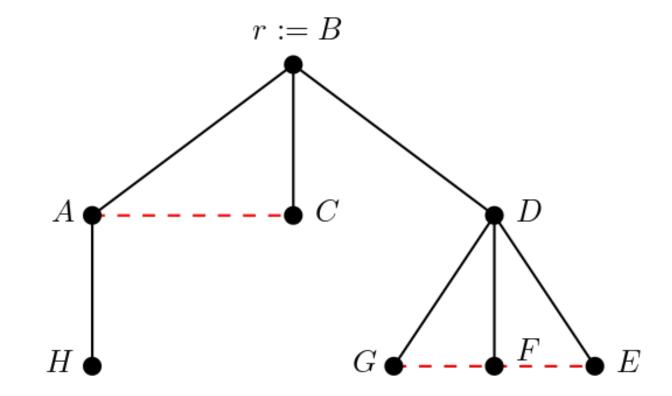


- We need to count shortest paths (that use a specific edge).
- Girvan-Newman Algorithm
  - Count shortest paths from a given start vertex.
  - This is done in 3 steps.
  - We repeat this for every vertex.
  - Eventually, we will have counted each shortest path twice.

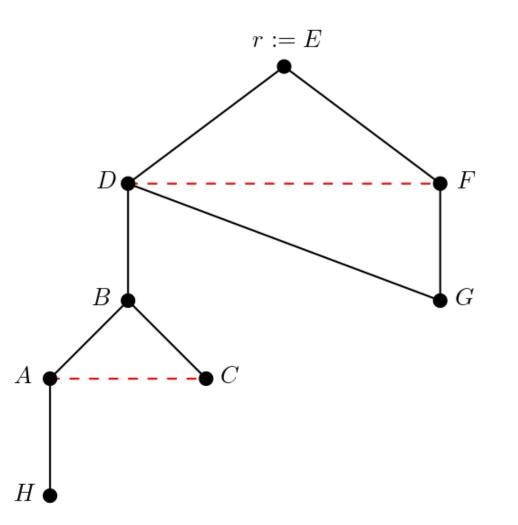
- Let *G* be the given graph with |V(G)| = n and |E(G)| = m for some  $m, n \in \mathbb{N}$ . We **fix a vertex** of *G*, call it *r*.
- Perform a **breadth-first search** (BFS) in *G* with *r* as the root.
- Instead of storing a breadth-first search tree, we store precisely all those edges that lie on some shortest path starting in *r*.
- 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 O(m).

DTU









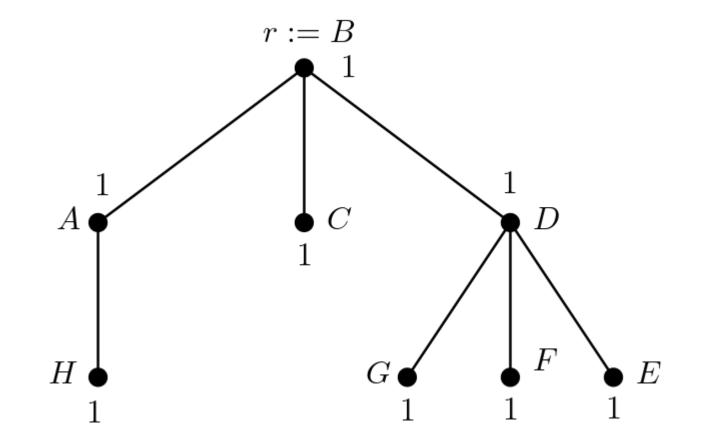
For each vertex v, count # of shortest paths from r ending in v.

- Label r with  $\ell_2(r) := 1$ . (Note that r has distance 0 to itself.)
- Let v be a vertex in distance class  $D_i$  for i > 0. Now label v with:

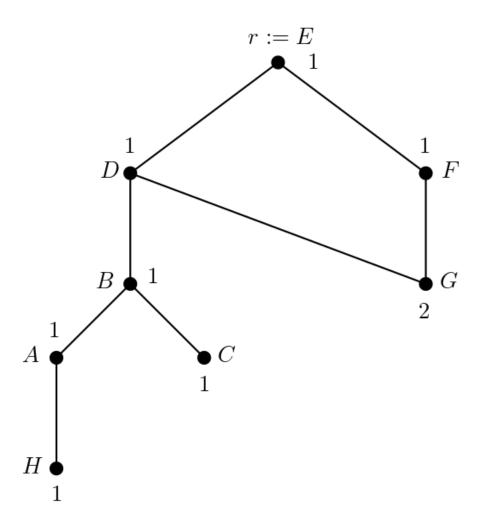
$$\ell_2(v) := \sum_{\substack{w \in D_{i-1} \\ vw \in E(G)}} \ell_2(w)$$

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









#### **Computing betweenness for edges: Step 3**

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

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

To label all edges with this count, we use another auxiliary labelling  $\ell_3$  for the vertices.

### Computing betweenness for edges: Step 3 Intuition:

- Think of  $\ell_3$  and  $b_r$  as flows.
- **BUT** instead of Kirchhoff's law, each vertex consumes a flow of 1.
- We demand that each vertex without neighbours in later distance classes receives a flow of 1.
- Each other vertex must receive (1 + what is sent further).
- How is the total flow (-1) which enters a vertex *w* split among the edges *vw* that enter *w*:

- via the fraction 
$$\frac{\ell_2(v)}{\ell_2(w)}$$
.

#### **Computing betweenness for edges: Step 3**

- Label each vertex v that has no neighbour in a later distance class with:  $\ell_3(v) \coloneqq 1$ .
- Let v be a vertex in distance class  $D_i$  for i > 0 with a neighbour in  $D_{i+1}$ . Now label v with:

$$\ell_3(v) \coloneqq 1 + \sum_{\substack{w \in D_{i+1} \\ vw \in E(G)}} b_r(vw)$$

# DTU

#### **Girvan-Newman Algorithm: Step 3**

- Label each vertex v that has no neighbour in a later distance class with:  $\ell_3(v) \coloneqq 1$ .
- Let v be a vertex in distance class  $D_i$  for i > 0 with a neighbour in  $D_{i+1}$ . Now label v with:

$$\ell_3(v)\coloneqq 1+\sum_{\substack{w\in D_{i+1}\\vw\in E(G)}}b_r(vw)$$

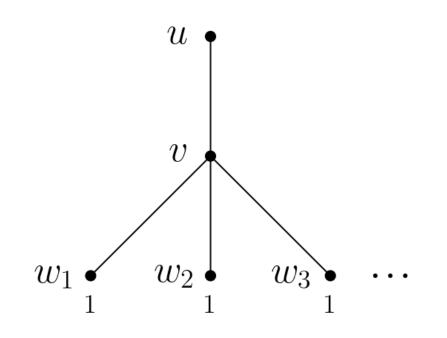
• Let  $w \in D_{i+1}$  and let  $v_1, ..., v_k$  be the neighbours of w in  $D_i$ . Let  $\ell_2$  denote the labelling we have assigned in Step 2. Now label each edge  $v_i w$  by

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

• Let  $\ell_3(w_i) = 1$ .

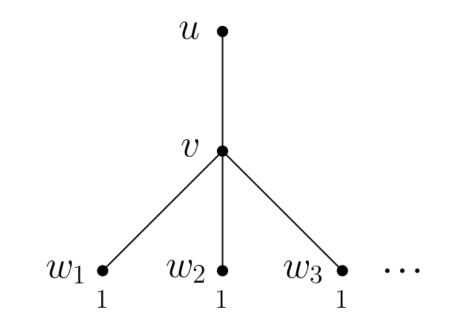
• 
$$b_r(vw_i) = 1 \cdot \frac{\ell_2(v)}{\ell_2(w_i)}$$

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

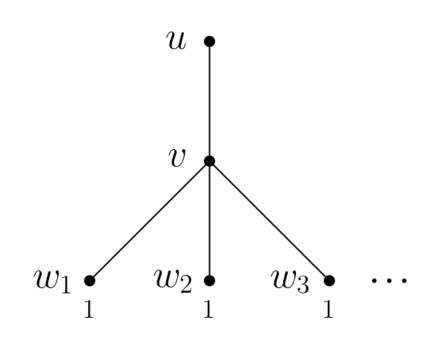


• Let  $\ell_3(w_i) = 1$ .

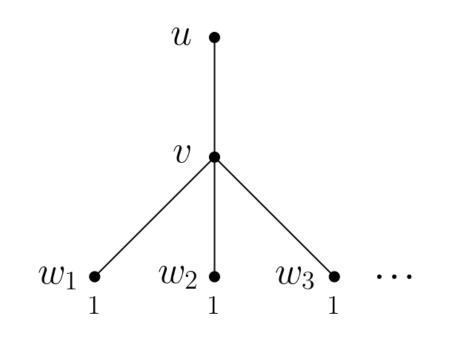
• 
$$b_r(uv) = \ell_3(v) \cdot \frac{\ell_2(u)}{\ell_2(v)} =$$



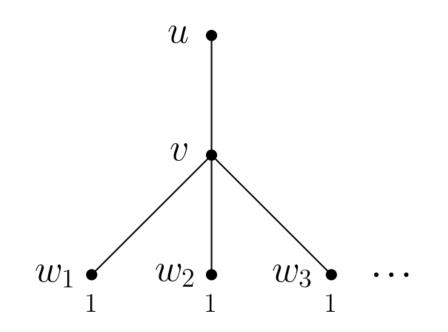
• Let  $\ell_3(w_i) = 1$ . •  $b_r(uv) = \ell_3(v) \cdot \frac{\ell_2(u)}{\ell_2(v)} =$  $= \frac{\ell_2(u)}{\ell_2(v)} + \frac{\ell_2(u)}{\ell_2(v)} \sum_{w_i} b_r(vw_i) =$ 



• Let  $\ell_3(w_i) = 1$ . •  $b_r(uv) = \ell_3(v) \cdot \frac{\ell_2(u)}{\ell_2(v)} =$  $=\frac{\ell_2(u)}{\ell_2(v)}+\frac{\ell_2(u)}{\ell_2(v)}\sum b_r(vw_i)=$  $= \frac{\ell_2(u)}{\ell_2(v)} + \frac{\ell_2(u)}{\ell_2(v)} \sum \frac{\ell_2(v)}{\ell_2(w_i)} =$ 

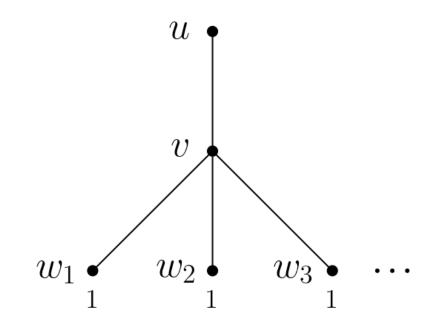


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•  $b_r(uv) = \ell_3(v) \cdot \frac{\ell_2(u)}{\ell_2(v)} =$  $=\frac{\ell_2(u)}{\ell_2(v)} + \frac{\ell_2(u)}{\ell_2(v)} \sum b_r(vw_i) =$  $= \frac{\ell_2(u)}{\ell_2(v)} + \frac{\ell_2(u)}{\ell_2(v)} \sum \frac{\ell_2(v)}{\ell_2(w_i)} =$  $= \frac{\ell_2(u)}{\ell_2(v)} + \sum_{w_i} \frac{\ell_2(u)}{\ell_2(w_i)}$ 

• Let  $\ell_3(w_i) = 1$ .



So  $b_r(uv)$  really counts the fraction of all shortest paths from r that use uv.

# DTU

#### **Computing betweenness for edges**

- In order to compute the betweenness centrality for an edge *e*, we have to perform the three previous steps for every vertex as root.
- Set  $b_r(e) = 0$  if e is not contained in the BFS structure.
- Then we get:

$$b(e) = \frac{1}{2} \sum_{r \in V(G)} b_r(e)$$

- Note that we need to divide by 2 since we count each shortest path twice, namely for each of the two ways of how to traverse the path.
- The running time for the betweenness computation is O(nm). So if our graph is not sparse, then  $O(nm) = O(n^3)$ .
- 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)  $C = (C_1, ..., C_k)$  of V(G) into communities (clusters)  $C_i$ .
- Rough idea: Define *modularity* Q(G, C) as a measure via:

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

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

#### Model for a random graph

- Let G be a graph. Define a random (multi)graph R<sub>d</sub>(G) on the same vertex set which keeps all vertex degrees (# edges incident with a vertex), i.e.:
- 1.  $V(\mathcal{R}_d(G)) = V(G)$ .
- 2.  $d_{\mathcal{R}_d(G)}(v) = d_G(v)$  for every  $v \in V(G)$ .
- Here let  $d_G(v)$  denote the # edges incident with vertex v in G. Hence,  $d_{\mathcal{R}_d(G)}(v)$  denotes the # edges incident with v in  $\mathcal{R}_d(G)$ .
- Idea of building  $\mathcal{R}_d(G)$ : Cut the edges at every vertex and rewire them randomly, allowing multiple edges and loops.

#### Model for a random graph

- Let  $v, w \in V(G)$  and let |E(G)| = m. We enumerate the edges incident with v within G from 1 to  $d_G(v)$ .
- Probability that the *i*-th edge incident with *v* is rewired to some edge incident with *w*:

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

• 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**

- Given a graph *G* with |E(G)| = m and a clustering  $C = (C_1, ..., C_k)$  of V(G) into communities  $C_i$ .
- Define **modularity** Q(G, C) as:

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

- Here  $A_{vw}$  is the indicator function:  $A_{vw} = \begin{cases} 1, & \text{if } vw \in E(C_i) \\ 0, & \text{if } vw \notin E(C_i) \end{cases}$
- We scale the sum by  $\frac{1}{2m}$  to get the range for Q(G, C) within [-1, 1].
- Usually: Q(G, C) > 0,3 is an indicator for good community structure.



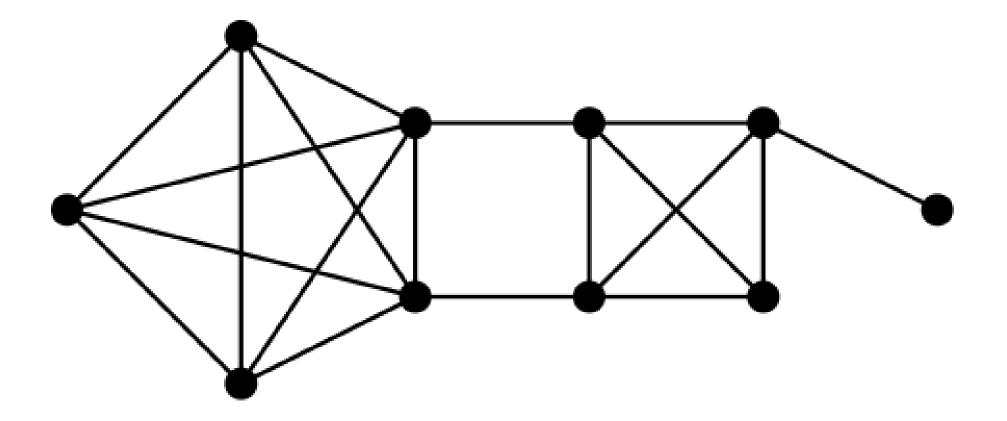
# Spectral clustering

#### **Spectral clustering**

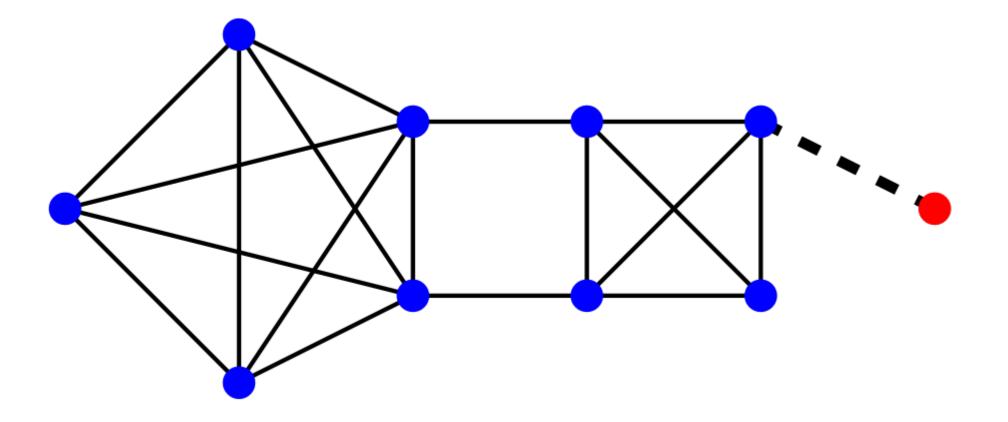
- Let G be a simple undirected graph.
- Task: Partition V(G) into two classes (clusters) such that:
  - 1. we maximise the # of edges within the clusters, and
  - 2. we minimise the # of edges between the clusters.
- For two vertex sets  $A, B \subseteq V(G)$  let E(A, B) denote the set of edges that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

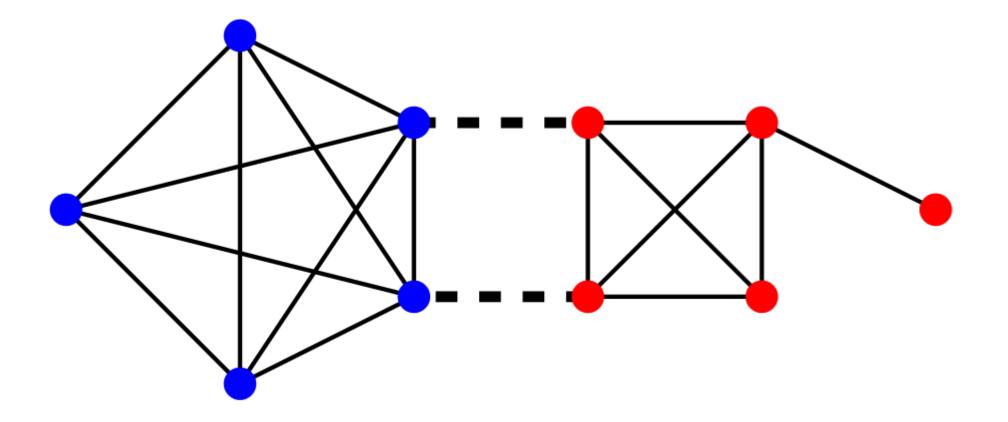












- Better: Consider *normalised cuts* and minimise.
- Let *E*(*A*, *B*) be a cut of G. Then the *normalised cut value* is:

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

Here  $vol(A) \coloneqq \sum_{v \in A} d(v)$ .

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

DTU

#### Spectral clustering: "good" cut

• Let *E*(*A*, *B*) be a cut of G. Then the *normalised cut value* is:

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

Here 
$$vol(A) \coloneqq \sum_{v \in A} d(v)$$
.

Or consider: RatioCut

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

#### Adjacency matrix of a graph

- Let *G* be a simple undirected graph with |V(G)| = n. Enumerate the vertices of *G* by  $v_1, ..., v_n$ .
- 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  $a_{ij} = 0$ .

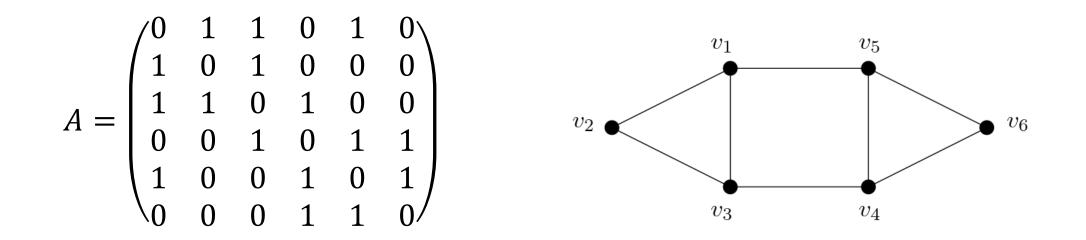
• If Ax = y, then the following holds for the *i*-th component  $y_i$  of *y*:  $y_i = \sum_{j=1}^n a_{ij} x_j = \sum_{v_i v_j \in E(G)} x_j$ 

70



#### Adjacency matrix of a graph

Example:



#### 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  $\Lambda = {\lambda_1, ..., \lambda_n} \subseteq \mathbb{R}$  of its **eigenvalues**. Usually we sort  $\Lambda$  by  $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ .
- Recap (eigenvalue  $\lambda$  and one eigenvector x of it):

$$Ax = \lambda \cdot x$$

#### **Recap: symmetric matrices**

#### • A(G) = 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  $\ge 0$ ).
- Fact: A is positive semidefinite iff  $x^T A x \ge 0$  for all  $x \ne 0$ .

# **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 *d*-regular).

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

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

Actually:

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

### **Some intuition:** *d***-regular graphs**

• As special case: Let *G* be *d*-regular with precisely **2 components**, say *A* and *B*.

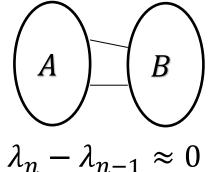
$$A \cdot \underbrace{\left(1, \dots, 1\right)}_{A}, \underbrace{0, \dots, 0}_{B}\right)^{T} = d \cdot \underbrace{\left(1, \dots, 1\right)}_{A}, \underbrace{0, \dots, 0}_{B}\right)^{T}$$
$$A \cdot \underbrace{\left(0, \dots, 0\right)}_{A}, \underbrace{1, \dots, 1}_{B}\right)^{T} = d \cdot \underbrace{\left(0, \dots, 0\right)}_{A}, \underbrace{1, \dots, 1}_{B}\right)^{T}$$

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

• Intuition:

$$\left(\begin{array}{c} A \\ B \\ \lambda_n - \lambda_{n-1} = 0 \end{array}\right)$$

few edges



#### **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  $L = L(G) \in \mathbb{R}^{n \times n}$  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  $(1, ..., 1)^T$ .
- *L* is positive semidefinite, hence  $x^T L x \ge 0$  for all  $x \ne 0$ ..

#### **General case**

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

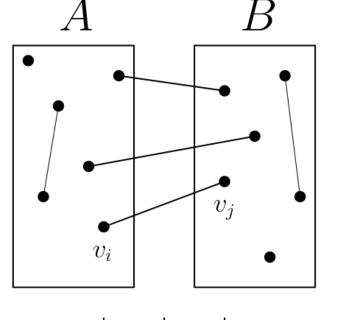
$$\lambda_2 = \min_{x} x^T L x = \sum_{v_i v_j \in E(G)} (x_i - x_j)^2$$

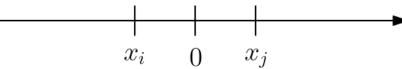
- Furthermore, a minimising vector x is an eigenvector for  $\lambda_2$ .
- **Partitioning:** Put all  $v_i$  with  $x_i < 0$  into set *A*, the rest into set *B*. This yields bipartition of V(G).

#### **General case**

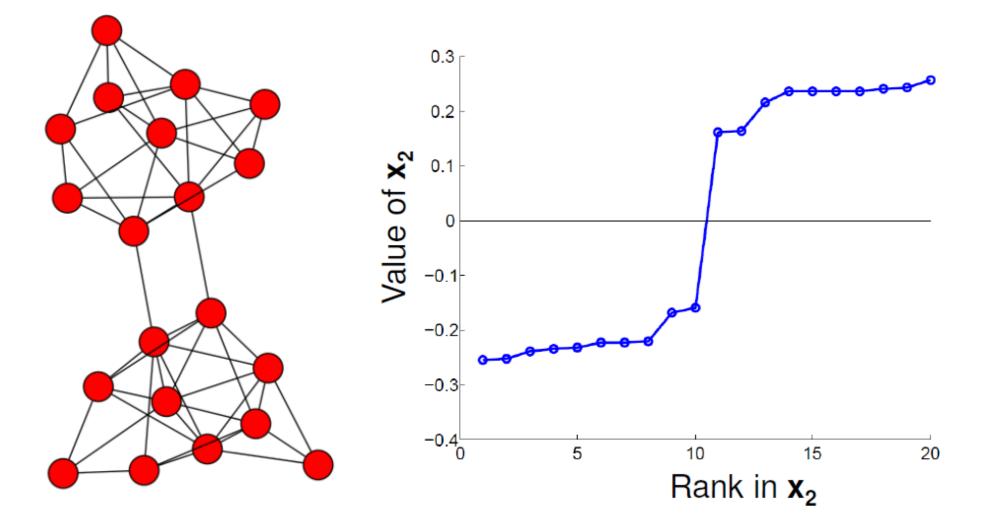
$$\lambda_2 = \min_{\substack{x \\ \sum_i x_i = 0}} x^T L x = \sum_{\substack{v_i v_j \in E(G)}} (x_i - x_j)^2$$

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

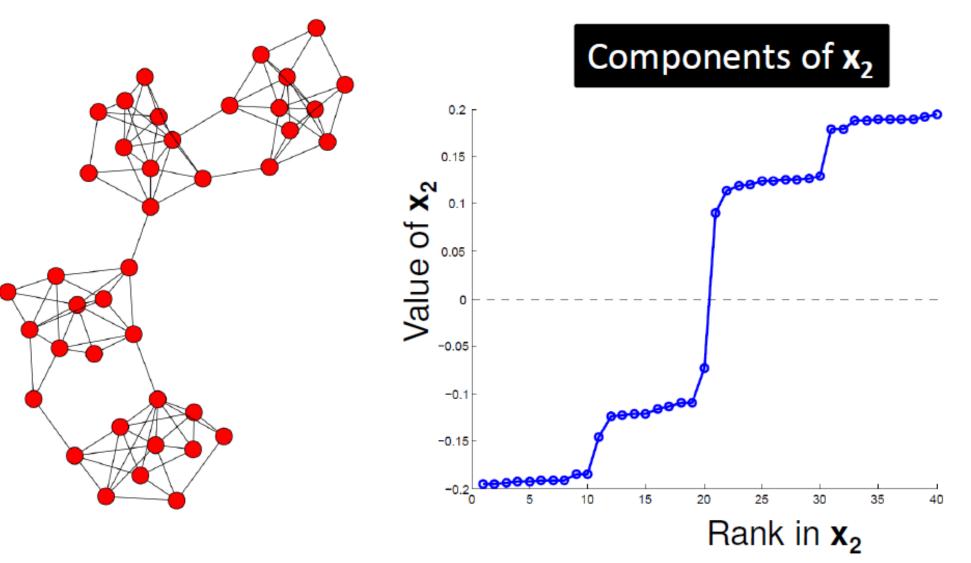












# Indication for good balanced partition

• Let E(A, B) be a cut of G. Then define:

$$\alpha = \alpha(A, B) = \frac{|E(A, B)|}{\min\{|A|, |B|\}}$$

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

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

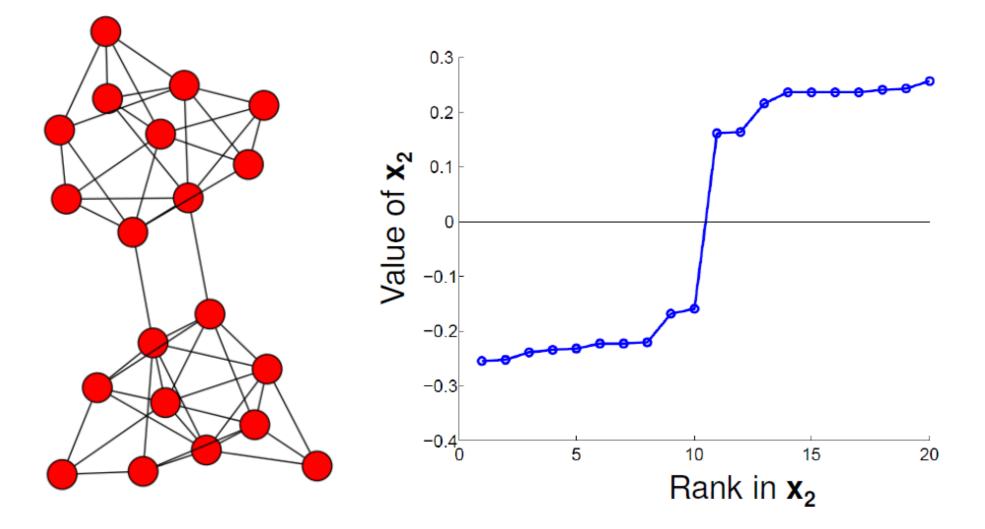
• Hence, we approximately (at most factor 2) find some balanced (w.r.t.  $\alpha$ ) cut E(A, B) via an eigenvector of L corresponding to  $\lambda_2$ .

# 

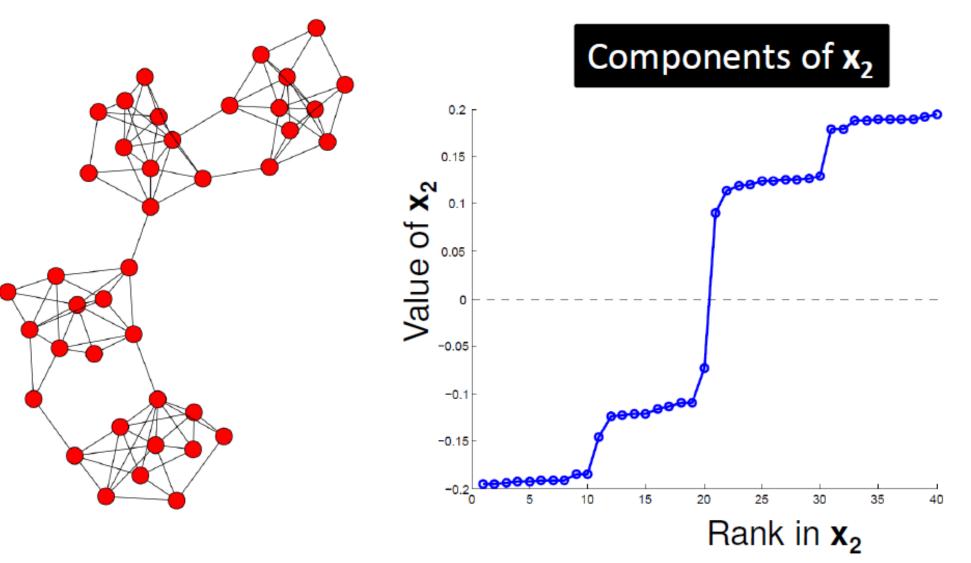
# Spectral clustering mixed with *k*-means

- Often: building the bipartition (A, B) for V(G) from the components of the eigenvector  $x_2$  of  $\lambda_2$  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  $\mathbb{R}^{k-1}$ .









# 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.

### **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).
- 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.
- 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.