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Social Network Analysis: Graph Clustering

Lecture follows [1]. Citations of [1] are mostly omitted because of simplicity

Graph Clustering

- Given directed, weighted graph G=(V,E,w); A graph clustering **C**={C_1, C_2, ..., C_k} is a partition of V into non-empty subsets C_i;
- Notations:
  - E(C_i,C_j): Set of edges in G from C_i to C_j;
  - $E(\mathbf{C}) = \cup_{i=1,\dots,k} E(C\_i)$: Set of intra-cluster edges;
  - $\overline{E(\mathbf{C})} = E \setminus E(\mathbf{C})$: Set of inter-cluster edges;
  - $m(\mathbf{C}) = |E(\mathbf{C})|$; $\overline{m}(\mathbf{C}) = |\overline{E(\mathbf{C})}|$;
  - G([C_i]): subgraph induced by C_i;
  - **C** with k=1: *1-clustering*; **C** with k=|V|: *singletons*; (both: *Trivial clustering);* **C** with k=2: *cut;*
  - **A**(G): Set of all possible clusterings on G;

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- Notations (continued):
  - Let **C_1**={C_1, C_2, ..., C_k} and **C_2**={C'_1, C'_2, ..., C'_l}:
    C_1 ≤ **C_2** ↔ ∀i ∃j : C_i ⊆C'_j;
    C_1: *refinement of* **C_2; C_2:** *coarsening of* **C_1;**
  - *Chain* (comparable set) of clusterings: *hierarchy;*
  - Hierarchy is *total* ←→ Both trivial clusterings are contained;
  - Hierarchy that contains one clustering for each {1,2,...,|V|}: *complete;*
  - S(V): *(Proper) Cut function*: Cutting the node-set in two (non-empty) subsets: S(V) and V \ S(V);

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Quality Measures for Clusterings

- Quality measure: Objective function **A**(G) → $\mathbb{R}$ that formalizes the clustering paradigm in a special way

- G= (V,E,w): Weight function w: E→ $\mathbb{R}^+$ is interpreted as "similarity" (higher weights correspond to more intense tie); also possible: negative weights = dissimilarity; or w: E → [0,1] or w: E → [-1,1] etc.

- Distinguish between no edge and edge with weight zero;

- Notation: $w(E) = \sum_{e \in E} w(e)$

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6: Graph Clustering

- General framework for a quality index of a clustering:

$$index(\mathbf{C}) = \frac{f(\mathbf{C}) + g(\mathbf{C})}{\max\{f(\mathbf{C}') + g(\mathbf{C}') : \mathbf{C}' \in \mathbf{A}(G)\}}$$

- $f : \mathbf{A}(G) \rightarrow \mathbb{R}^+$ measures intra cluster density (coherence);
  $g : \mathbf{A}(G) \rightarrow \mathbb{R}^+$ measures inter cluster sparseness (decoherence);

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Coverage

- First quality measure: Coverage

$$\gamma(\mathbf{C}) = \frac{w(E(\mathbf{C}))}{w(E)} = \frac{\sum_{e \in E(\mathbf{C})} w(e)}{\sum_{e \in E} w(e)}$$

- Thus: f = w(E(**C**)) and g = 0; → only accumulated intra cluster density is measured
- Maximum value 1 achieved for **C**={V} (1-clustering)
- A clustering has coverage $\gamma(\mathbf{C})=1$ iff $\overline{E}(\mathbf{C})=\varnothing$ (clustering is composed of connected components of G) or $w(\overline{E}(\mathbf{C}))=0$
- **C** with k>1 can be transformed into **C´** with k´<k and γ(**C**) ≤ γ(**C´**) by merging two clusters in **C** → optimal non-trivial **C** is a minimum cut
- → „Monotonic“ behavior of coverage → coverage is not a good sole quality index

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Conductance

- Clustering paradigm reformulated: Clusters should be well connected (many edges need to be removed to make it unconnected); few inter cluster edges (ideally none)
- Conductance: Measure for bottlenecks (Bottleneck: Cut that separates V into roughly same size halves and “cuts across” relatively few edges)
- Let **C**={C_1, V \ C_1} be a cut. Conductance φ of **C** is defined as

$$\varphi(\mathbf{C}) = \begin{cases} 1 & \text{if } C\_1 \in \{\varnothing, V\} \\ 0 & \text{if } C\_1 \notin \{\varnothing, V\},\ w(\overline{E(\mathbf{C})})=0 \\ \dfrac{w(\overline{E(\mathbf{C})})}{\min\left(\sum_{e \in E(C\_1, V)} w(e), \sum_{e \in E(V \setminus C\_1, V)} w(e)\right)} & \text{otherwise} \end{cases}$$

the smaller φ(**C**), the more „bottlenecky“ is **C**

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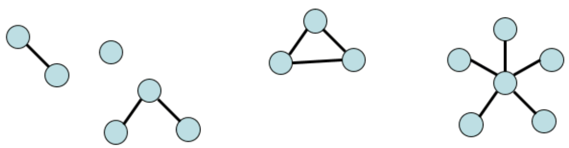
- Conductance φ of G is defined as

$$\varphi(G) = \min_{C\_1 \subseteq V} \varphi(C\_1, V \setminus C\_1)$$

- Small conductance ←→”good cut possible”
- All unconnected graphs have conductance 0
- Theorem: If G is undirected and positively weighted, G has maximum conductance φ(G)=1 iff G is connected and has at most three nodes or is a star.



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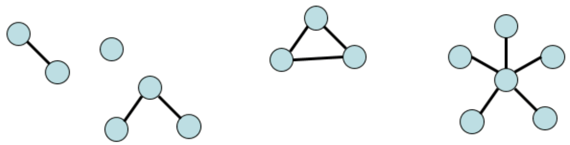

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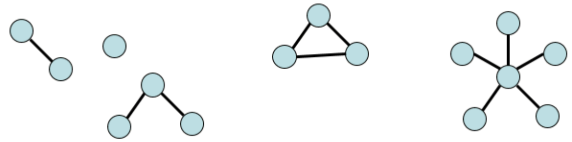

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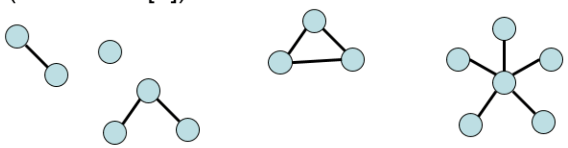

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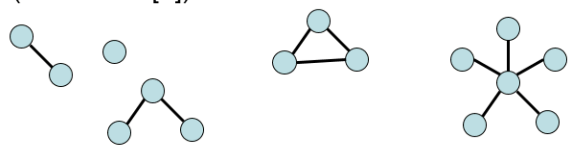

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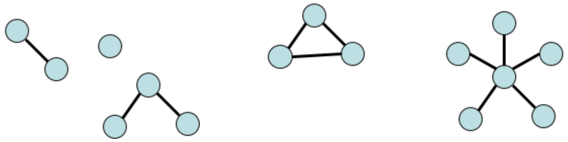

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Conductance

- Conductance appears to be a good element for a quality measure, but: calculating it is NP hard ☹ but: it can be approximated with guarantee $O((\log |V|)^{1/2})$ (see [1]) (This means: approximation * $O((\log |V|)^{1/2})$ = true value)

- The conductance of a complete graph is asymptotically 0.5: Let n be an integer:

$$\varphi(K_n) = \begin{cases} 0.5\frac{n}{n-1} & \text{if } n \text{ is even} \\ 0.5 + \frac{1}{n-1} & \text{if } n \text{ is odd} \end{cases}$$

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- With conductance we can define two appropriate quality measures for clusterings:

- First measure: g=0 and $f(\mathbf{C}) = \min_{1\le i\le k} \varphi(G[C\_i])$

- If the measure is small: At least one of the clusters (more precisely: the induced subgraph) contains at least one bottleneck → This cluster is too coarse →Use minimum conductance cut to cut this cluster in "halves"

- From theorem before: Only clusterings where the clusters induce subgraphs that are stars or have size at most three have f=1 (f is called *intra cluster conductance*)

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- Second measure: f=0 and

$$g(\mathbf{C}) = \begin{cases} 1 & \text{if } \mathbf{C} = \{V\} \\ 1 - \max_{1 \le i \le k} \varphi(\mathrm{C\_i},\ V \setminus \mathrm{C\_i}) & \text{otherwise} \end{cases}$$

- If the measure is small: At least one of the clusters (more precisely: the induced subgraph) has many connections to outside → The clustering is too fine →Merge clusters
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Performance

- Main idea: Clustering paradigm → Count “correctly classified pairs of nodes”. A pair of nodes is correctly classified if:
  - It is in the same cluster AND connected by an edge → f counts the number of edges within clusters
  - If it is not in the same cluster AND not connected by an edge →g counts the number of non-existent edges between clusters

$$f(\mathbf{C}) = \sum_{i=1}^{k} |E(\mathrm{C\_i})|$$

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$$f(\mathbf{C}) = \sum_{i=1}^{k} |E(\mathrm{C\_i})|$$

$$g(\mathbf{C}) = \sum_{u,v \in V} [(u,v) \notin E] * [u \in \mathrm{C\_i}, v \in \mathrm{C\_j}, i \neq j]$$

Iverson-notation: [L]=1 if L is true

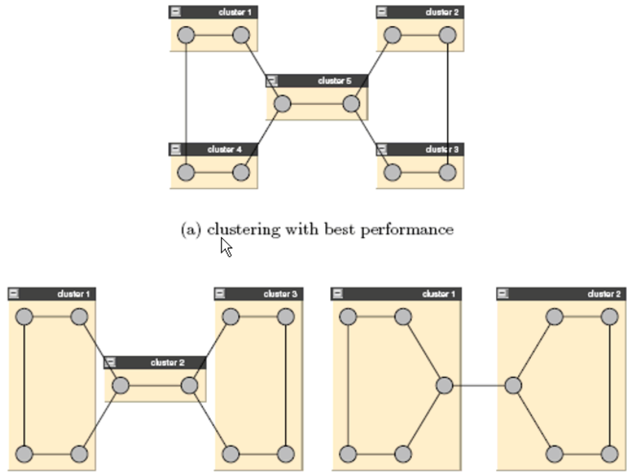
Performance

- Calculating the maximum of f+g is NP-hard (In fact calculating the maximum of f+g would in essence be calculating the optimal clustering) →use |V| (|V|-1) as normalization for quality measure
- The performance index is then:

$$\mathrm{perf}(\mathbf{C}) = \frac{f(\mathbf{C}) + g(\mathbf{C})}{|V|(|V|-1)}$$

- Problems with Performance: when graph is sparse (example: planar graphs: |E| is linear in |V|). Tendency: Performance delivers many small clusters

Performance



(a) clustering with best performance

(b) intuitive clustering (c) another intuitive clustering

Fig. 8.4. A situation where the clustering with optimal performance is a refinement (Figure 8.4(b)) of an intuitive clustering and is skew (Figure 8.4(c)) to another intuitive clustering

Performance

- If using weighted edges → some modifications:
  - use weights normalized to 1 → Max weight M = 1

$$f(\mathbf{C}) = \sum_{i=1}^{k} w(E(C\_i))$$

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Performance

- In that version g neglects the individual inter-cluster edges → Introduce g_w

$$g'(\mathbf{C}) = g(\mathbf{C}) + \underbrace{M\,|\overline{E(\mathbf{C})}| - w(\overline{E(\mathbf{C})})}_{g_w(\mathbf{C})}$$

- Overall index is then:

$$\text{perf}_w(\mathbf{C}) = \frac{f(\mathbf{C}) + g(\mathbf{C}) + \vartheta\, g_w(\mathbf{C})}{M(|V|(|V|-1))}$$

- other possibility: minimize incorrectly classified edges (dual problem)

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Other Indices

- If density measure π on graphs is available:

$$\begin{aligned} \text{worst case: } & \min_i\{\pi(G[C_1]), \ldots, \pi(G[C_k])\} \\ \text{average case: } & \frac{1}{k}\sum_i \pi(G[C_i]) \\ \text{best case: } & \max_i\{\pi(G[C_1]), \ldots, \pi(G[C_k])\} \end{aligned}$$

- (especially suitable in metric spaces)

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- What have we seen so far? Measures for cluster quality
- But how do we compute such clusters?
- First group of methods: Greedy approaches

greedy minimization:

```
let L0 be a feasible solution;
i ←0;
while({L | L∈N(Li), c(L)<c(Li)} ≠ Ø) {
        Li+1 ← argminL∈N(Li) c(L);
        i ← i+1;
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```

Space of all solutions L that can be constructed from solution L_i

c(L) is the cost of solution L

Graph Clustering Algorithms

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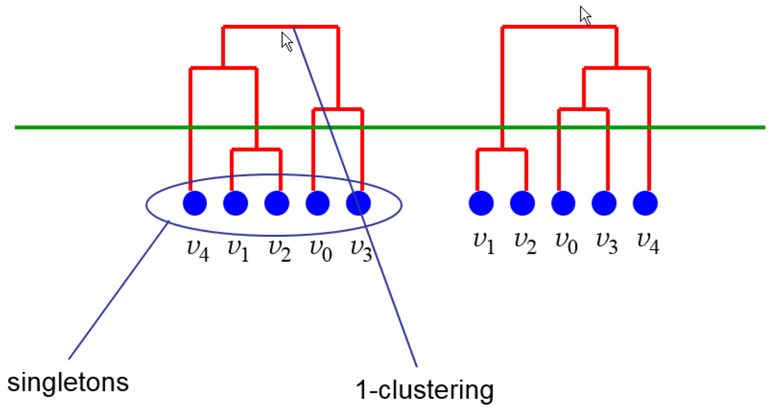
- For greedy maximization substitute argmax and >
- What function do we use as c(L) → cluster quality measures modeling the clustering paradigm
- How do we construct solutions (clusterings) from other solutions: Merging or splitting of clusters → a hierarchy of clusters results → "Dendrogram"

- Advantage of Dendrograms: Can be "**cut**" at any desired number of clusters.



Graph Clustering Algorithms

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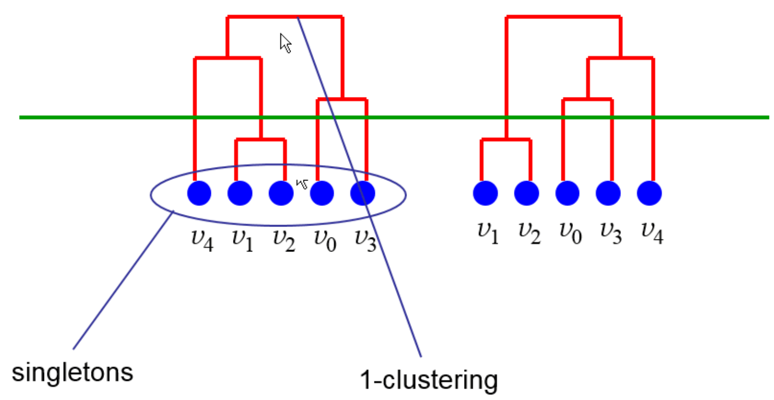

Graph Clustering Algorithms

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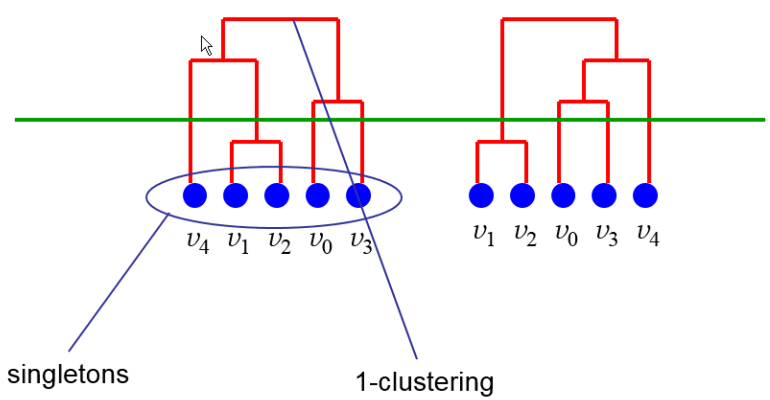

Graph Clustering Algorithms

- Linkage (Agglomeration): Iteratively coarsens a given clustering by merging two clusters until 1-clustering is reached ("bottom up")
- Splitting (Division): Iteratively refines a given clustering by splitting one cluster until slingleton clustering is reached ("top down").

- Linkage:

  P(V) := 2^V =: power-set

  - Given: G=(V,E,w); initial clustering $\mathbf{C}_1$;
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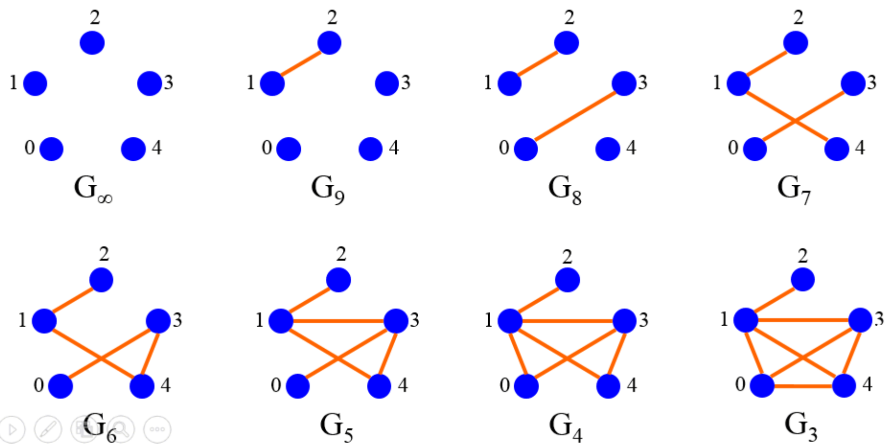
Linkage

- Example

weight matrix:

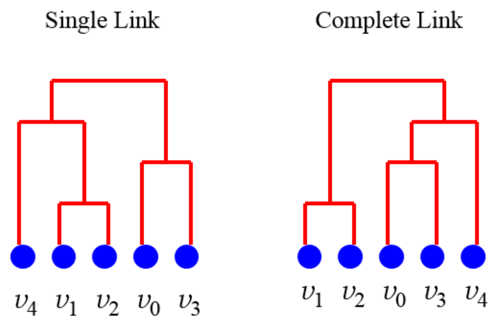
	v_0	v_1	v_2	v_3	v_4
v_0	∞	4	2	8	3
v_1	4	∞	9	5	7
v_2	2	9	∞	0	1
v_3	8	5	0	∞	6
v_4	3	7	1	6	∞

Threshold graphs:



Linkage

Resulting dendrograms:



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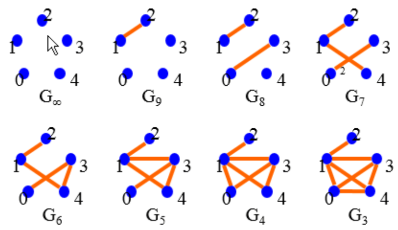
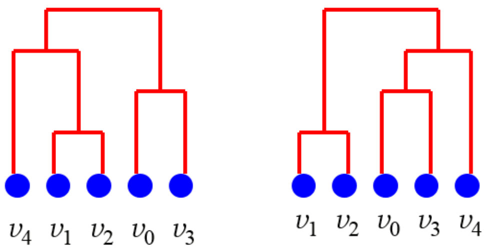


Resulting dendrograms:

Single Link   Complete Link



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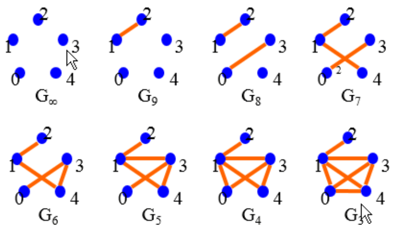

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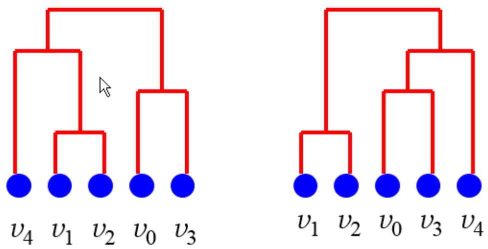

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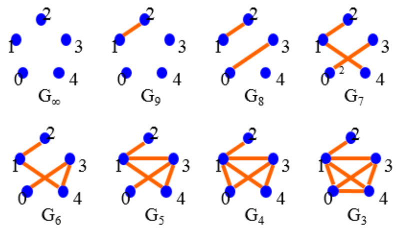

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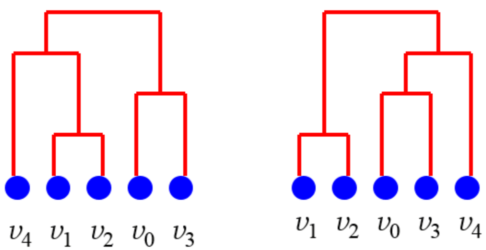

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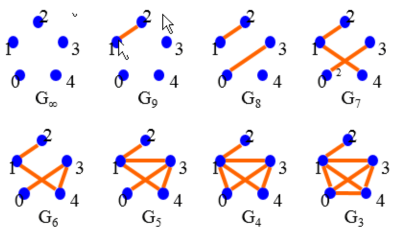

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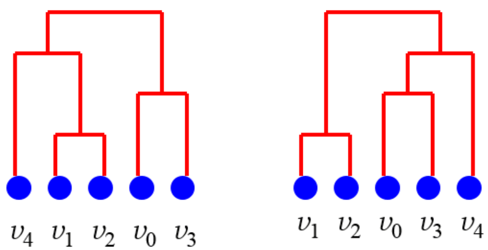

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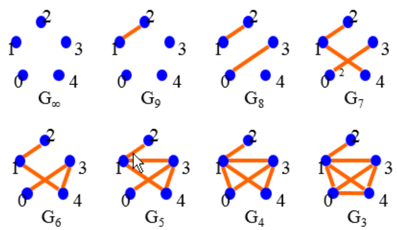

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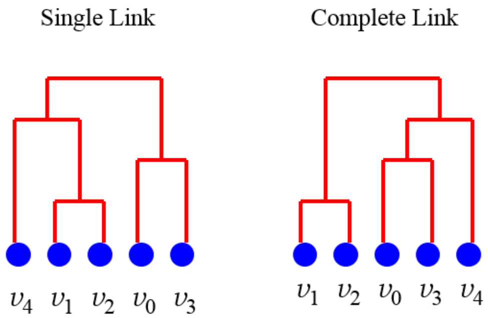

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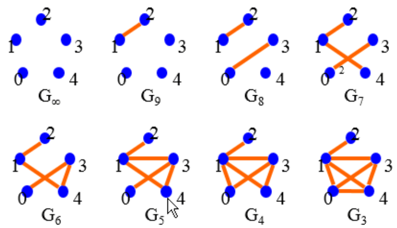

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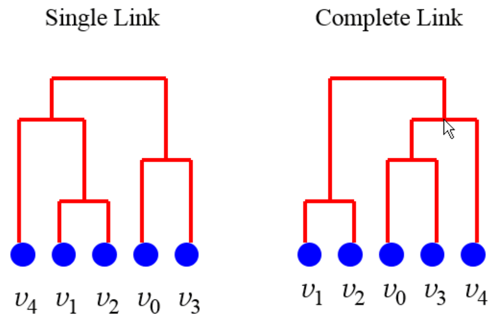

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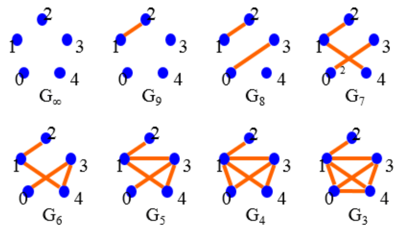

Linkage

- Instead of the weight matrix

weight matrix:

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we may as well use an "equivalent" distance matrix $d(i,j) = d_{ij}$, e.g.

$$\begin{pmatrix} 0 & 6 & 8 & 2 & 7 \\ 6 & 0 & 1 & 5 & 3 \\ 8 & 1 & 0 & 10 & 9 \\ 2 & 5 & 10 & 0 & 4 \\ 7 & 3 & 9 & 4 & 0 \end{pmatrix}$$

and would have to modify the threshold graph based algorithm(replace < with > and ≥ with ≤ and ∞ with 0) (or set weight = 1/distance). Then this algorithm implements precisely the aforementioned cost function

$$c_{local}(C_i, C_j) = \begin{matrix} \max \\ \min \end{matrix} \{ d(u,v) \mid u \in C_i, v \in C_j \}$$

Complete Linkage   Single Linkage

Splitting

- Given: $G=(V,E,w)$; initial clustering $\mathbf{C}_1$;
- Given: Either c_{global}: $A(G) \rightarrow \mathbb{R}^+$

  c_{local}: $P(V) \times P(V) \rightarrow \mathbb{R}^+$ (for splitting operations) or

  c_{global}: $A(G) \rightarrow \mathbb{R}^+$ and cut function $S: P(V) \rightarrow P(V)$ or

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- $i \rightarrow i+1$: Split that cluster where the resulting clustering yields the minimum global cost or

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Splitting

C_x: one of the clusters

one “half” of the split of C_x

strictly global

strictly local

semi global

semi local

one “half” of the cut (split) of some C_x, defining the cut

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Splitting

- Cut function avoids having to test all possible splits
  - Variants of Cut functions:

$$S(V) := \underset{\emptyset \neq V' \subset V}{\operatorname{argmin}} \; \omega(E(V', V \setminus V'))$$

$$S_{\text{ratio}}(V) := \underset{\emptyset \neq V' \subset V}{\operatorname{argmin}} \; \frac{\omega(E(V', V \setminus V'))}{|V'| \cdot (|V| - |V'|)}$$ [1]

$$S_{\text{balanced}}(V) := \underset{\emptyset \neq V' \subset V}{\operatorname{argmin}} \; \frac{\omega(E(V', V \setminus V'))}{\min(|V'|, (|V| - |V'|))}$$

$$S_{\text{conductance}}(V) := \underset{\emptyset \neq V' \subset V}{\operatorname{argmax}} \; \delta(V') = \underset{V' \subset V}{\operatorname{argmin}} \; \varphi(V', V \setminus V')$$

inter cluster conductance (slide 14):

$$g(\mathbf{C} = \{V', V \setminus V'\}) = \delta(V') = \begin{cases} 1 & \text{if } \mathbf{C} = \{V, \{\}\} \\ 1 - \varphi(V', V \setminus V') & \text{otherwise} \end{cases}$$

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Shifting

shifting minimization:

```
let L0 be a feasible solution;
i ←0;
while({L | L∈N(Li)} ≠ Ø){
      choose Li+1 from N(Li)according to ☺;
      i ← i+1;
}
```

- Choosing schema ☺ can be either based on potential function φ, on random selection or based on genetic algorithms with fitness function etc.
- Potential function φ: A(G) x A(G) → $\mathbb{R}$ based: Chose a new clustering $\mathbf{C}_{i+1}$ so that $\varphi(\mathbf{C}_i, \mathbf{C}_{i+1}) > 0$

Newman Girvan Method: Centrality-based Splitting + Modularity

Last example of this part: bringing it all together (see [3]):

- Observations → critique on agglomerative methods: fail to cluster peripheral nodes correctly [3] → Newman Girvan method: Divisive hierarchical clustering (splitting) + Modularity:

1. Calculate edge betweenness for all edges
2. Remove edge with highest edge betweenness
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→ dendrogram

- Use Modularity as intra cluster coherence (f) cluster validity measure (g=0) to optimally cut dendrogram:

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Newman Girvan Method: Centrality-based Splitting + Modularity

Last example of this part: bringing it all together (see [3]):

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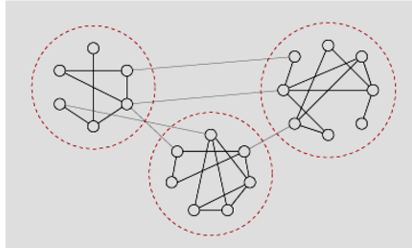

[3]

- k clusters → k x k symmetric matrix **e**: e_{ij} = |E(C_i,C_j)| / |E| : fraction of edges between communities
- $\mathrm{Tr}\,\mathbf{e} = \sum_i' e_{ii}$: fraction of edges within communities
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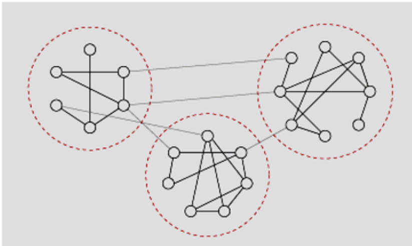

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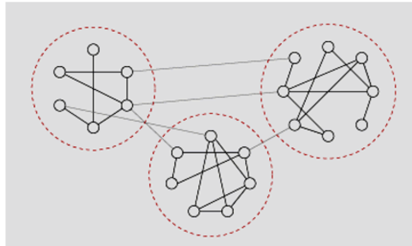

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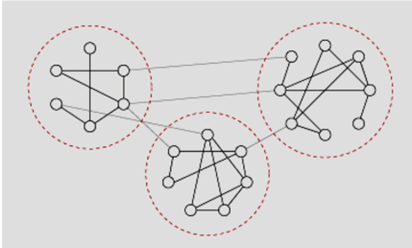

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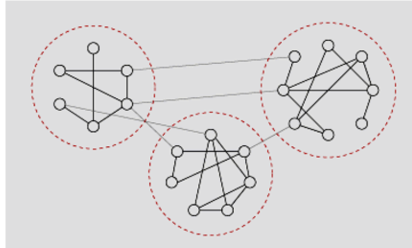

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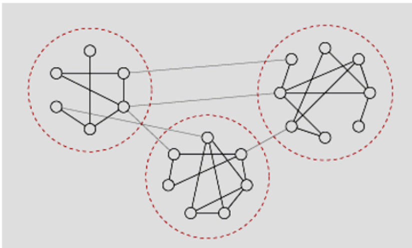

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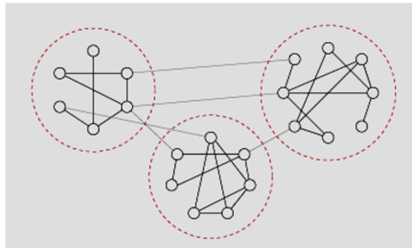

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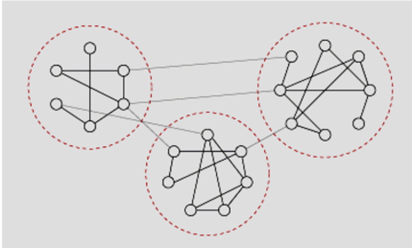

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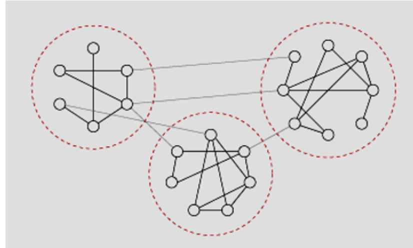

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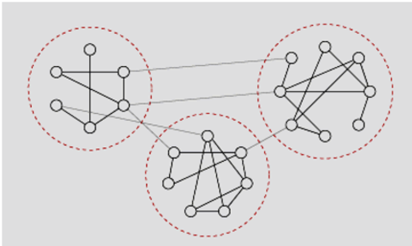

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How to compute Modularity with a given (weighted) adjacency matrix?

- Real graph: Fraction of edges within clusters:

  |E(C_i)| / |E| = $\frac{\sum_{ij} A_{ij}\delta(c_i,c_j)}{\sum_{ij} A_{ij}} = \frac{1}{2m}\sum_{ij} A_{ij}\delta(c_i,c_j)$ $m = \frac{1}{2}\sum_{ij} A_{ij}$,

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  $k_v = \sum_w A_{vw}$.

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- → with the new formulation we can compute modularity for weighted graphs

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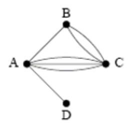
Modularity:

- In [1]: different notion (not keeping a_i fixed): $\sum_{i=1}^{k}\left(|E(C_i)| - m\frac{|C_i|\cdot(|C_i|-1)}{n\cdot(n-1)}\right)$

- In [4]: Newman's version for weighted graphs:
  idea: use multiple edges to model weights



$$\equiv \begin{array}{c} \begin{matrix} A & B & C & D \end{matrix} \\ \begin{pmatrix} 0 & 1 & 3 & 1 \\ 1 & 0 & 2 & 0 \\ 3 & 2 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \end{array} \begin{matrix} A \\ B \\ C \\ D \end{matrix}$$

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