Script **generated by TTT**

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Conductance

- With conductance we can define two appropriate quality measures for clusterings:
- First measure: g=0 and $f(\mathbf{C}) = \min_{1 \le i \le k} \varphi(G[\text{C\_i}])$
- 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*)

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

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

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

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

- 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

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

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

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

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$\delta(C_i, C_j)$

or, more precisely,

$\delta(i, j) = \delta_{ij}$

(Kronecker-symbol)

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- 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:

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

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

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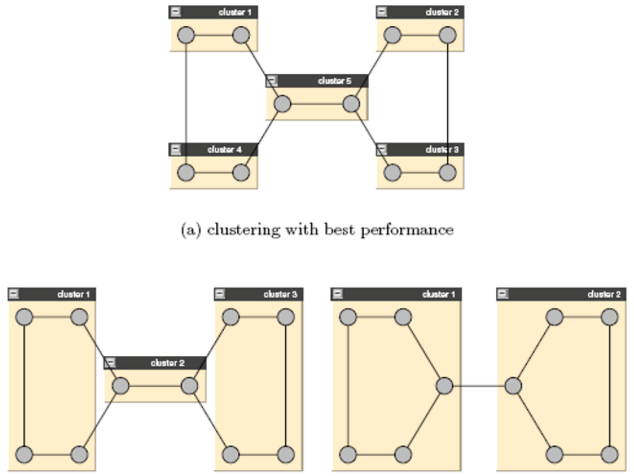

(a) clustering with best performance

(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

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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:}\quad & \min_i\{\pi(G[C_1]),\ldots,\pi(G[C_k])\}\\
\text{average case:}\quad & \frac{1}{k}\sum_i \pi(G[C_i])\\
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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:

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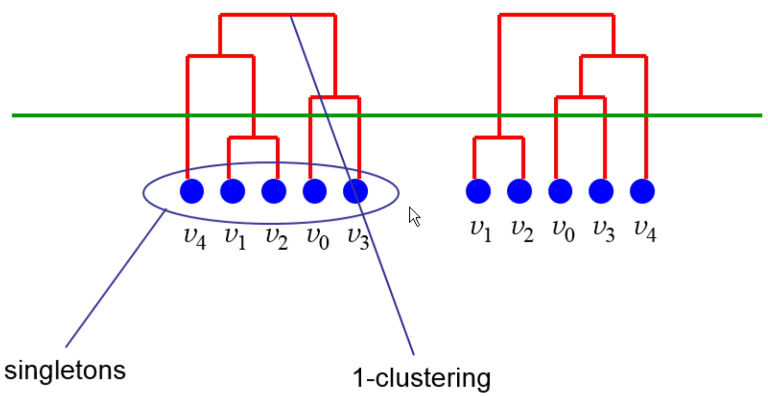
- Advantage of Dendrograms: Can be "**cut**" at any desired number of clusters.



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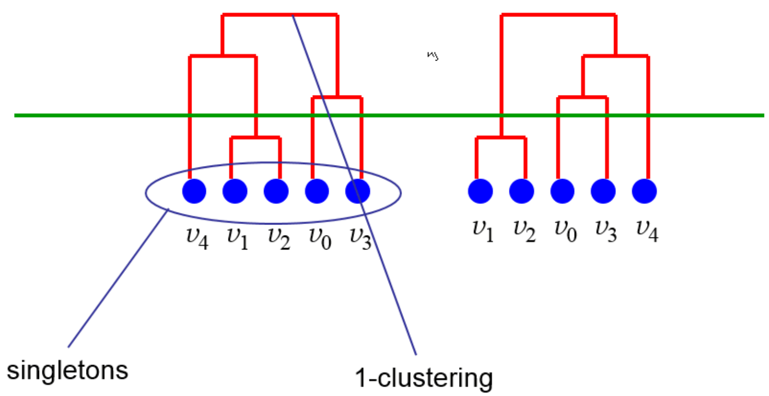

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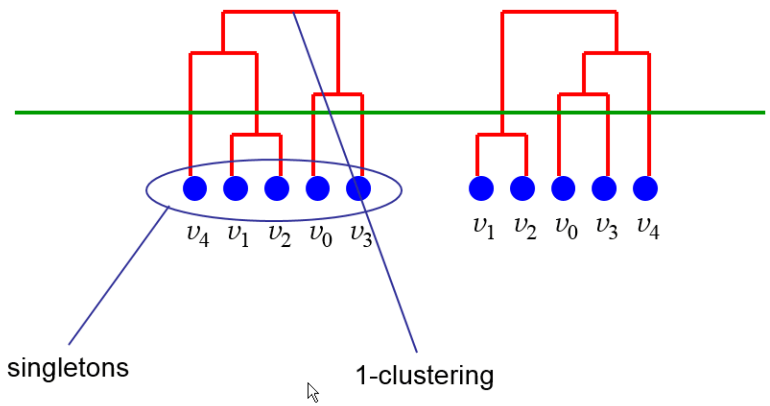

- Linkage (Agglomeration): Iteratively coarsens a given clustering by merging two clusters until 1-clustering is reached ("bottom up")
- Splitting (Division): Iteratively refines a given clustering by splitting one cluster until slingleton clustering is reached ("top down").

- Linkage:

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

  - Given: G=(V,E,w); initial clustering $\mathbf{C}_1$;
  - Given: Either c_{global}: A(G) → $\mathbb{R}^+$ or c_{local}: P(V) x P(V) → $\mathbb{R}^+$ (for merging operations)
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Variants / realizations of Linkage:

- Let d(u,v) denote the minimal path length between nodes u and v then local cost function:

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

max: Complete Linkage

min: Single Linkage

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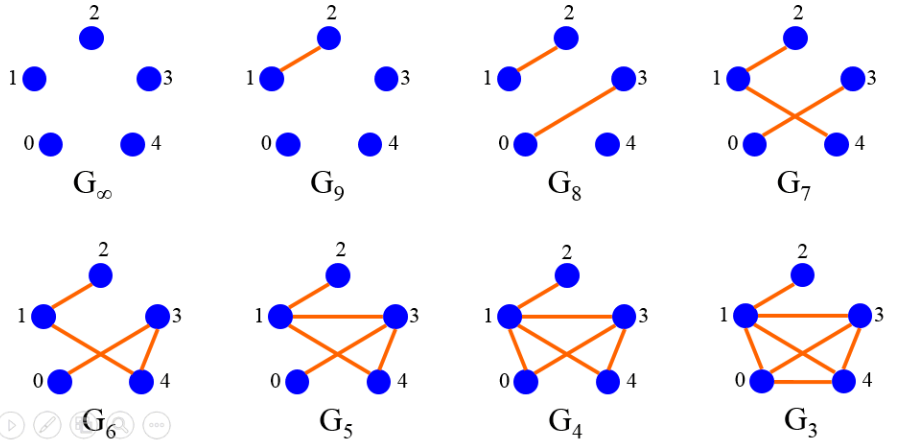
Linkage

- 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:



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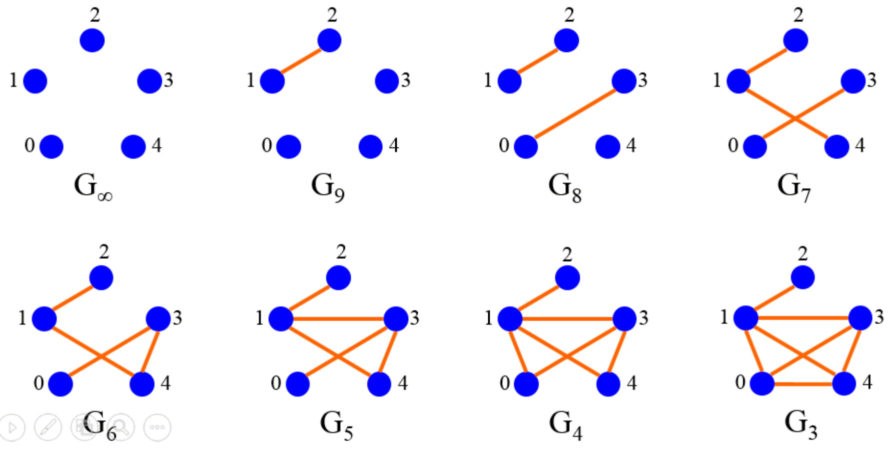

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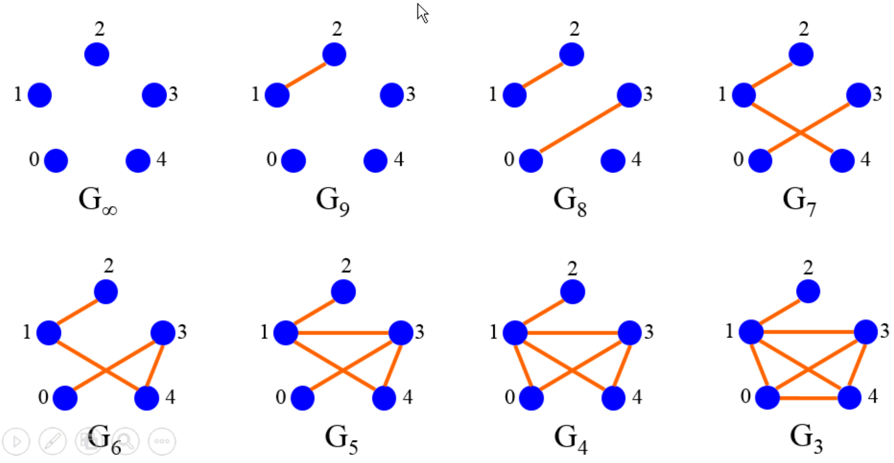


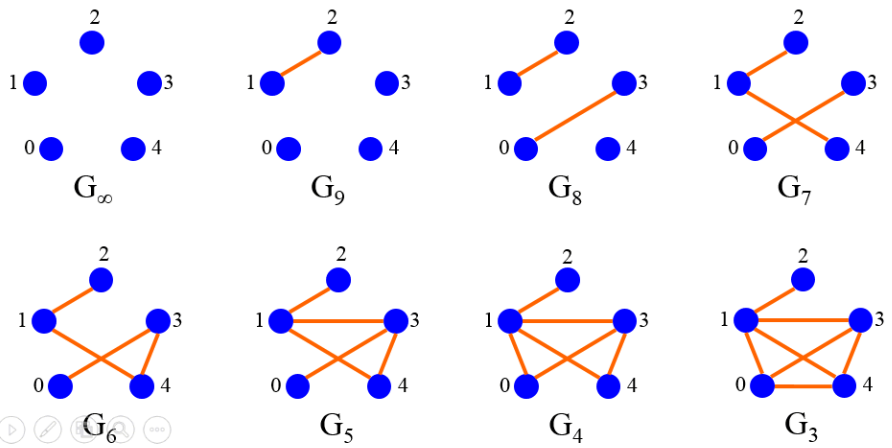
Linkage

- Example

weight matrix:

$$\begin{array}{c} \begin{matrix} v_0 & v_1 & v_2 & v_3 & v_4 \end{matrix} \\ \begin{pmatrix} \infty & 4 & 2 & 8 & 3 \\ 4 & \infty & 9 & 5 & 7 \\ 2 & 9 & \infty & 0 & 1 \\ 8 & 5 & 0 & \infty & 6 \\ 3 & 7 & 1 & 6 & \infty \end{pmatrix} \begin{matrix} v_0 \\ v_1 \\ v_2 \\ v_3 \\ v_4 \end{matrix} \end{array}$$

Threshold graphs:



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- Example

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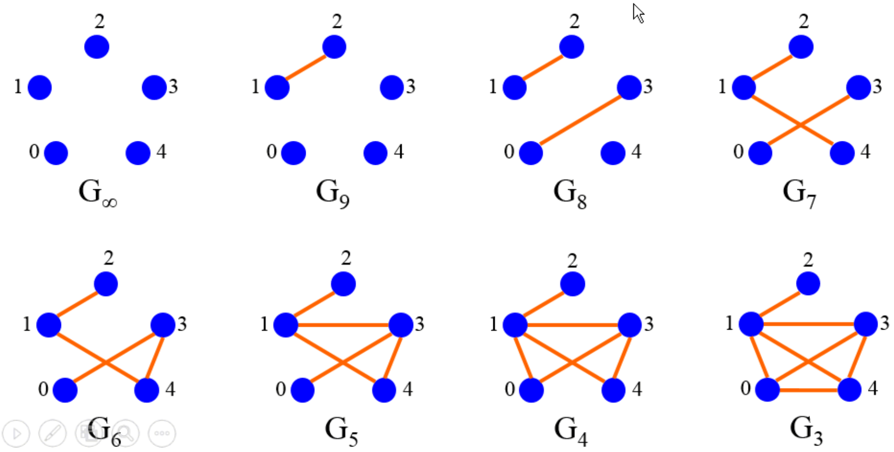

- Example

weight matrix:

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

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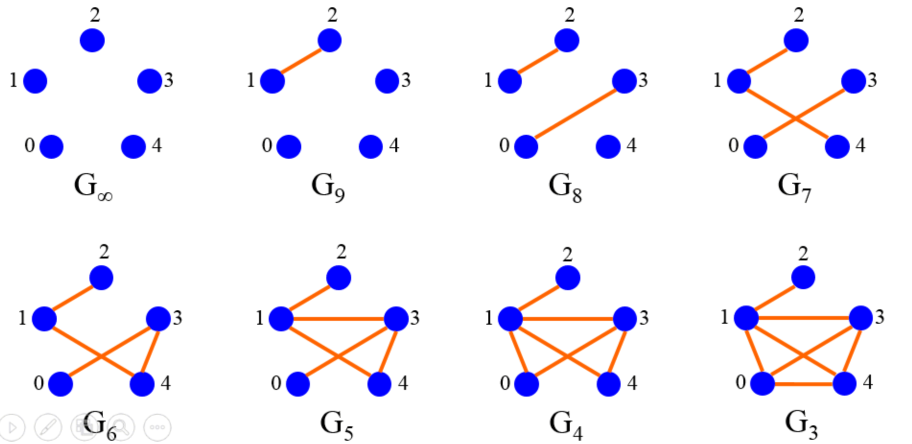

Linkage

- Example

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	v_0	v_1	v_2	v_3	v_4	
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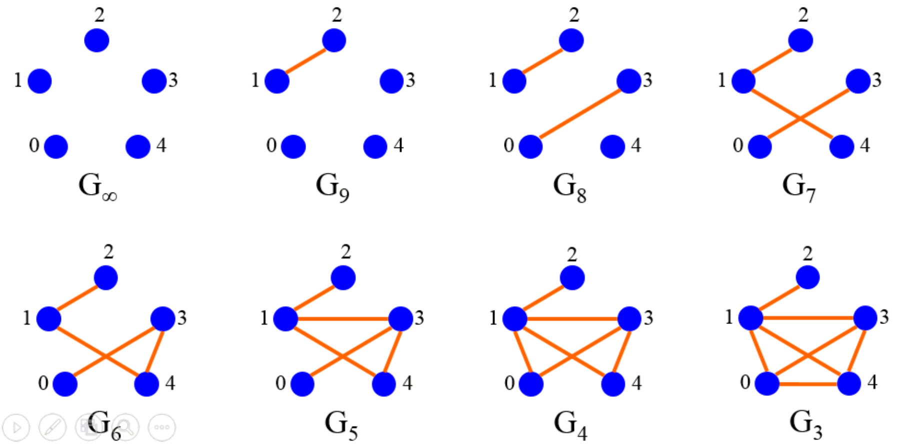
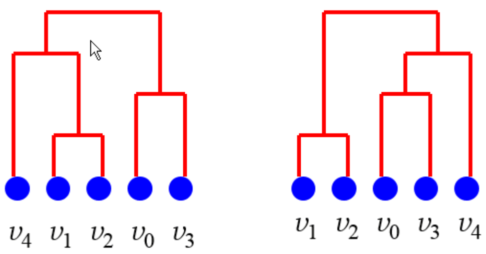


Linkage

Resulting dendrograms:

Single Link

Complete Link



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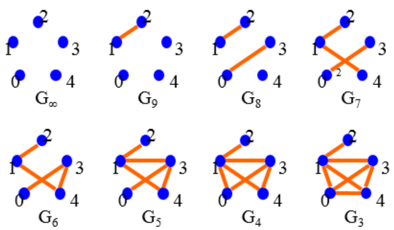

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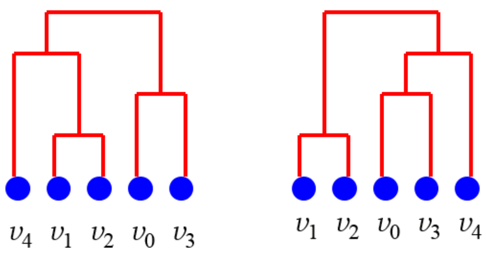

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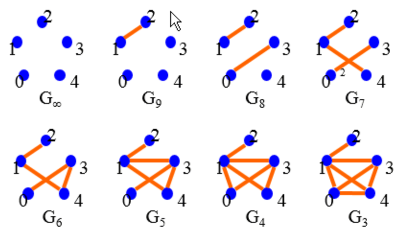

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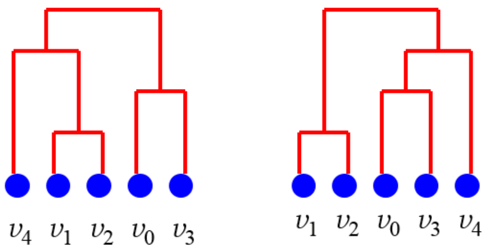

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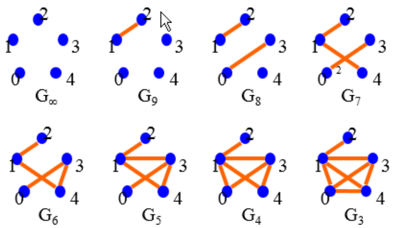

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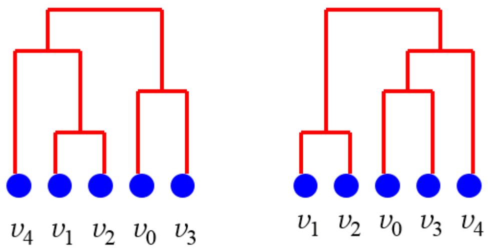

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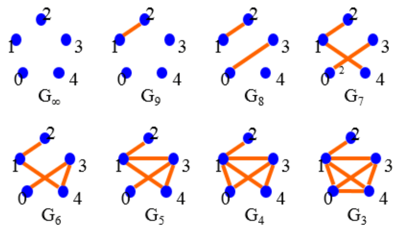

Linkage

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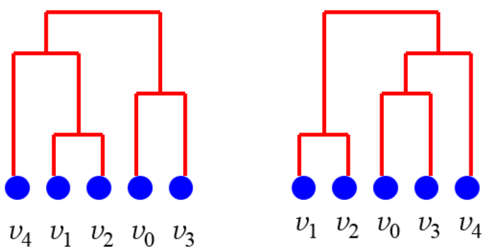

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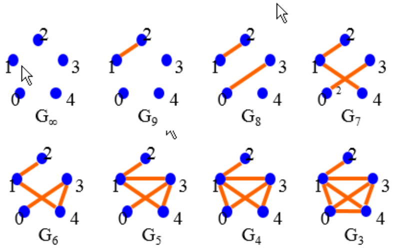

Linkage

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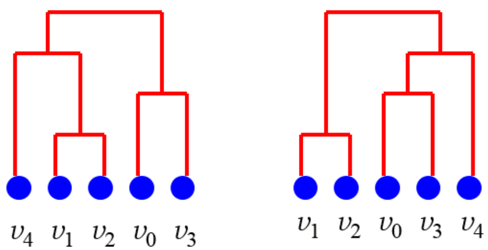

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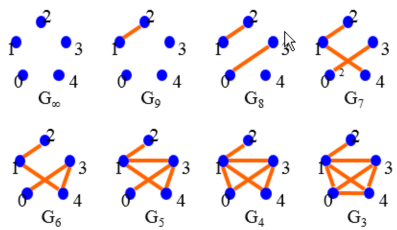

Linkage

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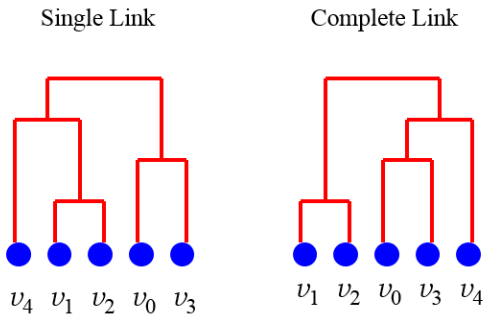

weight matrix:

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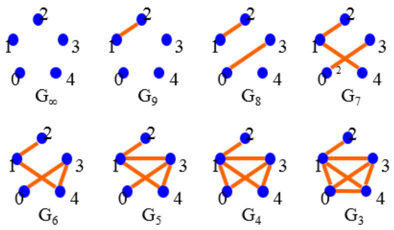

Linkage

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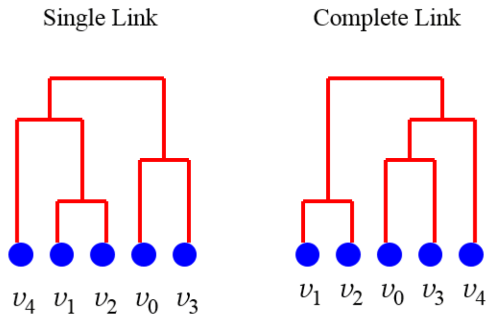

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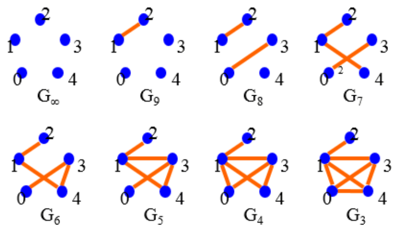

Linkage

- Instead of the weight matrix

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	∞

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

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

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

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

max: Complete Linkage   min: Single Linkage

Splitting

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

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

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

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

  split the cluster with the minimum local splitting cost or

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C_x: one of the clusters

one "half" of the split of C_x

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strictly global

strictly local

semi global

semi local

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  - Variants of Cut functions:

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

$$S_{\text{ratio}}(V) := \operatorname*{argmin}_{\emptyset \neq V' \subset V} \frac{\omega(E(V', V \setminus V'))}{|V'| \cdot (|V| - |V'|)}$$

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

[1]

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

- Instead of merge / split now the following actions are allowed:
  - Move node from one cluster to another
  - Move node from one cluster to form a own singleton cluster
  - Exchange cluster assignments of two nodes

Shifting

- Potential function may use compound operations (make intermediate operations "free of charge") → If many global extrema in potential function exist → May be easier to reach global extremum (Free operations may be analogous to simulated annealing's "temperature shaking")
- Shifting is more often used as refinement of an existing quite good clustering than to compute a new one.

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shifting minimization:

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let L0 be a feasible solution;
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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
3. Recalculate edge betweennes, goto 1.

→ dendrogram

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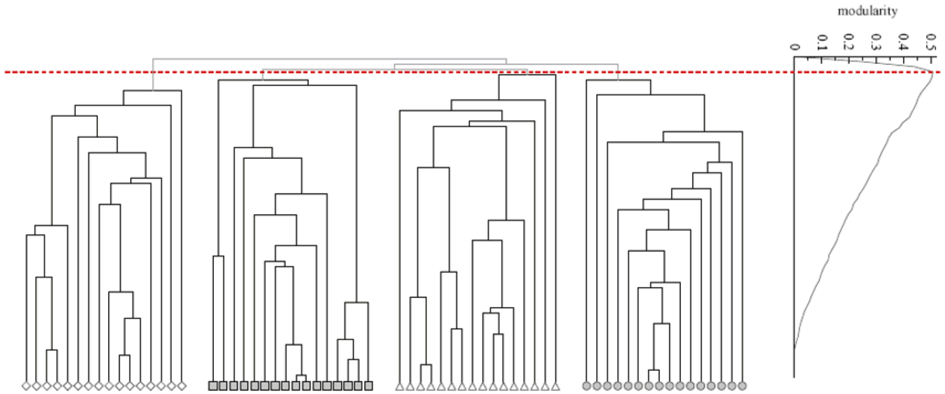

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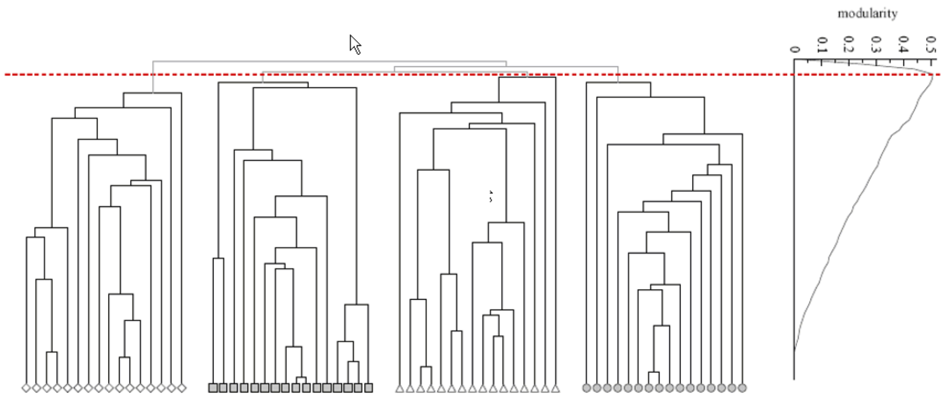

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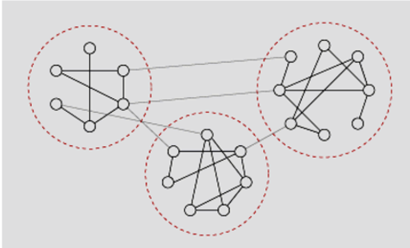

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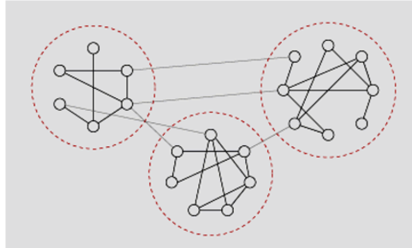

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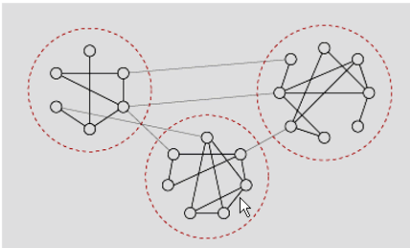

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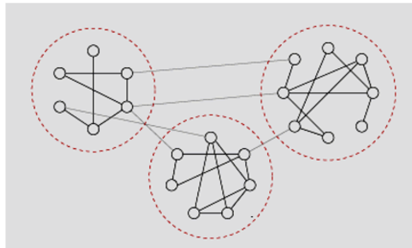

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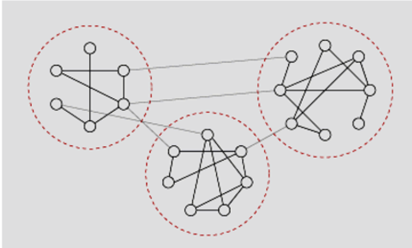

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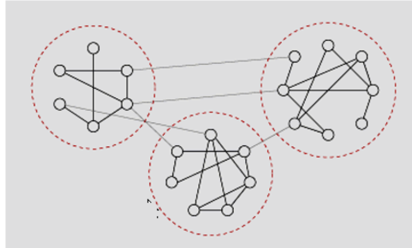

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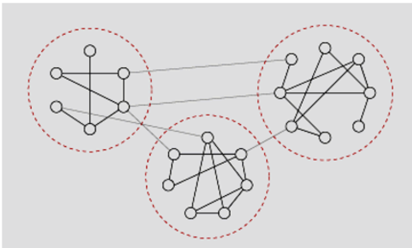

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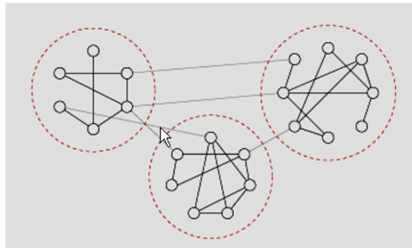

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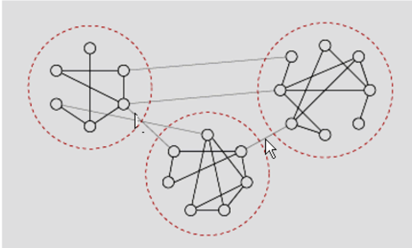

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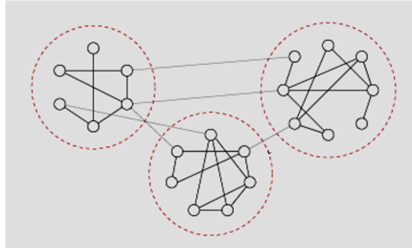

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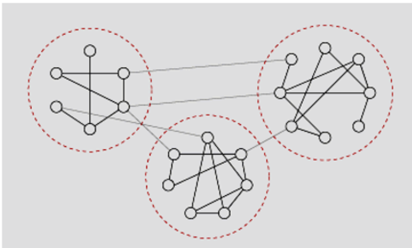

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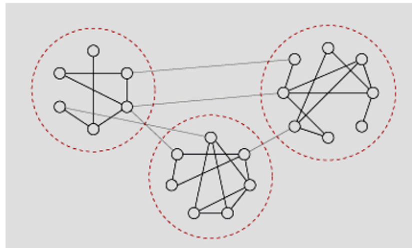

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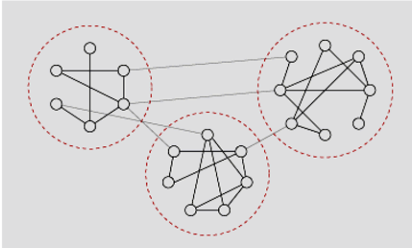

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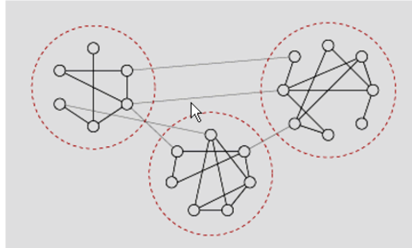

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