Clustering - II

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1. Hierarchies
2. Dendrograms

Definition

Let S be a set. A *hierarchy on the set* S is a collection of sets $\mathcal{H} \subseteq \mathcal{P}(S)$ that satisfies the following conditions:

i. the members of $\mathcal{H}$ are nonempty sets;
ii. $S \in \mathcal{H}$;
iii. for every $x \in S$, we have $\{x\} \in \mathcal{H}$;
iv. if $H, H' \in \mathcal{H}$ and $H \cap H' \neq \emptyset$, then we have either $H \subseteq H'$ or $H' \subseteq H$.

Trees and Hierarchies

A standard technique for constructing a hierarchy on a set S starts with a rooted tree $(\mathcal{T}, v_0)$ whose nodes are labeled by subsets of the set S. Let V be the set of vertices of the tree $\mathcal{T}$. The function $\mu : V \longrightarrow \mathcal{P}(S)$, which gives the label $\mu(v)$ of each node $v \in V$, is defined as follows:

i. the tree $\mathcal{T}$ has $|S|$ leaves, and each leaf v is labeled by a distinct singleton $\mu(v) = \{x\}$ for $x \in S$;

ii. if an interior vertex v of the tree has the descendants $v_1, v_2, \ldots, v_n$, then $\mu(v) = \bigcup_{i=1}^{n} \mu(v_i)$.

The set of labels $\mathcal{H}_\mathcal{T}$ of the rooted tree $(\mathcal{T}, v_0)$ forms a hierarchy on S.

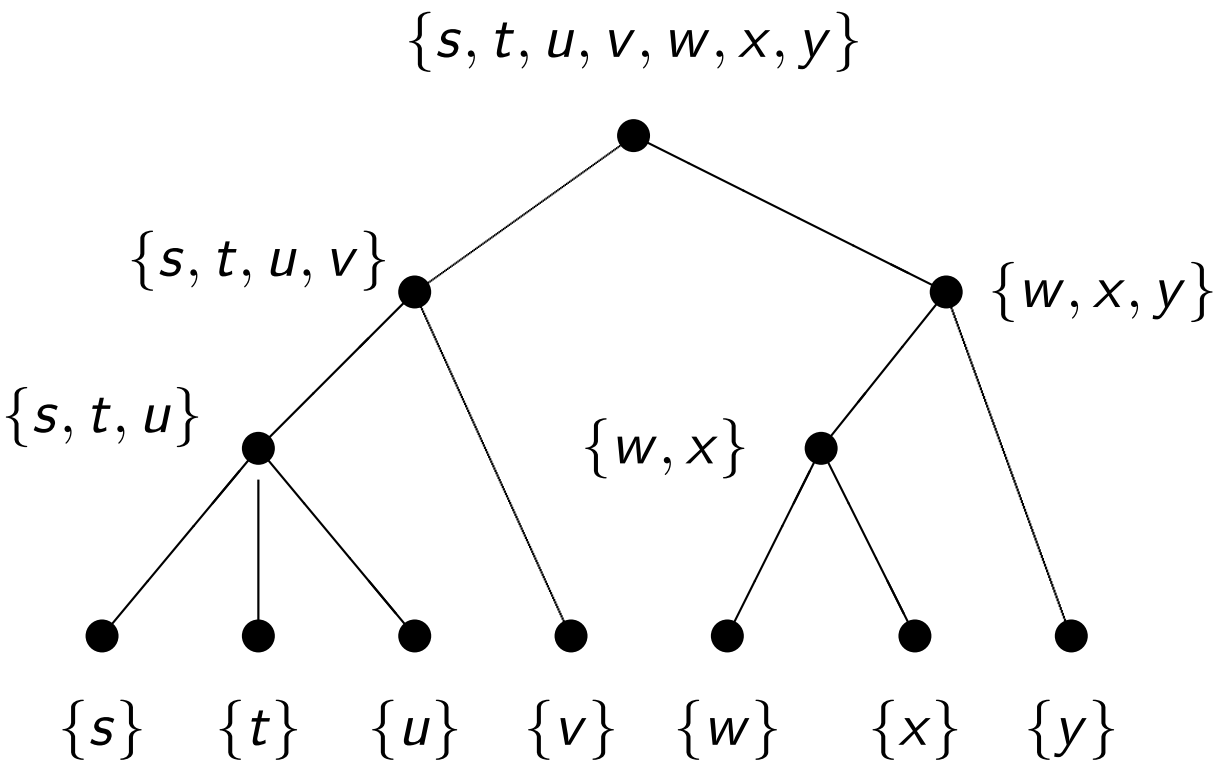
- Each singleton $\{x\}$ is a label of a leaf.
- Every vertex is labeled by the set of labels of the leaves that descend from that vertex.
- The root v_0 of the tree is labeled by S.

Suppose that H, H' are labels of the nodes u, v of $\mathcal{T}$, respectively. If $H \cap H' \neq \emptyset$, then the vertices u, v have a common descendant. In a tree, this can take place only if u is a descendant of v or v is a descendant of u; that is, only if $H \subseteq H'$, or $H' \subseteq H$, respectively.

Example

Let $S = \{s, t, u, v, w, x, y\}$ and let $\mathcal{T}$ be a tree. It is easy to verify that the family of subsets of S that label the nodes of $\mathcal{T}$ is a hierarchy on the set S.

$$\begin{aligned}\mathcal{H} \;=\; & \{\{s\},\{t\},\{u\},\{v\},\{w\},\{x\},\{y\},\\ & \{s,t,u\},\{w,x\},\{s,t,u,v\},\{w,x,y\},\{s,t,u,v,w,x,y\}\}\end{aligned}$$



Tree labeled by subsets of S.

Chains of partitions defined on a set generate hierarchies, as we show next.

Theorem

Let S be a set and let $C = (\pi_1, \pi_2, \ldots, \pi_n)$ be an increasing chain of partitions $(PART(S), \leqslant)$ such that $\pi_1 = \alpha_S$ and $\pi_n = \omega_S$. Then, the collection $\mathcal{H}_C = \bigcup_{i=1}^{n} \pi_i$ that consists of the blocks of all partitions in the chain is a hierarchy on S.

Proof

The blocks of any of the partitions are nonempty sets, so $\mathcal{H}_C$ satisfies the first condition of the Definition on Slide 3.
We have $S \in \mathcal{H}_C$ because S is the unique block of $\pi_n = \omega_S$. Also, since all singletons $\{x\}$ are blocks of $\alpha_S = \pi_1$, it follows that $\mathcal{H}_C$ satisfies the second and the third conditions of Definition on Slide3.
Finally, let H and H' be two sets of $\mathcal{H}_C$ such that $H \cap H' \neq \emptyset$. It is clear that these two sets cannot be blocks of the same partition. Thus, there exist two partitions π_i and π_j in the chain such that $H \in \pi_i$ and $H' \in \pi_j$. Suppose that $i < j$. Since every block of π_j is a union of blocks of π_i, H' is a union of blocks of π_i and $H \cap H' \neq \emptyset$ means that H is one of these blocks. Thus, $H \subseteq H'$.

Theorem on Slide 7 can be stated in terms of chains of equivalences; we give the following alternative formulation for convenience.

Theorem

Let S be a finite set and let $(\rho_1, \ldots, \rho_n)$ be a chain of equivalence relations on S such that $\rho_1 = \iota_S$ and $\rho_n = \theta_S$. Then, the collection of blocks of the equivalence relations ρ_r (that is, the set $\bigcup_{1 \leqslant r \leqslant n} S/\rho_r$) is a hierarchy on S.

Define the relation "$\prec$" on a hierarchy $\mathcal{H}$ on S by $H \prec K$ if $H, K \in \mathcal{H}$, $H \subset K$, and there is no set $L \in \mathcal{H}$ such that $H \subset L \subset K$.

Lemma

Let $\mathcal{H}$ be a hierarchy on a finite set S and let $L \in \mathcal{H}$. The collection $\mathcal{P}_L = \{H \in \mathcal{H} \mid H \prec L\}$ is a partition of the set L.

Proof: We claim that $L = \bigcup \mathcal{P}_L$. Indeed, it is clear that $\bigcup \mathcal{P}_L \subseteq L$. Conversely, suppose that $z \in L$ but $z \notin \bigcup \mathcal{P}_L$. Since $\{z\} \in \mathcal{H}$ and there is no $K \in \mathcal{P}_L$ such that $z \in K$, it follows that $\{z\} \in \mathcal{P}_L$, which contradicts the assumption that $z \notin \bigcup \mathcal{P}_L$. This means that $L = \bigcup \mathcal{P}_L$.
Let $K_0, K_1 \in \mathcal{P}_L$ be two distinct sets. These sets are disjoint since otherwise we would have either $K_0 \subset K_1$ or $K_1 \subset K_0$, and this would contradict the definition of $\mathcal{P}_L$.

Theorem

Let $\mathcal{H}$ be a hierarchy on a set S. The graph of the relation $\prec$ on $\mathcal{H}$ is a tree whose root is S; its leaves are the singletons $\{x\}$ for every $x \in S$.

Proof.

Since $\prec$ is an antisymmetric relation on $\mathcal{H}$, it is clear that the graph $(\mathcal{H}, \prec)$ is acyclic. Moreover, for each set $K \in \mathcal{H}$, there is a unique path that joins K to S, so the graph is indeed a rooted tree. □

Definition

Let $\mathcal{H}$ be a hierarchy on a set S. A *grading function* for $\mathcal{H}$ is a function $h : \mathcal{H} \longrightarrow \mathbb{R}$ that satisfies the following conditions:

i. $h(\{x\}) = 0$ for every $x \in S$, and

ii. if $H, K \in \mathcal{H}$ and $H \subset K$, then $h(H) < h(K)$.

If h is a grading function for a hierarchy $\mathcal{H}$, the pair $(\mathcal{H}, h)$ is a *graded hierarchy*.

Example

For the hierarchy $\mathcal{H}$ defined in Example on Slide 6 on the set $S = \{s, t, u, v, w, x, y\}$, the function $h : \mathcal{H} \longrightarrow \mathbb{R}$ given by

$$h(\{s\}) = h(\{t\}) = h(\{u\}) = h(\{v\}) = h(\{w\}) = h(\{x\}) = h(\{y\}) = 0,$$
$$h(\{s, t, u\}) = 3, h(\{w, x\}) = 4, h(\{s, t, u, v\}) = 5, h(\{w, x, y\}) = 6,$$
$$h(\{s, t, u, v, w, x, y\}) = 7,$$

is a grading function and the pair $(\mathcal{H}, h)$ is a graded hierarchy on S.

Theorem

Let S be a finite set and let $C = (\pi_1, \pi_2, \ldots, \pi_n)$ be an increasing chain of partitions $(PART(S), \leqslant)$ such that $\pi_1 = \alpha_S$ and $\pi_n = \omega_S$.
If $f : \{1, \ldots, n\} \longrightarrow \mathbb{R}_{\geqslant 0}$ is a function such that $f(1) = 0$, then the function $h : \mathcal{H}_C \longrightarrow \mathbb{R}_{\geqslant 0}$ given by $h(K) = f\left(\min\{j \mid K \in \pi_j\}\right)$ is a grading function for the hierarchy $\mathcal{H}_C$.

Proof: Since $\{x\} \in \pi_1 = \alpha_S$, it follows that $h(\{x\}) = 0$.
Suppose that $H, K \in \mathcal{H}_C$ and $H \subset K$. If $\ell = \min\{j \mid H \in \pi_j\}$ it is impossible for K to be a block of a partition that precedes π_ℓ. Therefore, $\ell < \min\{j \mid K \in \pi_j\}$, so $h(H) < h(K)$, and $(\mathcal{H}_C, h)$ is indeed a graded hierarchy.

A graded hierarchy defines an ultrametric, as shown next.

Theorem

Let $(\mathcal{H}, h)$ be a graded hierarchy on a finite set S. Define the function $d : S^2 \longrightarrow \mathbb{R}$ as $d(x, y) = \min\{h(U) \mid U \in \mathcal{H} \text{ and } \{x, y\} \subseteq U\}$ for $x, y \in S$. The mapping d is an ultrametric on S.

Observe that for every $x, y \in S$ there exists a set $H \in \mathcal{H}$ such that $\{x, y\} \subseteq H$ because $S \in \mathcal{H}$.
It is immediate that $d(x, x) = 0$. Conversely, suppose that $d(x, y) = 0$. Then, there exists $H \in \mathcal{H}$ such that $\{x, y\} \subseteq H$ and $h(H) = 0$. If $x \neq y$, then $\{x\} \subset H$, hence $0 = h(\{x\}) < h(H)$, which contradicts the fact that $h(H) = 0$. Thus, $x = y$.
The symmetry of d is immediate.
To prove the ultrametric inequality, let $x, y, z \in S$, and suppose that $d(x, y) = p$, $d(x, z) = q$, and $d(z, y) = r$. There exist $H, K, L \in \mathcal{H}$ such that $\{x, y\} \subseteq H$, $h(H) = p$, $\{x, z\} \subseteq K$, $h(K) = q$, and $\{z, y\} \subseteq L$, $h(L) = r$. Since $K \cap L \neq \emptyset$ (because both sets contain z), we have either $K \subseteq L$ or $L \subseteq K$, so $K \cup L$ equals either K or L and, in either case, $K \cup L \in \mathcal{H}$. Since $\{x, y\} \subseteq K \cup L$, it follows that

$$d(x, y) \leqslant h(K \cup L) = \max\{h(K), H(L)\} = \max\{d(x, z), d(z, y)\},$$

which is the ultrametric inequality.

Example

The values of the ultrametric generated by the graded hierarchy $(\mathcal{H}, h)$ on the set S introduced in Example given on Slide 13 are given in the following table:

d	s	t	u	v	w	x	y
s	0	3	3	5	7	7	7
t	3	0	3	5	7	7	7
u	3	3	0	5	7	7	7
v	5	5	5	0	7	7	7
w	7	7	7	7	0	4	6
x	7	7	7	7	4	0	6
y	7	7	7	7	6	6	0

Theorem

Let (S, d) be a finite ultrametric space. There exists a graded hierarchy $(\mathcal{H}, h)$ on S such that d is the ultrametric associated to $(\mathcal{H}, h)$.

Proof

Let $\mathcal{H}$ be the collection of equivalence classes of the equivalences $\eta_r = \{(x, y) \in S^2 \mid d(x, y) \leqslant r\}$ defined by the ultrametric d on the finite set S, where the index r takes its values in the range R_d of the ultrametric d. Define $h(E) = \min\{r \in R_d \mid E \in S/\eta_r\}$ for every equivalence class E. It is clear that $h(\{x\}) = 0$ because $\{x\}$ is an η_0-equivalence class for every $x \in S$.
Let $[x]_t$ be the equivalence class of x relative to the equivalence η_t.
Suppose that E and E' belong to the hierarchy and $E \subset E'$. We have $E = [x]_r$ and $E' = [x]_s$ for some $x \in X$. Since E is strictly included in E', there exists $z \in E' - E$ such that $d(x, z) \leqslant s$ and $d(x, z) > r$. This implies $r < s$. Therefore,

$$h(E) = \min\{r \in R_d \mid E \in S/\eta_r\} \leq \min\{s \in R_d \mid E' \in S/\eta_s\} = h(E'),$$

which proves that $(\mathcal{H}, h)$ is a graded hierarchy.

Proof (cont'd)

The ultrametric e generated by the graded hierarchy $(\mathcal{H}, h)$ is given by

$$\begin{aligned} e(x,y) &= \min\{h(B) \mid B \in \mathcal{H} \text{ and } \{x,y\} \subseteq B\} \\ &= \min\{r \mid (x,y) \in \eta_r\} = \min\{r \mid d(x,y) \leqslant r\} = d(x,y), \end{aligned}$$

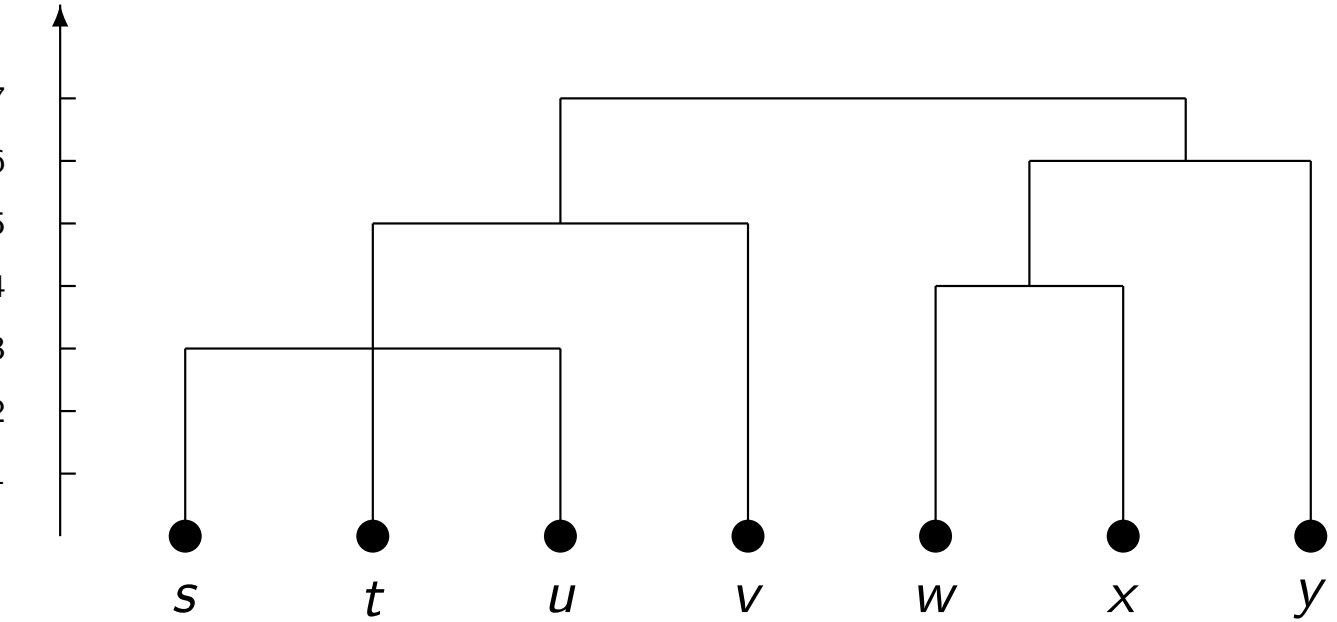
for $x, y \in S$; in other words, we have $e = d$.

Example

Starting from the ultrametric on the set $S = \{s, t, u, v, w, x, y\}$ defined by the table given in Example on Slide 17, we obtain the following quotient sets:

Values of r	S/η_r
$[0, 3)$	$\{s\}, \{t\}, \{u\}, \{v\}, \{w\}, \{x\}, \{y\}$
$[3, 4)$	$\{s, t, u\}, \{v\}, \{w\}, \{x\}, \{y\}$
$[4, 5)$	$\{s, t, u\}, \{v\}, \{w, x\}, \{y\}$
$[5, 6)$	$\{s, t, u, v\}, \{w, x\}, \{y\}$
$[6, 7)$	$\{s, t, u, v\}, \{w, x, y\}$
$[7, \infty)$	$\{s, t, u, v, w, x, y\}$

We shall draw the tree of a graded hierarchy $(\mathcal{H}, h)$ using a special representation known as a *dendrogram*.
In a dendrogram, an interior vertex K of the tree is represented by a horizontal line drawn at the height $h(K)$. For example, the dendrogram of the graded hierarchy of Example given on Slide 13 is shown next.
As we saw, the value $d(x, y)$ of the ultrametric d generated by a hierarchy $\mathcal{H}$ is the smallest height of a set of a hierarchy that contains both x and y. This allows us to "read" the value of the ultrametric generated by $\mathcal{H}$ directly from the dendrogram of the hierarchy.



Dendrogram of graded hierarchy of Example given on Slide 13