

# Machine Learning II

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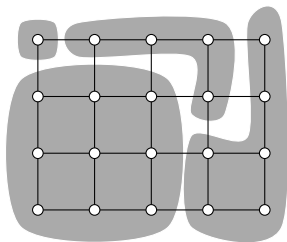
Machine Learning for Computer Vision  
TU Dresden



<https://mlcv.cs.tu-dresden.de/courses/26-summer/ml2/>

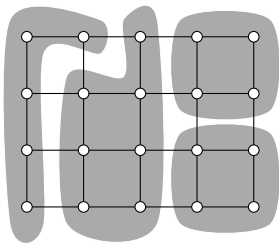
Summer Term 2026

## Clustering



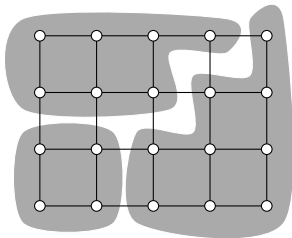
Clustering of a graph  $G = (V, E)$

## Clustering



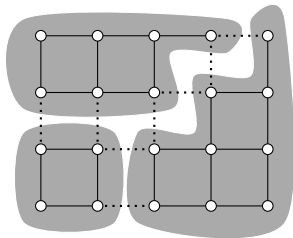
Clustering of a graph  $G = (V, E)$

## Clustering



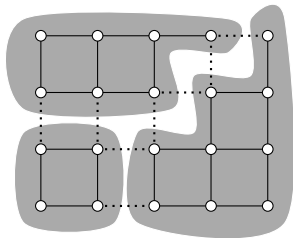
Clustering of a graph  $G = (V, E)$

## Clustering



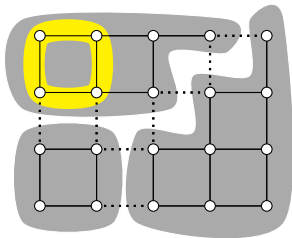
Clustering of a graph  $G = (V, E)$

## Clustering



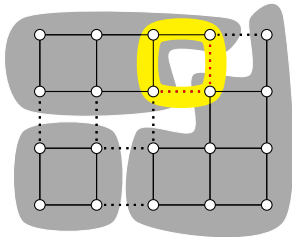
Multicut of a graph  $G = (V, E)$

## Clustering



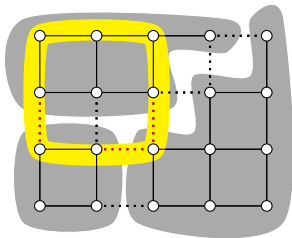
Multicut of a graph  $G = (V, E)$

## Clustering



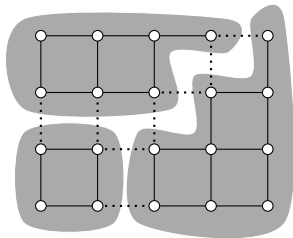
Multicut of a graph  $G = (V, E)$

## Clustering



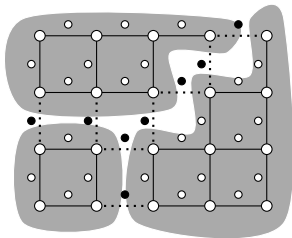
Multicut of a graph  $G = (V, E)$

## Clustering



Multicut of a graph  $G = (V, E)$

## Clustering



Multicut of a graph  $G = (V, E)$

**Definition 1.** Let  $G = (V, E)$  be any graph.

- A subgraph  $G' = (U, E')$  of  $G$  is called a **cluster** of  $G$  iff  $G'$  is non-empty, node-induced (i.e.  $E' = E \cap \binom{U}{2}$ ) and connected.
- A partition  $\Pi$  of the node set  $V$  is called a **clustering** of  $G$  iff for every  $U \in \Pi$  the subgraph  $(U, E \cap \binom{U}{2})$  of  $G$  induced by  $U$  is connected (and thus a component of  $G$ ).
- Let  $C_G$  denote the set of all clusterings of  $G$ .

**Definition 2.** Let  $G = (V, E)$  be any graph.

- For any  $M \subseteq E$ ,  $M$  is called a **multicut** of  $G$  iff for every cycle  $(V_C, E_C)$  of  $G$ :  $|E_C \cap M| \neq 1$ .
- Let  $M_G$  denote the set of all multicuts of  $G$ .

**Lemma 1.** Let  $G = (V, E)$  be any graph.

- For any clustering  $\Pi$  of  $G$ , the set  $\{ab \in E \mid \forall U \in \Pi: a \notin U \vee b \notin U\}$   
=:  $M_\Pi$  of those edges that straddle distinct clusters is a multicut of  $G$ .
- For any clustering  $\Pi$  of  $G$ , the multicut  $M_\Pi$  is said to be **induced** by  $\Pi$ .
- The map  $\Pi \mapsto M_\Pi$  from clusterings to induced multicuts is a **bijection** from  $C_G$  to  $M_G$ .

## Clustering

**Remark 1.** The characteristic function  $y \in \{0, 1\}^E$  of a multicut  $y^{-1}(1)$  makes explicit for every edge  $ab = e \in E$  whether the incident nodes  $a$  and  $b$  belong to the same clusters,  $y_e = 0$ , or distinct clusters,  $y_e = 1$ .

**Lemma 2.** For any  $y \in \{0, 1\}^E$ , the set  $y^{-1}(1)$  is a multicut of  $G$  iff the following inequalities are satisfied:

$$\forall (V_C, E_C) \in \text{cycles}(G) \quad \forall e \in E_C: \quad y_e \leq \sum_{e' \in E_C \setminus \{e\}} y_{e'} \quad (1)$$

**Learning and inferring clusterings:**

- Instead of the problem of learning and inferring clusterings, we consider the problem of learning and inferring multicuts. By Lemma 1, this is w.l.o.g..
- We reduce the problem of learning and inferring multicuts to the problem of learning and inferring decisions, by defining constrained data  $(S, X, x, Y)$  with

$$S = E \tag{2}$$

$$\mathcal{Y} = \left\{ y \in \{0, 1\}^E \mid \forall (V_C, E_C) \in \text{cycles}(G) \forall e \in E_C : y_e \leq \sum_{e' \in E_C \setminus \{e\}} y_{e'} \right\} . \tag{3}$$

- As inference problem, we obtain the **(minimum cost) multicut problem**

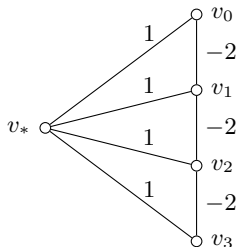
$$\min_{y \in \{0, 1\}^E} \sum_{e \in E} \underbrace{(-f_\theta(x_e))}_{=: c_e} y_e \tag{4}$$

$$\text{subject to } \forall (V_C, E_C) \in \text{cycles}(G) \forall e \in E_C : y_e \leq \sum_{e' \in E_C \setminus \{e\}} y_{e'} . \tag{5}$$

## Clustering

**Theorem 1.** The minimum cost multicut problem is NP-hard.

*Proof.* (Sketch) By reduction of **maximum independent set**:

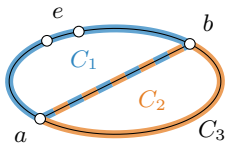


□

## Clustering

**Theorem 2** (Chopra and Rao 1993). In the minimum cost multicut problem, the inequalities (1) are redundant for chordal cycles.

*Proof.* (Sketch) Consider a cycle  $C_3$  with a chord  $ab$ .



By induction, (1) holds for  $C_1$  and  $C_2$ . For any  $e \in C_1 \setminus \{ab\}$ :

$$\begin{aligned} y_e &\leq \sum_{e' \in C_1 \setminus \{e\}} y_{e'} = y_{ab} + \sum_{e' \in C_1 \setminus \{e, ab\}} y_{e'} \\ &\leq \sum_{e' \in C_2 \setminus \{ab\}} y_{e'} + \sum_{e' \in C_1 \setminus \{e, ab\}} y_{e'} = \sum_{e' \in C_3 \setminus \{e\}} y_{e'} . \end{aligned}$$

For any  $e \in C_2 \setminus \{ab\}$ , the argument is analogous. □

**Corollary 1** (Chopra and Rao 1993). The multicut problem for a complete graph is isomorphic to the clique partition problem for the node set.

*Proof.* (Sketch) In a complete graph  $G = (V, E)$ , the chordless cycles are precisely the triangles.

The inequalities (1) for all triangles are written equivalently as

$$\forall a \in V \forall b \in V \setminus \{a\} \forall c \in V \setminus \{a, b\}: \quad y_{ac} \leq y_{ab} + y_{bc} \ .$$

Substituting  $1 - y'$  for  $y$  (i.e. swapping the roles of 0 and 1), yields the transitivity constraints of the clique partition problem:

$$\forall a \in V \forall b \in V \setminus \{a\} \forall c \in V \setminus \{a, b\}: \quad y'_{ab} + y'_{bc} - 1 \leq y'_{ac} \ .$$

□

**Definition 3.** For any graph  $G = (V, E)$  and any  $c \in \mathbb{R}^E$ , the **cycle relaxation** of the minimum cost multicut problem is

$$\min_{y \in \mathbb{R}^E} \langle c, y \rangle \quad (6)$$

$$\text{subject to } \forall (V_C, E_C) \in \text{cycles}(G) \forall e \in E_C: y_e \leq \sum_{e' \in E_C \setminus \{e\}} y_{e'} \quad (7)$$

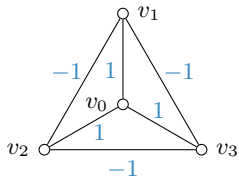
$$\forall e \in E: 0 \leq y_e \leq 1 . \quad (8)$$

**Remark 2.** The cycle relaxation of the minimum cost multicut problem

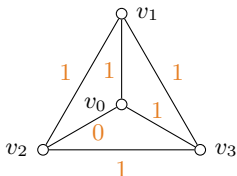
- can be solved by the simplex algorithm
- yields a lower bound on the minimum cost
- can be solved efficiently
- is not tight (see below)

## Clustering

**Example 1.** Instance of the multicut problem for an odd wheel:

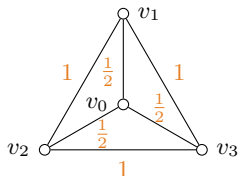


Instance



Solution

$$\langle c, y \rangle = -1$$



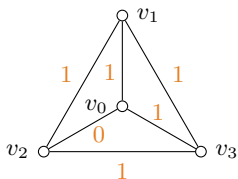
Solution to relaxation

$$\langle c, y \rangle = -\frac{3}{2}$$

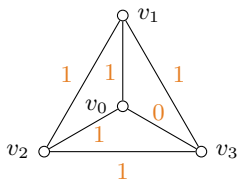
**Remark 3.** Approaches to working with LP relaxations that are not tight:

- branching
- cutting planes

**Example 2. Branching on  $y_{v_0v_2}$**



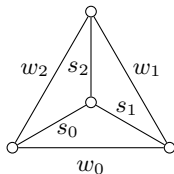
Solution to relaxation with  $y_{v_0v_2} = 0$   
 $\langle c, y \rangle = -1$



Solution to relaxation with  $y_{v_0v_2} = 1$   
 $\langle c, y \rangle = -1$

## Clustering

**Example 3.** An odd wheel inequality as a Chvátal-Gomory cutting plane:



From the cycle relaxation of the multicut problem, the inequalities

$$\begin{array}{ll} y_{w_0} \leq y_{s_0} + y_{s_1} & y_{w_0} \leq 1 \\ y_{w_1} \leq y_{s_1} + y_{s_2} & y_{w_1} \leq 1 \\ y_{w_2} \leq y_{s_2} + y_{s_0} & y_{w_2} \leq 1 \end{array}$$

together imply

$$\sum_j y_{w_j} - \sum_j y_{s_j} \leq \frac{3}{2}$$

For any integral feasible solution  $y$ , the lhs. is an integer. Thus:

$$\sum_j y_{w_j} - \sum_j y_{s_j} \leq \left\lfloor \frac{3}{2} \right\rfloor .$$

## Clustering

Next, we discuss partial optimality for clustering.

For ease of notation, we consider complete graphs, i.e., the clique partition problem.

## Clustering

**Definition 4.** For any  $A \neq \emptyset$  finite, any  $c: \binom{A}{2} \rightarrow \mathbb{R}$ ,

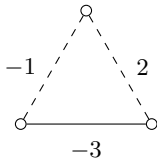
$$Y_A := \left\{ y: \binom{A}{2} \rightarrow \{0, 1\} \mid \forall a \in A \forall b \in A \setminus \{a\} \forall c \in A \setminus \{a, b\}: \right. \\ \left. y_{ab} + y_{bc} - 1 \leq y_{ac} \right\} \quad (9)$$

and  $\varphi_c: Y_A \rightarrow \mathbb{R}: y \mapsto \langle c, y \rangle$ ,

$$\min\{\varphi_c(y) \mid y \in Y_A\} \quad (10)$$

is called the instance of the **(clique) partition problem** wrt.  $A$  and  $c$ , which we abbreviate as  $\text{CPP}(A, c)$ .

**Example 4.**



## Clustering

For any set  $A$  and any  $U \subseteq A$ , we write

$$\partial U := \{\{u, a\} \in \binom{A}{2} \mid u \in U \wedge a \notin U\} . \quad (11)$$

**Definition 5.** Let  $A \neq \emptyset$  finite and  $U \subseteq A$ .

- The **elementary cut map** wrt.  $U$  is the  $\sigma_U: Y_A \rightarrow Y_A$  such that  $\forall y \in Y_A \forall \{a, b\} \in \binom{A}{2}$ :

$$\sigma_U(y)_{ab} = \begin{cases} 0 & \text{if } \{a, b\} \in \partial U \\ y_{ab} & \text{otherwise} \end{cases} . \quad (12)$$

- The **elementary join map** wrt.  $U$  is the  $\sigma'_U: Y_A \rightarrow Y_A$  such that  $\forall y \in Y_A \forall \{a, b\} \in \binom{A}{2}$ :

$$\sigma'_U(y)_{ab} = \begin{cases} 1 & \text{if } \{a, b\} \in \binom{U}{2} \\ 1 & \text{if } a \in U \wedge \exists u \in U: y_{ub} = 1 \\ 1 & \text{if } b \in U \wedge \exists u \in U: y_{ua} = 1 \\ 1 & \text{if } (\exists u \in U: y_{ua} = 1) \wedge \\ & (\exists u \in U: y_{ub} = 1) \\ y_{ab} & \text{otherwise} \end{cases} . \quad (13)$$

**Remark 4.**  $\sigma_U$  is well-defined, i.e.  $\sigma_U(Y_A) \subseteq Y_A$ .  $\sigma'_U$  is well-defined.  $\sigma'_U \circ \sigma_U$  is well-defined.

To begin with, we establish a trivial partial optimality condition for the clique partition problem:

**Lemma 3.** Let  $A \neq \emptyset$  finite and  $c: \binom{A}{2} \rightarrow \mathbb{R}$ . If there exists  $U \subseteq A$  such that

$$\forall \{a, b\} \in \partial U: \quad 0 \leq c_{ab} \quad , \quad (14)$$

there exists a solution  $y^*$  to  $\text{CPP}(A, c)$  such that

$$\forall \{a, b\} \in \partial U: \quad y_{ab}^* = 0 \quad . \quad (15)$$

## Clustering

*Proof.* For any  $y \in Y_A$ ,  $\sigma_U(y)$  satisfies (15). Moreover,  $\sigma_U$  is improving for  $\text{CPP}(A, c)$  because for any  $y \in Y_A$  and  $y' := \sigma_U(y)$ :

$$\varphi_c(y') - \varphi_c(y) = \sum_{\{a,b\} \in \binom{A}{2}} c_{ab} y'_{ab} - \sum_{\{a,b\} \in \binom{A}{2}} c_{ab} y_{ab} \quad (16)$$

$$= \sum_{\{a,b\} \in \binom{A}{2}} c_{ab} (y'_{ab} - y_{ab}) \quad (17)$$

$$= \sum_{\{a,b\} \in \partial U} c_{ab} (0 - y_{ab}) \quad (18)$$

$$= - \sum_{\{a,b\} \in \partial U} c_{ab} y_{ab} \quad (19)$$

$$\stackrel{(14)}{\leq} 0 . \quad (20)$$

□

## Clustering

For any  $r \in \mathbb{R}$ , we write

$$[r]_+ := \begin{cases} r & \text{if } r \geq 0 \\ 0 & \text{otherwise} \end{cases} \quad (21)$$

$$[r]_- := \begin{cases} 0 & \text{if } r \geq 0 \\ -r & \text{otherwise} \end{cases} . \quad (22)$$

Next, we establish a less trivial partial optimality condition for the CPP:

**Proposition 1.** Let  $A \neq \emptyset$  finite and  $c: \binom{A}{2} \rightarrow \mathbb{R}$ . If there exist  $U \subseteq A$  and  $\{u, v\} \in \partial U$  such that

$$\sum_{\{a,b\} \in \partial U \setminus \{\{u,v\}\}} [c_{ab}]_- \leq c_{uv} \quad , \quad (23)$$

there exists a solution  $y^*$  to  $\text{CPP}(A, c)$  such that  $y_{uv}^* = 0$ .

## Clustering

*Proof.* Let  $\xi: Y_A \rightarrow Y_A$  such that for all  $y \in Y_A$ :

$$\xi(y) = \begin{cases} y & \text{if } y_{uv} = 0 \\ \sigma_U(y) & \text{otherwise} \end{cases} . \quad (24)$$

For any  $y \in Y_A$  and  $y' := \xi(y)$ , we have  $y'_{uv} = 0$ .

Moreover,  $\xi$  is improving for  $\text{CPP}(A, c)$  because for all  $y \in Y_A$  and  $y' := \xi(y)$ , the following holds: If  $y_{ab} = 0$  then  $\varphi_c(y') - \varphi_c(y) = \varphi_c(y) - \varphi_c(y) = 0 \leq 0$ .

Otherwise:

$$\varphi_c(y') - \varphi_c(y) = \sum_{\{a,b\} \in \binom{A}{2}} c_{ab}(y'_{ab} - y_{ab}) \quad (25)$$

$$= c_{uv}(0 - 1) + \sum_{\{a,b\} \in \partial U \setminus \{\{u,v\}\}} c_{ab}(0 - y_{ab}) \quad (26)$$

$$= -c_{uv} - \sum_{\{a,b\} \in \partial U \setminus \{\{u,v\}\}} c_{ab} y_{ab} \quad (27)$$

$$\leq -c_{uv} + \sum_{\{a,b\} \in \partial U \setminus \{\{u,v\}\}} [c_{ab}]_- \quad (28)$$

$$\stackrel{(23)}{\leq} 0 . \quad (29)$$

□

Next, we establish a non-trivial partial optimality condition for the CPP:

**Lemma 4.** Let  $A \neq \emptyset$  finite and  $c: \binom{A}{2} \rightarrow \mathbb{R}$ . If there exist  $U \subseteq A$  such that

$$\sum_{\{u,a\} \in \partial U} [c_{ua}]_- \leq \min_{\{s,t\} \in \binom{U}{2}} \min_{\substack{y \in Y_U \\ y_{st}=0}} \sum_{\{u,v\} \in \binom{U}{2}} (-c_{uv})(1 - y_{uv}) , \quad (30)$$

there exists a solution  $y^*$  to  $\text{CPP}(A, c)$  such that  $\forall \{u, v\} \in \binom{U}{2}: y_{uv}^* = 1$ .

## Clustering

*Proof.* Let  $\xi: Y_A \rightarrow Y_A$  such that for all  $y \in Y_A$ :

$$\xi(y) := \begin{cases} (\sigma'_U \circ \sigma_U)(y) & \text{if } \exists \{u, v\} \in \binom{U}{2}: y_{uv} = 0 \\ y & \text{otherwise} \end{cases} . \quad (31)$$

For any  $y \in Y_A$ ,  $y' := \xi(y)$  and all  $\{u, v\} \in \binom{U}{2}$ , we have  $y'_{uv} = 1$ .

Moreover,  $\xi$  is improving because for all  $y \in Y_A$  and  $y' := \xi(y)$ , the following condition holds: If  $\forall \{u, v\} \in \binom{U}{2}: y_{uv} = 1$  then

$\varphi_c(y') - \varphi_c(y) = \varphi_c(y) - \varphi_c(y) = 0 \leq 0$ . Otherwise:

$$\varphi_c(y') - \varphi_c(y) = \sum_{\{u,a\} \in \partial U} c_{ua}(0 - y_{ua}) + \sum_{\{u,v\} \in \binom{U}{2}} c_{uv}(1 - y_{uv}) \quad (32)$$

$$\leq \sum_{\{u,a\} \in \partial U} [c_{ua}]_- + \max_{\{s,t\} \in \binom{U}{2}} \max_{\substack{y \in Y_U \\ y_{st} = 0}} \sum_{\{u,v\} \in \binom{U}{2}} c_{uv}(1 - y_{uv}) \quad (33)$$

$$\leq \sum_{\{u,a\} \in \partial U} [c_{ua}]_- - \min_{\{s,t\} \in \binom{U}{2}} \min_{\substack{y \in Y_U \\ y_{st} = 0}} \sum_{\{u,v\} \in \binom{U}{2}} (-c_{uv})(1 - y_{uv}) \quad (34)$$

$$\stackrel{(30)}{\leq} 0 . \quad (35)$$

□

Even if set  $U \subseteq A$  is given, Condition (30) of Lemma 4 cannot be checked efficiently: In general, the calculation of

$$\min_{\{s,t\} \in \binom{U}{2}} \min_{\substack{y \in Y_U \\ y_{st}=0}} \sum_{\{u,v\} \in \binom{U}{2}} (-c_{uv})(1 - y_{uv}) \quad (36)$$

requires solving CPPs with the additional constraint  $y_{st} = 0$ .

However, in the special case where  $\forall \{u,v\} \in \binom{U}{2}: c_{uv} \leq 0$ , these problems become minimum  $st$ -cut problems that can be solved efficiently.

Hence, one way of applying Lemma 4 algorithmically is in two steps:

1. heuristically search for a set  $U$  such that
  - inside  $U$ , all costs are non-positive
  - on the boundary of  $U$ , the sum of the negative costs is large.
2. efficiently test (30) for this  $U$