Methods of Network Analysis

Clustering and Blockmodeling

2. Approaches to Clustering

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Approaches to Clustering

- local optimization
- dynamic programming
- hierarchical methods; agglomerative methods; Lance-Williams formula; dendrogram; inversions; adding methods
- leaders and the dynamic clusters method
- graph theory (next, 3. lecture);

Local optimization

Often for a given optimization problem (Φ, P) there exist rules which relate to each element of the set Φ some elements of Φ. We call them *local transformations*.

The elements which can be obtained from a given element are called *neighbor*s – local transformations determine the *neighborhood relation* $S \subseteq \Phi \times \Phi$ in the set Φ.
The *neighborhood* of element $\mathrm{X} \in \Phi$ is called the set $S(\mathrm{X}) = \{\mathrm{Y} : \mathrm{X}S\mathrm{Y}\}$.
The element $\mathrm{X} \in \Phi$ is a *local minimum* for the *neighborhood structure* (Φ, S) iff

$$\forall \mathrm{Y} \in S(\mathrm{X}) : P(\mathrm{X}) \leq P(\mathrm{Y})$$

In the following we shall assume that S is reflexive, $\forall \mathrm{X} \in \Phi : \mathrm{X}S\mathrm{X}$.

They are the basis of the *local optimization procedure*

> select X_0; $\mathrm{X} := \mathrm{X}_0$;
> **while** $\exists \mathrm{Y} \in S(\mathrm{X}) : P(\mathrm{Y}) < P(\mathrm{X})$ **do** $\mathrm{X} := \mathrm{Y}$;

which starting in an element of $\mathrm{X}_0 \in \Phi$ repeats moving to an element determined by local transformation which has better value of the criterion function until no such element exists.

Clustering neigborhoods

Usually the neighborhood relation in local optimization clustering procedures over $P_k(\mathbf{U})$ is determined by the following two transformations:

- *transition*: clustering $\mathbf{C}'$ is obtained from $\mathbf{C}$ by moving a unit from one cluster to another

$$\mathbf{C}' = (\mathbf{C} \setminus \{C_u, C_v\}) \cup \{C_u \setminus \{\mathrm{X}_s\}, C_v \cup \{\mathrm{X}_s\}\}$$

- *transposition*: clustering $\mathbf{C}'$ is obtained from $\mathbf{C}$ by interchanging two units from different clusters

$$\mathbf{C}' = (\mathbf{C} \setminus \{C_u, C_v\}) \cup \{(C_u \setminus \{\mathrm{X}_p\}) \cup \{\mathrm{X}_q\}, (C_v \setminus \{\mathrm{X}_q\}) \cup \{\mathrm{X}_p\}\}$$

The transpositions preserve the number of units in clusters.

Hints

Two basic implementation approaches are usually used: *stored data* approach and *stored dissimilarity matrix* approach.

If the constraints are not too stringent, the relocation method can be applied directly on $\mathbf{\Phi}$; otherwise, we can transform using *penalty function method* the problem to an equivalent nonconstrained problem (P_k, Q) with $Q(\mathbf{C}) = P(\mathbf{C}) + \alpha K(\mathbf{C})$ where $\alpha > 0$ is a large constant and $K(\mathbf{C}) = 0$, for $\mathbf{C} \in \Phi$, and $K(\mathbf{C}) > 0$ otherwise.

There exist several improvements of the basic relocation algorithm: simulated annealing, tabu search, . . . (Aarts and Lenstra, 1997).

The *initial clustering* $\mathbf{C}_0$ can be given; most often we generate it randomly.
Let $c[s] = u \Leftrightarrow \mathrm{X}_s \in C_u$. Fill the vector c with the desired number of units in each cluster and shuffle it:

for $p := n$ **downto** 2 **do begin** $q := random(1, p); swap(c[p], c[q])$ **end**;

Quick scanning of neighbors

Testing $P(\mathbf{C}') < P(\mathbf{C})$ is equivalent to $P(\mathbf{C}) - P(\mathbf{C}') > 0$.
For the S criterion function

$$\Delta P(\mathbf{C}, \mathbf{C}') = P(\mathbf{C}) - P(\mathbf{C}') = p(C_u) + p(C_v) - p(C'_u) - p(C'_v)$$

Additional simplifications can be done considering relations between C_u and C'_u, and between C_v and C'_v.

Let us illustrate this on the generalized Ward's method. For this purpose it is useful to introduce the quantity

$$a(C_u, C_v) = \sum_{\mathrm{X} \in C_u, \mathrm{Y} \in C_v} w(\mathrm{X}) \cdot w(\mathrm{Y}) \cdot d(\mathrm{X}, \mathrm{Y})$$

Using the quantity $a(C_u, C_v)$ we can express $p(C)$ in the form $p(C) = \frac{a(C,C)}{2w(C)}$ and the equality mentioned in the introduction of the generalized Ward clustering problem: if $C_u \cap C_v = \emptyset$ then

$$w(C_u \cup C_v) \cdot p(C_u \cup C_v) = w(C_u) \cdot p(C_u) + w(C_v) \cdot p(C_v) + a(C_u, C_v)$$

Δ for the generalized Ward's method

Let us analyze the transition of a unit X_s from cluster C_u to cluster C_v:
We have $C_u' = C_u \setminus \{\mathrm{X}_s\}$, $C_v' = C_v \cup \{X_s\}$,

$$w(C_u) \cdot p(C_u) = w(C_u') \cdot p(C_u') + a(\mathrm{X}_s, C_u') = (w(C_u) - w(\mathrm{X}_s)) \cdot p(C_u') + a(\mathrm{X}_s, C_u')$$

and

$$w(C_v') \cdot p(C_v') = w(C_v) \cdot p(C_v) + a(\mathrm{X}_s, C_v)$$

From $d(\mathrm{X}_s, \mathrm{X}_s) = 0$ it follows $a(\mathrm{X}_s, C_u) = a(\mathrm{X}_s, C_u')$. Therefore

$$p(C_u') = \frac{w(C_u) \cdot p(C_u) - a(\mathrm{X}_s, C_u)}{w(C_u) - w(\mathrm{X}_s)} \qquad p(C_v') = \frac{w(C_v) \cdot p(C_v) + a(\mathrm{X}_s, C_v)}{w(C_v) + w(\mathrm{X}_s)}$$

and finally

$$\Delta P(\mathbf{C}, \mathbf{C}') = p(C_u) + p(C_v) - p(C_u') - p(C_v') =$$

$$= \frac{w(\mathrm{X}_s) \cdot p(C_v) - a(\mathrm{X}_s, C_v)}{w(C_v) + w(\mathrm{X}_s)} - \frac{w(\mathrm{X}_s) \cdot p(C_u) - a(\mathrm{X}_s, C_u)}{w(C_u) - w(\mathrm{X}_s)}$$

In the case when d is the squared Euclidean distance it is possible to derive also expression for corrections of centers (Späth, 1977).

Dynamic programming

Suppose that $\mathrm{Min}(\mathbf{\Phi}_k, P) \neq \emptyset$, $k = 1, 2, \ldots$. Denoting $P^*(\mathbf{U}, k) = P(\mathbf{C}_k^*(\mathbf{U}))$ we can derive the generalized *Jensen equality* (Batagelj, Korenjak and Klavžar, 1994):

$$P^*(\mathbf{U}, k) = \begin{cases} p(\mathbf{U}) & \{\mathbf{U}\} \in \mathbf{\Phi}_1 \\ \min\limits_{\substack{\emptyset \subset C \subset \mathbf{U} \\ \exists \mathbf{C} \in \mathbf{\Phi}_{k-1}(\mathbf{U} \setminus C) : \mathbf{C} \cup \{C\} \in \mathbf{\Phi}_k(\mathbf{U})}} (P^*(\mathbf{U} \setminus C, k-1) \oplus p(C)) & k > 1 \end{cases}$$

This is a *dynamic programming* (Bellman) equation which, for some special constrained problems, that keep the size of $\mathbf{\Phi}_k$ small, allows us to solve the clustering problem by the adapted Fisher's algorithm.

Hierarchical methods

The set of feasible clusterings $\mathbf{\Phi}$ determines the *feasibility predicate* $\Phi(\mathbf{C}) \equiv \mathbf{C} \in \mathbf{\Phi}$ defined on $\mathcal{P}(\mathcal{P}(\mathbf{U}) \setminus \{\emptyset\})$; and conversely $\mathbf{\Phi} \equiv \{\mathbf{C} \in \mathcal{P}(\mathcal{P}(\mathbf{U}) \setminus \{\emptyset\}) : \Phi(\mathbf{C})\}$.

In the set $\mathbf{\Phi}$ the relation of *clustering inclusion* $\sqsubseteq$ can be introduced by

$$\mathbf{C}_1 \sqsubseteq \mathbf{C}_2 \equiv \forall C_1 \in \mathbf{C}_1, C_2 \in \mathbf{C}_2 : C_1 \cap C_2 \in \{\emptyset, C_1\}$$

we say also that the clustering $\mathbf{C}_1$ is a *refinement* of the clustering $\mathbf{C}_2$.

It is well known that $(P(\mathbf{U}), \sqsubseteq)$ is a partially ordered set (even more, semimodular lattice). Because any subset of partially ordered set is also partially ordered, we have: Let $\mathbf{\Phi} \subseteq P(\mathbf{U})$ then $(\mathbf{\Phi}, \sqsubseteq)$ is a partially ordered set.

The clustering inclusion determines two related relations (on $\mathbf{\Phi}$):

$\mathbf{C}_1 \sqsubset \mathbf{C}_2 \equiv \mathbf{C}_1 \sqsubseteq \mathbf{C}_2 \wedge \mathbf{C}_1 \neq \mathbf{C}_2$ – strict inclusion, and

$\mathbf{C}_1 \sqsubset\!\!\cdot\, \mathbf{C}_2 \equiv \mathbf{C}_1 \sqsubset \mathbf{C}_2 \wedge \neg\exists \mathbf{C} \in \mathbf{\Phi} : (\mathbf{C}_1 \sqsubset \mathbf{C} \wedge \mathbf{C} \sqsubset \mathbf{C}_2)$ – predecessor.

Conditions on the structure of the set of feasible clusterings

We shall assume that the set of feasible clusterings $\mathbf{\Phi} \subseteq P(\mathbf{U})$ satisfies the following conditions:

F1. $\mathbf{O} \equiv \{\{X\} : X \in \mathbf{U}\} \in \mathbf{\Phi}$

F2. The feasibility predicate Φ is *local* – it has the form $\Phi(\mathbf{C}) = \bigwedge_{C \in \mathbf{C}} \varphi(C)$ where $\varphi(C)$ is a predicate defined on $\mathcal{P}(\mathbf{U}) \setminus \{\emptyset\}$ (clusters).

The intuitive meaning of $\varphi(C)$ is: $\varphi(C) \equiv$ the cluster C is 'good'. Therefore the locality condition can be read: a 'good' clustering $\mathbf{C} \in \mathbf{\Phi}$ consists of 'good' clusters.

F3. The predicate Φ has the property of *binary heredity* with respect to the *fusibility* predicate $\psi(C_1, C_2)$, i.e.,

$$C_1 \cap C_2 = \emptyset \wedge \varphi(C_1) \wedge \varphi(C_2) \wedge \psi(C_1, C_2) \Rightarrow \varphi(C_1 \cup C_2)$$

This condition means: in a 'good' clustering, a fusion of two 'fusible' clusters produces a 'good' clustering.

…conditions

F4. The predicate ψ is *compatible* with clustering inclusion $\sqsubseteq$, i.e.,

$$\forall \mathbf{C}_1, \mathbf{C}_2 \in \mathbf{\Phi} : (\mathbf{C}_1 \sqsubset \mathbf{C}_2 \wedge \mathbf{C}_1 \setminus \mathbf{C}_2 = \{C_1, C_2\} \Rightarrow \psi(C_1, C_2) \vee \psi(C_2, C_1))$$

F5. The *interpolation* property holds in $\mathbf{\Phi}$, i.e., $\forall \mathbf{C}_1, \mathbf{C}_2 \in \mathbf{\Phi}$:

$$(\mathbf{C}_1 \sqsubset \mathbf{C}_2 \wedge \mathrm{card}(\mathbf{C}_1) > \mathrm{card}(\mathbf{C}_2) + 1 \Rightarrow \exists \mathbf{C} \in \mathbf{\Phi} : (\mathbf{C}_1 \sqsubset \mathbf{C} \wedge \mathbf{C} \sqsubset \mathbf{C}_2))$$

These conditions provide a framework in which the hierarchical methods can be applied also for constrained clustering problems $\mathbf{\Phi}_k(\mathbf{U}) \subset P_k(\mathbf{U})$.

In the ordinary problem both predicates $\varphi(C)$ and $\psi(C_p, C_q)$ are always true – all conditions F1-F5 are satisfied.

Criterion functions compatible with a dissimilarity between clusters

We shall call a *dissimilarity between clusters* a function $D : (C_1, C_2) \to \mathbb{R}_0^+$ which is symmetric, i.e., $D(C_1, C_2) = D(C_2, C_1)$.

Let $(\mathbb{R}_0^+, \oplus, 0, \leq)$ be an ordered abelian monoid. Then the criterion function $P(\mathbf{C}) = \bigoplus_{C\in\mathbf{C}} p(C)$, $\forall X \in \mathbf{U} : p(\{X\}) = 0$ is *compatible* with dissimilarity D over $\mathbf{\Phi}$ iff for all $C \subseteq \mathbf{U}$ holds:

$$\varphi(C) \wedge \mathrm{card}(C) > 1 \Rightarrow p(C) = \min_{(C_1,C_2)\in\Psi(C)} (p(C_1) \oplus p(C_2) \oplus D(C_1, C_2))$$

Theorem 2.1 *A* S *criterion function is compatible with dissimilarity D defined by*

$$D(C_p, C_q) = p(C_p \cup C_q) - p(C_p) - p(C_q)$$

In this case, let $\mathbf{C}' = \mathbf{C} \setminus \{C_p, C_q\} \cup \{C_p \cup C_q\}$, $C_p, C_q \in \mathbf{C}$, *then*

$$P(\mathbf{C}') - P(\mathbf{C}) = D(C_p, C_q)$$

Greedy approximation

Theorem 2.2 *Let P be compatible with D over $\mathbf{\Phi}$, $\oplus$ distributes over* min, *and F1 – F5 hold, then*

$$P(\mathbf{C}_k^*) = \min_{\mathbf{C}\in\mathbf{\Phi}_k} P(\mathbf{C}) = \min_{\substack{C_1,C_2\in\mathbf{C}\in\mathbf{\Phi}_{k+1}\\ \psi(C_1,C_2)}} (P(\mathbf{C}) \oplus D(C_1,C_2))$$

The equality from theorem 2.1 can also be written in the form

$$P(\mathbf{C}_k^*) = \min_{\mathbf{C}\in\mathbf{\Phi}_{k+1}} (P(\mathbf{C}) \oplus \min_{\substack{C_1,C_2\in\mathbf{C}\\ \psi(C_1,C_2)}} D(C_1,C_2))$$

from where we can see the following 'greedy' approximation:

$$P(\mathbf{C}_k^*) \approx P(\mathbf{C}_{k+1}^*) \oplus \min_{\substack{C_1,C_2\in\mathbf{C}_{k+1}^*\\ \psi(C_1,C_2)}} D(C_1,C_2)$$

which is the basis for the following agglomerative (binary) procedure for solving the clustering problem.

Agglomerative methods

1. $k := n$; $\mathbf{C}(k) := \{\{X\} : X \in \mathbf{U}\}$;
2. **while** $\exists C_i, C_j \in \mathbf{C}(k)\colon (i \neq j \wedge \psi(C_i, C_j))$ **repeat**

 2.1. $(C_p, C_q) := \text{argmin}\{D(C_i, C_j)\colon i \neq j \wedge \psi(C_i, C_j)\}$;

 2.2. $C := C_p \cup C_q$; $k := k - 1$;

 2.3. $\mathbf{C}(k) := \mathbf{C}(k+1) \setminus \{C_p, C_q\} \cup \{C\}$;

 2.4. determine $D(C, C_s)$ for all $C_s \in \mathbf{C}(k)$

3. $m := k$

Note that, because it is based on an approximation, this procedure is not an exact procedure for solving the clustering problem.

For another, *probabilistic* view on agglomerative methods see Kamvar, Klein, Manning (2002).

Divisive methods work in the reverse direction. The problem here is how to efficiently find a good split (C_p, C_q) of cluster C.

Some dissimilarities between clusters

We shall use the generalized Ward's c.e.f.

$$p(C) = \frac{1}{2w(C)} \sum_{X,Y \in C} w(X) \cdot w(Y) \cdot d(X,Y)$$

and the notion of the *generalized center* $\overline{C}$ of the cluster C, for which the dissimilarity to any cluster or unit U is defined by

$$d(U, \overline{C}) = d(\overline{C}, U) = \frac{1}{w(C)} (\sum_{X \in C} w(X) \cdot d(X,U) - p(C))$$

Minimal: $D^m(C_u, C_v) = \min_{X \in C_u, Y \in C_v} d(X,Y)$

Maximal: $D^M(C_u, C_v) = \max_{X \in C_u, Y \in C_v} d(X,Y)$

Average: $D^a(C_u, C_v) = \frac{1}{w(C_u)w(C_v)} \sum_{X \in C_u, Y \in C_v} w(X) \cdot w(Y) \cdot d(X,Y)$

... some dissimilarities

Gower-Bock: $D^G(C_u, C_v) = d(\overline{C}_u, \overline{C}_v) = D^a(C_u, C_v) - \frac{p(C_u)}{w(C_u)} - \frac{p(C_v)}{w(C_v)}$

Ward: $D^W(C_u, C_v) = \frac{w(C_u)w(C_v)}{w(C_u \cup C_v)} D^G(\overline{C}_u, \overline{C}_v)$

Inertia: $D^I(C_u, C_v) = p(C_u \cup C_v)$

Variance: $D^V(C_u, C_v) = \mathrm{var}(C_u \cup C_v) = \frac{p(C_u \cup C_v)}{w(C_u \cup C_v)}$

Weighted increase of variance:

$$D^v(C_u, C_v) = \mathrm{var}(C_u \cup C_v) - \frac{w(C_u) \cdot \mathrm{var}(C_u) + w(C_v) \cdot \mathrm{var}(C_v)}{w(C_u \cup C_v)} = \frac{D^W(C_u, C_v)}{w(C_u \cup C_v)}$$

For all of them *Lance-Williams-Jambu formula* holds:

$$\begin{aligned} D(C_p \cup C_q, C_s) \quad &= \quad \alpha_1 D(C_p, C_s) + \alpha_2 D(C_q, C_s) + \beta D(C_p, C_q) + \\ &\quad + \gamma |D(C_p, C_s) - D(C_q, C_s)| + \delta_1 v(C_p) + \delta_2 v(C_q) + \delta_3 v(C_s) \end{aligned}$$

Lance-Williams-Jambu coefficients

method	α_1	α_2	β	γ	δ_t	$v(C_t)$
minimum	$\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	0	–
maximum	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$	0	–
average	$\frac{w_p}{w_{pq}}$	$\frac{w_q}{w_{pq}}$	0	0	0	–
Gower-Bock	$\frac{w_p}{w_{pq}}$	$\frac{w_q}{w_{pq}}$	$-\frac{w_p w_q}{w_{pq}^2}$	0	0	–
Ward	$\frac{w_{ps}}{w_{pqs}}$	$\frac{w_{qs}}{w_{pqs}}$	$-\frac{w_s}{w_{pqs}}$	0	0	–
inertia	$\frac{w_{ps}}{w_{pqs}}$	$\frac{w_{qs}}{w_{pqs}}$	$\frac{w_{pq}}{w_{pqs}}$	0	$-\frac{w_t}{w_{pqs}}$	$p(C_t)$
variance	$\frac{w_{ps}^2}{w_{pqs}^2}$	$\frac{w_{qs}^2}{w_{pqs}^2}$	$\frac{w_{pq}^2}{w_{pqs}^2}$	0	$-\frac{w_t}{w_{pqs}^2}$	$p(C_t)$
w.i. variance	$\frac{w_{ps}^2}{w_{pqs}^2}$	$\frac{w_{qs}^2}{w_{pqs}^2}$	$-\frac{w_s w_{pq}}{w_{pqs}^2}$	0	0	–

$$w_p = w(C_p),\ w_{pq} = w(C_p \cup C_q),\ w_{pqs} = w(C_p \cup C_q \cup C_s)$$

Hierarchies

The agglomerative clustering procedure produces a series of feasible clusterings $\mathbf{C}(n), \mathbf{C}(n-1), \ldots, \mathbf{C}(m)$ with $\mathbf{C}(m) \in \mathrm{Max}\,\mathbf{\Phi}$ (maximal elements for $\sqsubseteq$).

Their union $\mathcal{T} = \bigcup_{k=m}^{n} \mathbf{C}(k)$ is called a *hierarchy* and has the property

$$\forall C_p, C_q \in \mathcal{T} : C_p \cap C_q \in \{\emptyset, C_p, C_q\}$$

The set inclusion $\subseteq$ is a *tree* or *hierarchical* order on $\mathcal{T}$. The hierarchy $\mathcal{T}$ is *complete* iff $\mathbf{U} \in \mathcal{T}$.

For $W \subseteq \mathbf{U}$ we define the *smallest cluster* $C_{\mathcal{T}}(W)$ from $\mathcal{T}$ containing W as:

c1. $\quad W \subseteq C_{\mathcal{T}}(W)$

c2. $\quad \forall C \in \mathcal{T} : (W \subseteq C \Rightarrow C_{\mathcal{T}}(W) \subseteq C)$

$C_{\mathcal{T}}$ is a *closure* on $\mathcal{T}$ with a special property

$$\mathrm{Z} \notin C_{\mathcal{T}}(\{\mathrm{X}, \mathrm{Y}\}) \Rightarrow C_{\mathcal{T}}(\{\mathrm{X}, \mathrm{Y}\}) \subset C_{\mathcal{T}}(\{\mathrm{X}, \mathrm{Y}, \mathrm{Z}\}) = C_{\mathcal{T}}(\{\mathrm{X}, \mathrm{Z}\}) = C_{\mathcal{T}}(\{\mathrm{Y}, \mathrm{Z}\})$$

Level functions

A mapping $h : \mathcal{T} \to \mathbb{R}_0^+$ is a *level function* on $\mathcal{T}$ iff

l1. $\forall \mathrm{X} \in \mathbf{U} : h(\{\mathrm{X}\}) = 0$

l2. $C_p \subseteq C_q \Rightarrow h(C_p) \leq h(C_q)$

A simple example of level function is $h(C) = \mathrm{card}(C) - 1$.

Every hierarchy / level function determines an ultrametric dissimilarity on $\mathbf{U}$

$$\delta(\mathrm{X}, \mathrm{Y}) = h(C_{\mathcal{T}}(\{\mathrm{X}, \mathrm{Y}\}))$$

The converse is also true (see Dieudonne (1960)): Let d be an ultrametric on $\mathbf{U}$. Denote $\overline{B}(\mathrm{X}, r) = \{\mathrm{Y} \in \mathbf{U} : d(\mathrm{X}, \mathrm{Y}) \leq r\}$. Then for any given set $A \subset \mathbb{R}^+$ the set

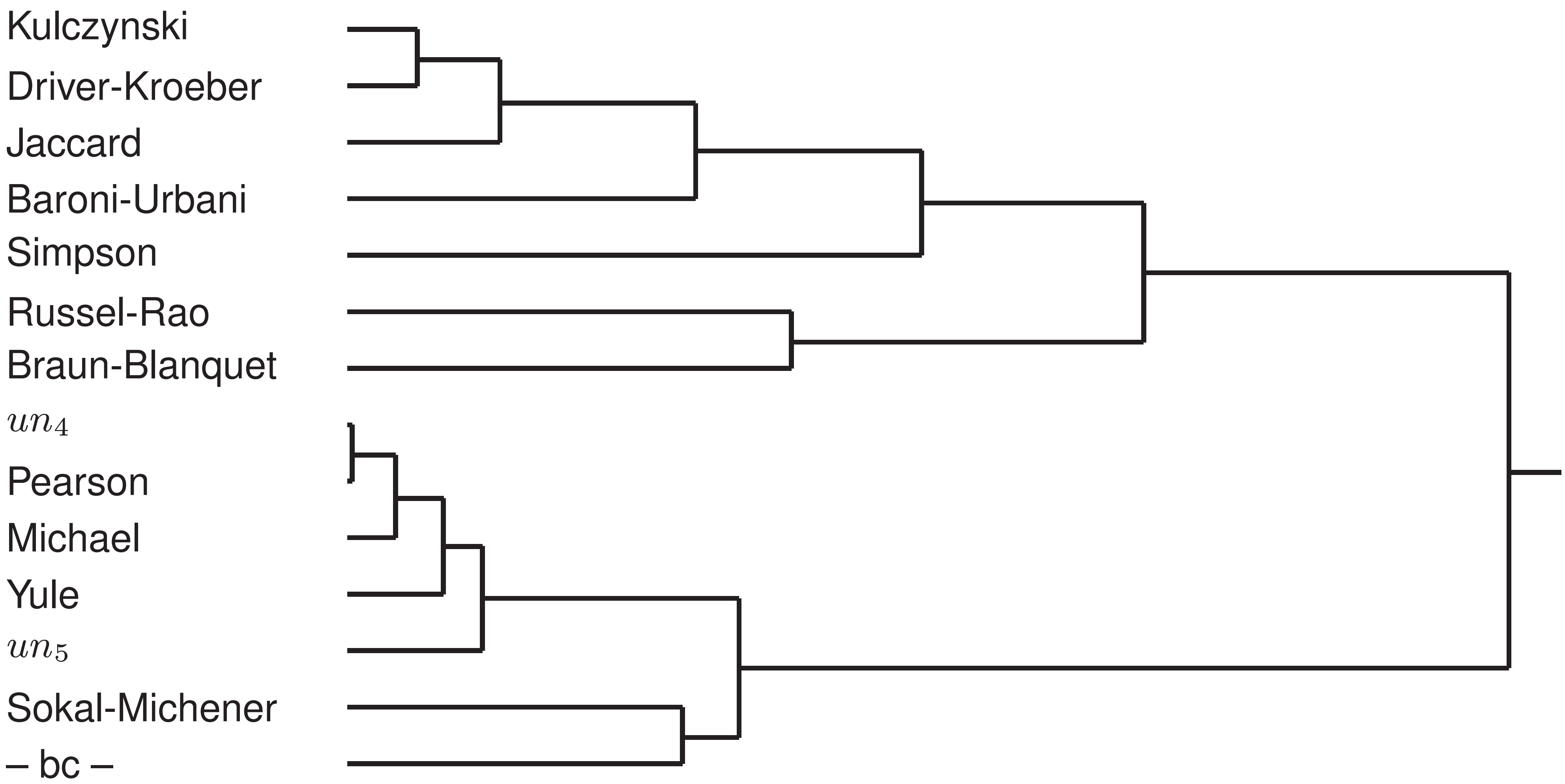
$$\mathbf{C}(A) = \{\overline{B}(\mathrm{X}, r) : \mathrm{X} \in \mathbf{U}, r \in A\} \cup \{\{\mathbf{U}\}\} \cup \{\{\mathrm{X}\} : \mathrm{X} \in \mathbf{U}\}$$

is a complete hierarchy, and $h(C) = \mathrm{diam}(C)$ is a level function.

The pair $(\mathcal{T}, h)$ is called a *dendrogram* or a *clustering tree* because it can be visualized as a tree.

Association coefficients, Monte Carlo, $m = 15$

CLUSE – maximum $[0.00, 0.33]$



Inversions

Unfortunately the function $h_D(C) = D(C_p, C_q)$, $C = C_p \cup C_q$ is not always a level function – for some Ds the *inversions*, $D(C_p, C_q) > D(C_p \cup C_q, C_s)$, are possible.

Batagelj (1981) showed:

Theorem 2.3 *h_D is a level function for the Lance-Williams procedure $(\alpha_1, \alpha_2, \beta, \gamma)$ iff:*

(i) $\gamma + \min(\alpha_1, \alpha_2) \geq 0$

(ii) $\alpha_1 + \alpha_2 \geq 0$

(iii) $\alpha_1 + \alpha_2 + \beta \geq 1$

The dissimilarity D has the *reducibility* property (Bruynooghe, 1977) iff

$$D(C_p, C_q) \leq t,\ D(C_p, C_s) \geq t,\ D(C_q, C_s) \geq t \ \Rightarrow\ D(C_p \cup C_q, C_s) \geq t$$

Theorem 2.4 *If a dissimilarity D has the reducibility property then h_D is a level function.*

Adding hierarchical methods

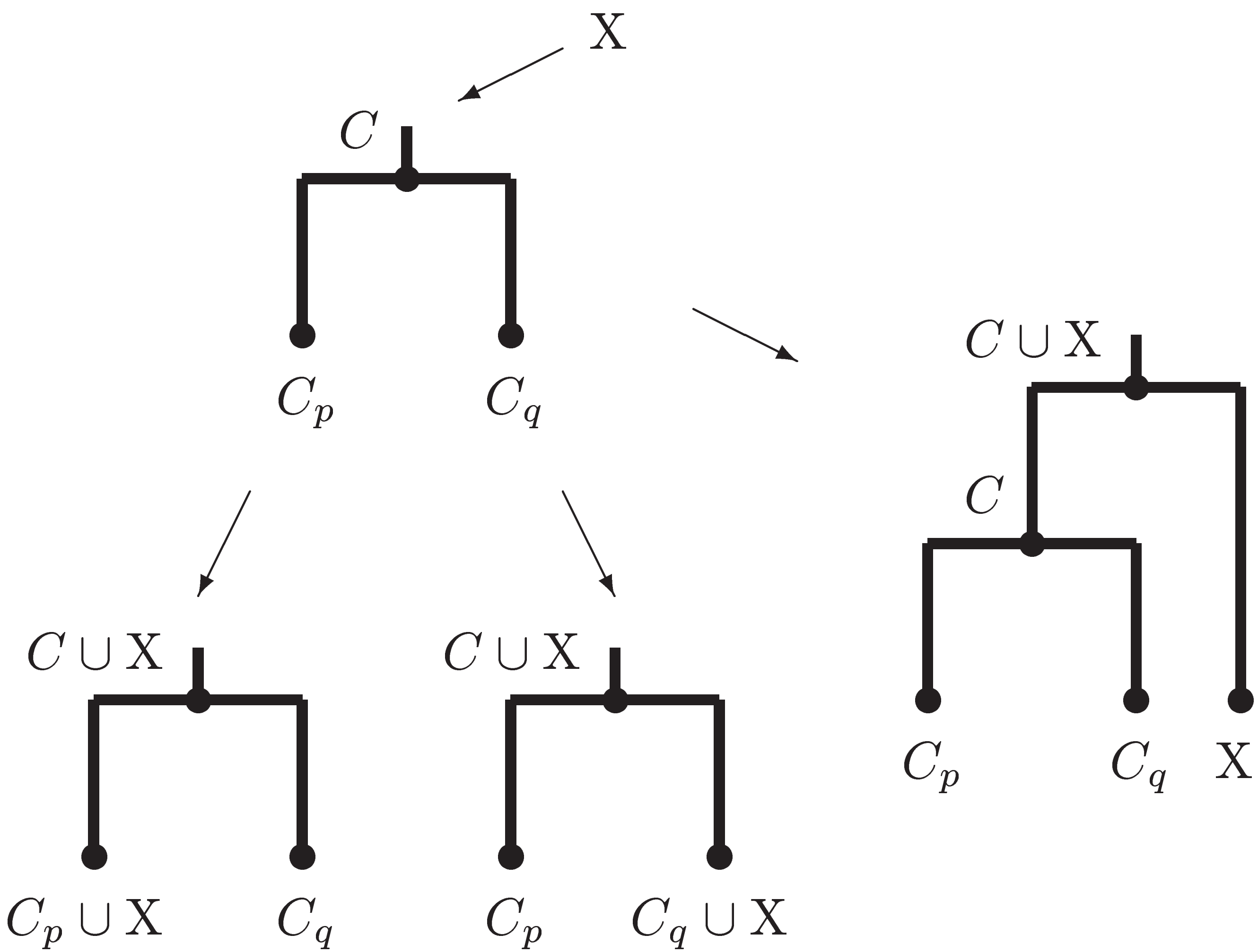
Suppose that we already built a clustering tree $\mathcal{T}$ over the set of units $\mathbf{U}$. To add a new unit X to the tree $\mathcal{T}$ we start in the root and branch down. Assume that we reached the node corresponding to cluster C, which was obtained by joining subclusters C_p and C_q. There are three possibilities: or to add X to C_p, or to add X to C_q, or to form a new cluster $\{X\}$.

Consider again the 'greedy approximation' $P(\mathbf{C}^\bullet_k) = P(\mathbf{C}^\bullet_{k+1}) + D(C_p, C_q)$ where $D(C_p, C_q) = \min_{C_u, C_v \in \mathbf{C}^\bullet_{k+1}} D(C_u, C_v)$ and $\mathbf{C}^\bullet_i$ are greedy solutions.

Since we wish to minimize the value of criterion P it follows from the greedy relation that we have to select the case corresponding to the maximal among values $D(C_p \cup \{X\}, C_q)$, $D(C_q \cup \{X\}, C_p)$ and $D(C_p \cup C_q, \{X\})$.

This is a basis for the adding clustering method. We start with a tree on the first two units and then successively add to it the remaining units. The unit X is included into all clusters through which we branch it down.

... adding hierarchical methods



About the minimal solutions of (P_k, SR)

Theorem 2.5 *In the (locally with respect to transitions) minimal clustering for the problem* (P_k, SR)

$$\mathrm{SR.} \qquad P(\mathbf{C}) = \sum_{C \in \mathbf{C}} \sum_{\mathrm{X} \in C} w(\mathrm{X}) \cdot d(\mathrm{X}, \overline{C})$$

each unit is assigned to the nearest representative: Let $\mathbf{C}^\bullet$ *be (locally with respect to transitions) minimal clustering then it holds:*

$$\forall C_u \in \mathbf{C}^\bullet \forall \mathrm{X} \in C_u \forall C_v \in \mathbf{C}^\bullet \setminus \{C_u\} : d(\mathrm{X}, \overline{C}_u) \leq d(\mathrm{X}, \overline{C}_v)$$

Proof

Let $\mathbf{C}' = (\mathbf{C}^\bullet \setminus \{C_u, C_v\}) \cup \{C_u \setminus \{\mathrm{X}\}, C_v \cup \{\mathrm{X}\}\}$ be any clustering neighbouring with respect to transitions to the clustering $\mathbf{C}^\bullet$. From the theorem assumptions $P(\mathbf{C}^\bullet) \leq P(\mathbf{C}')$ and the type of criterion function we have:

$$p(C_u) + p(C_v) \leq p(C_u \setminus \mathrm{X}) + p(C_v \cup \mathrm{X})$$

and by proposition 1.4.b: $\leq p(C_u) - w(\mathrm{X}).d(\mathrm{X}, \overline{C}_u) + p(C_v \cup \mathrm{X})$.
Therefore $p(C_v) \leq p(C_v \cup \mathrm{X}) - w(\mathrm{X}).d(\mathrm{X}, \overline{C}_u)$, and

$$\begin{aligned} w(\mathrm{X}).d(\mathrm{X}, \overline{C}_u) &\leq p(C_v \cup \mathrm{X}) - p(C_v) = \\ &= p(C_v \cup \mathrm{X}) - (p(C_v) + w(\mathrm{X}).d(\mathrm{X}, \overline{C}_v)) + w(\mathrm{X}).d(\mathrm{X}, \overline{C}_v) \\ &= w(\mathrm{X}).d(\mathrm{X}, \overline{C}_v) + (p(C_v \cup \mathrm{X}) - \sum_{\mathrm{Y} \in C_v \cup \mathrm{X}} w(\mathrm{Y}).d(\mathrm{Y}, \overline{C}_v)) \end{aligned}$$

By the definition of cluster-error function of type R the second term in the last line is negative. Therefore

$$\leq w(\mathrm{X}).d(\mathrm{X}, \overline{C}_v)$$

Dividing by $w(\mathrm{X}) > 0$ we finally get

$$d(\mathrm{X}, \overline{C}_u) \leq d(\mathrm{X}, \overline{C}_v)$$

Leaders method

In order to support our intuition in further development we shall briefly describe a simple version of dynamic clusters method – the *leaders* or k-means method, which is the basis of the ISODATA program (one among the most popular clustering programs) and several recent 'data-mining' methods. In the leaders method the criterion function has the form SR.

The basic scheme of leaders method is simple:

determine $\mathbf{C}_0$; $\mathbf{C} := \mathbf{C}_0$;
repeat
  determine for each $C \in \mathbf{C}$ its leader $\overline{C}$;
  the new clustering $\mathbf{C}$ is obtained by assigning each unit
    to its nearest leader
until leaders stabilize

To obtain a 'good' solution and an impression of its quality we can repeat this procedure with different (random) $\mathbf{C}_0$.

The dynamic clusters method

The dynamic clusters method is a generalization of the above scheme. Let us denote:

Λ	– set of *representatives*
$\mathbf{L} \subseteq \Lambda$	– *representation*
Ψ	– set of *feasible representations*
$W : \Phi \times \Psi \to \mathbb{R}_0^+$	– *extended criterion function*
$G : \Phi \times \Psi \to \Psi$	– *representation function*
$F : \Phi \times \Psi \to \Phi$	– *clustering function*

and

Basic scheme of the dynamic clusters method

the following conditions have to be satisfied:

W0. $P(\mathbf{C}) = \min_{\mathrm{L} \in \Psi} W(\mathbf{C}, \mathrm{L})$

the functions G and F tend to improve (diminish) the value of the extended criterion function W:

W1. $W(\mathbf{C}, G(\mathbf{C}, \mathrm{L})) \leq W(\mathbf{C}, \mathrm{L})$

W2. $W(F(\mathbf{C}, \mathrm{L}), \mathrm{L}) \leq W(\mathbf{C}, \mathrm{L})$

then the *dynamic clusters method* can be described by the scheme:

$\mathbf{C} := \mathbf{C}_0; \mathrm{L} := \mathrm{L}_0;$

repeat

$\quad \mathrm{L} := G(\mathbf{C}, \mathrm{L});$

$\quad \mathbf{C} := F(\mathbf{C}, \mathrm{L})$

until the clustering stabilizes

Properties of DCM

To this scheme corresponds the sequence $v_n = (\mathbf{C}_n, \mathrm{L}_n), n \in \mathbb{N}$ determined by relations

$$\mathrm{L}_{n+1} = G(\mathbf{C}_n, \mathrm{L}_n) \quad \text{and} \quad \mathbf{C}_{n+1} = F(\mathbf{C}_n, \mathrm{L}_{n+1})$$

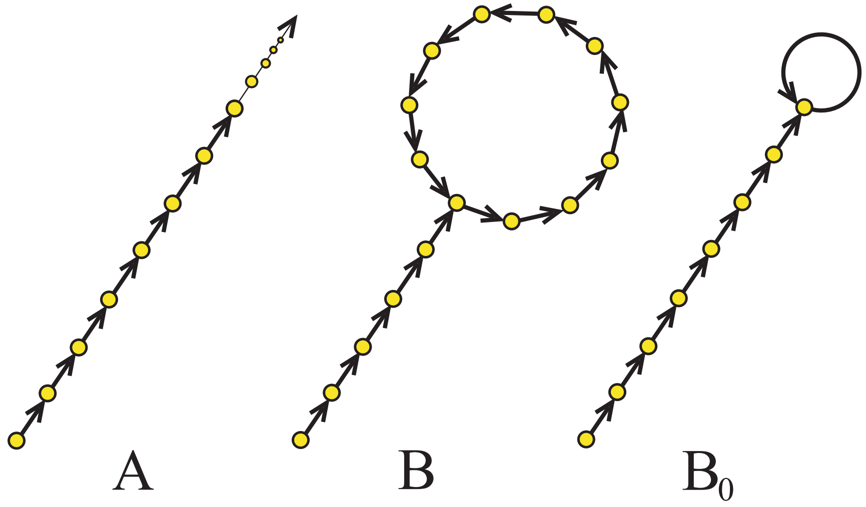
and the sequence of values of the extended criterion function $u_n = W(\mathbf{C}_n, \mathrm{L}_n)$. Let us also denote $u^* = P(\mathbf{C}^*)$. Then it holds:

Theorem 2.6 *For every* $n \in \mathbb{N}$, $u_{n+1} \leq u_n$, $u^* \leq u_n$, *and if for* $k > m$, $v_k = v_m$ *then* $\forall n \geq m : u_n = u_m$.

The Theorem 2.6 states that the sequence u_n is monotonically decreasing and bounded, therefore it is convergent. Note that the limit of u_n is not necessarily u^* – the dynamic clusters method is a local optimization method.

... types of of DCM sequences

Type A: $\neg\exists k, m \in \mathbb{N}, k > m : v_k = v_m$
Type B: $\exists k, m \in \mathbb{N}, k > m : v_k = v_m$
Type B$_0$: Type B with $k = m + 1$



The DCM sequence (v_n) is of type B if

- sets Φ and Ψ are both finite.
  For example, when we select a representative of C among its members.
- $\exists \delta > 0 : \forall n \in \mathbb{N} : (v_{n+1} \neq v_n \Rightarrow u_n - u_{n+1} > \delta)$

Because the sets $\mathbf{U}$ and consequently Φ are finite we expect from a good dynamic clusters procedure to stabilize in finite number of steps – is of type B.

Additional requirement

The conditions W0, W1 and W2 are not strong enough to ensure this. We shall try to compensate the possibility that the set of representations Ψ is infinite by the additional requirement:

W3. $W(\mathbf{C}, G(\mathbf{C}, \mathrm{L})) = W(\mathbf{C}, \mathrm{L}) \Rightarrow \mathrm{L} = G(\mathbf{C}, \mathrm{L})$

With this requirement the 'symmetry' between Φ and Ψ is distroyed. We could reestablish it by the requirement:

W4. $W(F(\mathbf{C}, \mathrm{L}, \mathrm{L})) = W(\mathbf{C}, \mathrm{L}) \Rightarrow \mathbf{C} = F(\mathbf{C}, \mathrm{L})$

but it turns out that W4 often fails. For this reason we shall avoid it.

Theorem 2.7 *If W3 holds and if there exists $m \in \mathbb{N}$ such that $u_{m+1} = u_m$, then also* $\mathrm{L}_{m+1} = \mathrm{L}_m$.

Simple clustering and representation functions

Usually, in the applications of the DCM, the clustering function takes the form $F : \Psi \to \Phi$. In this case the condition W2 simplifies to: $W(F(\mathrm{L}), \mathrm{L}) \leq W(\mathbf{C}, \mathrm{L})$ which can be expressed also as $F(\mathrm{L}) \in \mathrm{Min}_{\mathbf{C}\in\Phi} W(\mathbf{C}, \mathrm{L})$. For such, *simple* clustering functions it holds:

Theorem 2.8 *If the clustering function F is simple and if there exists $m \in \mathbb{N}$ such that $\mathrm{L}_{m+1} = \mathrm{L}_m$, then for every $n \geq m : v_n = v_m$.*

What can be said about the case when G is *simple* – has the form $G : \Phi \to \Psi$?

Theorem 2.9 *If W3 holds and the representation function G is simple then:*

a. $G(\mathbf{C}) = \arg\min_{\mathrm{L}\in\Psi} W(\mathbf{C}, \mathrm{L})$

b. $\exists k, m \in \mathbb{N}, k > m \forall i \in \mathbb{N} : v_{k+i} = v_{m+i}$

c. $\exists m \in \mathbb{N} \forall n \geq m : u_n = u_m$

d. *if also F is simple then* $\exists m \in \mathbb{N} \forall n \geq m : v_n = v_m$

Original DCM

In the original dynamic clusters method (Diday, 1979) both functions F and G are simple – $F : \Psi \to \Phi$ and $G : \Phi \to \Psi$.

We proved, if also W3 holds and the functions F and G are simple, then:

G0. $G(\mathbf{C}) = \operatorname*{argmin}_{\mathrm{L} \in \Psi} W(\mathbf{C}, \mathrm{L})$

and

F0. $F(\mathrm{L}) \in \mathrm{Min}_{\mathbf{C} \in \Phi} W(\mathbf{C}, \mathrm{L})$

In other words, given an extended criterion function W, the relations G0 and F0 define an appropriate pair of functions G and F such that the DCM stabilizes in finite number of steps.

...Clustering and Networks

In the next, 3. lecture we shall discuss

- clustering with relational constraint
- transforming data into graphs (neighbors)
- clustering of networks; dissimilarities between graphs (networks)
- clustering of vertices / links; dissimilarities between vertices
- clustering in large networks