

Machine Learning I

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Machine Learning for Computer Vision
TU Dresden



Winter Term 2022/2023

Clustering

Contents.

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Clustering

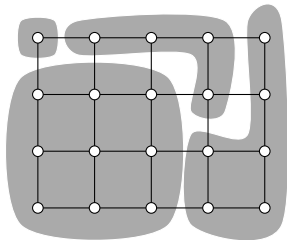
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- ▶ This part of the course is about the problem of **decomposing (clustering)** a graph into **components (clusters)**, without knowing the number, size or any other property of the clusters.
- ▶ This generalizes the problem of partitioning a set. It specializes to the latter for complete graphs.

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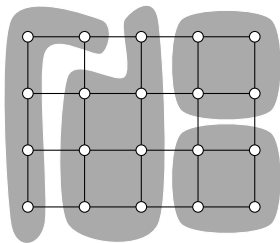
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- ▶ This generalizes the problem of partitioning a set. It specializes to the latter for complete graphs.
- ▶ Analogously, the problem of decomposing a graph is introduced as an **unsupervised learning** problem w.r.t. **constrained data**.

Clustering



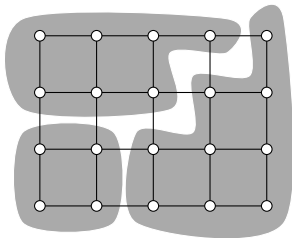
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Clustering



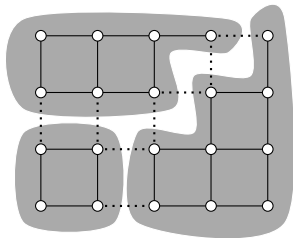
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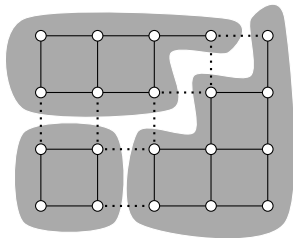
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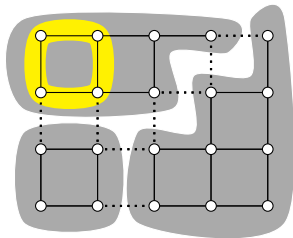
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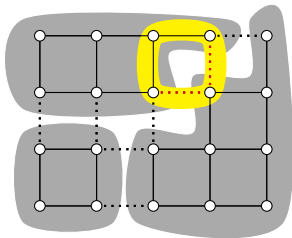
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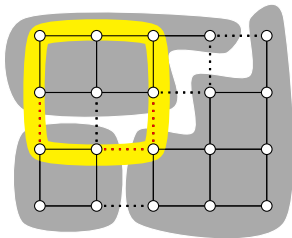
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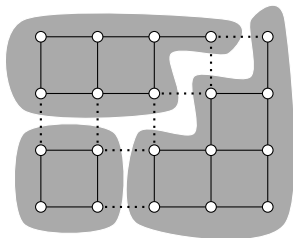
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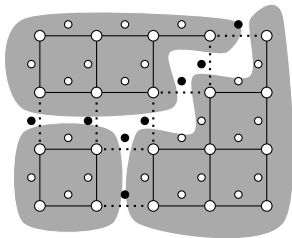
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- ▶ We denote by D_G the set of all decompositions of G .

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Lemma.

- ▶ For any decomposition of a graph G , the set of those edges that straddle distinct components is a multicut of G . This multicut is said to be **induced** by the decomposition.
- ▶ The map from decompositions to induced multicuts is a **bijection** from D_G to M_G .

Clustering

Remarks:

- ▶ The characteristic function $y: E \rightarrow \{0, 1\}$ of a multicut $y^{-1}(1)$ decides, for every edge $\{a, b\} = e \in E$, whether the incident nodes a and b belong to the same component ($y_e = 0$) or distinct components ($y_e = 1$).

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Lemma. For any $y: E \rightarrow \{0, 1\}$, the set $y^{-1}(1)$ of those edges that are mapped to 1 is a multicut of G iff the following inequalities are satisfied:

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

Constrained Data

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

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

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

Clustering

Family of functions

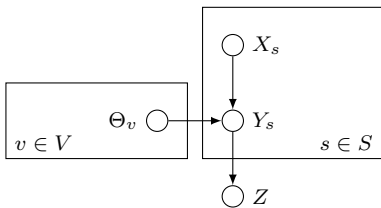
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Family of functions

- ▶ We consider a finite, non-empty set V , called a set of **attributes**, and the **attribute space** $X = \mathbb{R}^V$
- ▶ We consider **linear functions**. Specifically, we consider $\Theta = \mathbb{R}^V$ and $f : \Theta \rightarrow \mathbb{R}^X$ such that

$$\forall \theta \in \Theta \quad \forall \hat{x} \in \mathbb{R}^V : \quad f_{\theta}(\hat{x}) = \sum_{v \in V} \theta_v \hat{x}_v = \langle \theta, \hat{x} \rangle . \quad (4)$$

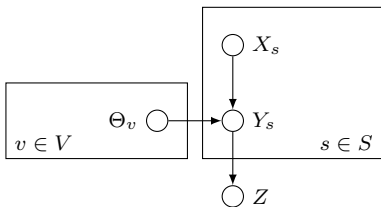
Clustering



Random Variables

- For any $\{a, b\} = s \in S = E$, let X_s be a random variable whose value is a vector $x_s \in \mathbb{R}^V$, the **attribute vector** of s .

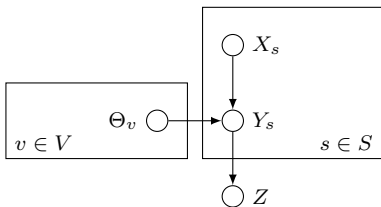
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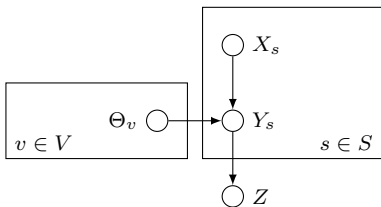
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- ▶ For any $v \in V$, let Θ_v be a random variable whose value is a real number $\theta_v \in \mathbb{R}$, a **parameter** of the function we seek to learn.

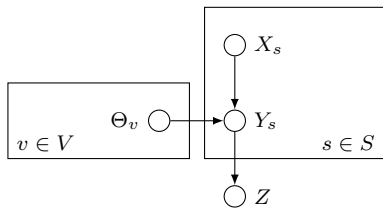
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- ▶ For any $v \in V$, let Θ_v be a random variable whose value is a real number $\theta_v \in \mathbb{R}$, a **parameter** of the function we seek to learn.
- ▶ Let Z be a random variable whose value is a subset $\mathcal{Z} \subseteq \{0, 1\}^S$ called the set of **feasible decisions**. For clustering, we are interested in $\mathcal{Z} = \mathcal{Y}$, the set characterizing multicuts of G .

Clustering



Factorization

$$P(X, Y, Z, \Theta) = P(Z | Y) \prod_{s \in S} P(Y_s | X_s, \Theta) \prod_{v \in V} P(\Theta_v) \prod_{s \in S} P(X_s)$$

Clustering

Factorization

- ▶ Supervised learning:

$$P(\Theta \mid X, Y, Z)$$

Clustering

Factorization

- Supervised learning:

$$\begin{aligned} P(\Theta | X, Y, Z) &= \frac{P(X, Y, Z, \Theta)}{P(X, Y, Z)} \\ &= \frac{P(Z | Y) P(Y | X, \Theta) P(X) P(\Theta)}{P(Z | X, Y) P(X, Y)} \\ &= \frac{P(Z | Y) P(Y | X, \Theta) P(X) P(\Theta)}{P(Z | Y) P(X, Y)} \\ &= \frac{P(Y | X, \Theta) P(X) P(\Theta)}{P(X, Y)} \\ &\propto P(Y | X, \Theta) P(\Theta) \\ &= \prod_{s \in S} P(Y_s | X_s, \Theta) \prod_{v \in V} P(\Theta_v) \end{aligned}$$

Clustering

Factorization

► Inference:

$$P(Y | X, Z, \theta)$$

Clustering

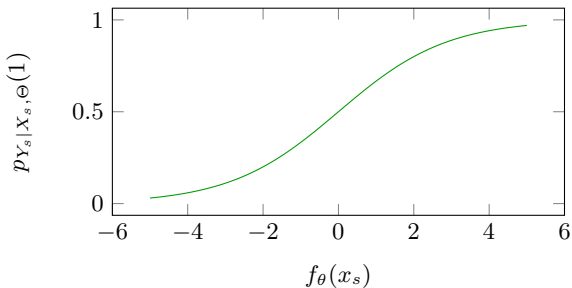
Factorization

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$$\begin{aligned} P(Y | X, Z, \theta) &= \frac{P(X, Y, Z, \Theta)}{P(X, Z, \Theta)} \\ &= \frac{P(Z | Y) P(Y | X, \Theta) P(X) P(\Theta)}{P(X, Z, \Theta)} \\ &\propto P(Z | Y) P(Y | X, \Theta) \\ &= P(Z | Y) \prod_{s \in S} P(Y_s | X_s, \Theta) \end{aligned}$$

► **Logistic distribution**

$$\forall s \in S: \quad p_{Y_s|X_s, \theta}(1) = \frac{1}{1 + 2^{-f_\theta(x_s)}} \quad (5)$$

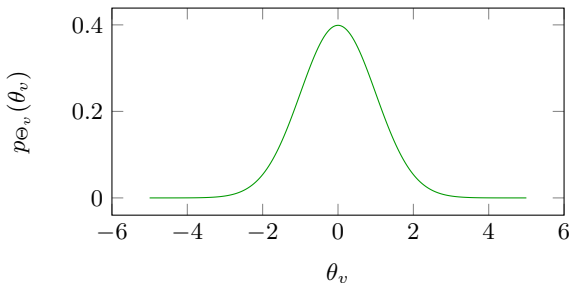


Clustering

Distributions

- **Normal distribution** with $\sigma \in \mathbb{R}^+$:

$$\forall v \in V : \quad p_{\Theta_v}(\theta_v) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\theta_v^2/2\sigma^2} \quad (6)$$



Clustering

Distributions

► **Uniform distribution on a subset**

$$\forall \mathcal{Z} \subseteq \{0, 1\}^S \quad \forall y \in \{0, 1\}^S \quad p_{\mathcal{Z}|Y}(\mathcal{Z}, y) \propto \begin{cases} 1 & \text{if } y \in \mathcal{Z} \\ 0 & \text{otherwise} \end{cases}$$

Note that $p_{\mathcal{Z}|Y}(\mathcal{Y}, y)$ is non-zero iff the labeling $y: S \rightarrow \{0, 1\}$ defines an multicut of G .

Clustering

Lemma. Estimating maximally probable parameters θ , given attributes x and decisions y , i.e.,

$$\operatorname{argmax}_{\theta \in \mathbb{R}^V} p_{\Theta|X,Y,Z}(\theta, x, y, \mathcal{Y})$$

is an l_2 -regularized logistic regression problem.

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Proof. Analogous to the case of deciding, we obtain:

$$\begin{aligned} & \operatorname{argmax}_{\theta \in \mathbb{R}^V} p_{\Theta|X,Y,Z}(\theta, x, y, \mathcal{Y}) \\ &= \operatorname{argmin}_{\theta \in \mathbb{R}^V} \sum_{s \in S} \left(-y_s f_{\theta}(x_s) + \log \left(1 + 2^{f_{\theta}(x_s)} \right) \right) + \frac{\log e}{2\sigma^2} \|\theta\|_2^2 . \end{aligned}$$

Clustering

Lemma. Estimating maximally probable decisions y , given attributes x , given the set of feasible decisions \mathcal{Y} , and given parameters θ , i.e.,

$$\operatorname{argmax}_{y \in \{0,1\}^S} p_{Y|X,Z,\Theta}(y, x, \mathcal{Y}, \theta) \quad (7)$$

assumes the form of the **minimum cost multicut problem**:

$$\operatorname{argmin}_{y: E \rightarrow \{0,1\}} \sum_{e \in E} (-\langle \theta, x_e \rangle) y_e \quad (8)$$

$$\text{subject to } \forall C \in \text{cycles}(G) \forall e \in C: y_e \leq \sum_{e' \in C \setminus \{e\}} y_{e'} \quad (9)$$

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

Bansal et al. (2004) reduce this problem to the k terminal cut problem whose NP-hardness is an important result Dahlhaus et al. (1994).

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For simplicity, we define $c : E \rightarrow \mathbb{R}$ such that

$$\forall e \in S: \quad c_e = -\langle \theta, x_e \rangle \quad (10)$$

and write the (linear) cost function $\varphi : \{0, 1\}^E \rightarrow \mathbb{R}$ such that

$$\forall y \in \{0, 1\}^E: \quad \varphi(y) = \sum_{e \in E} c_e y_e \quad (11)$$

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- ▶ It searches for decompositions with lower cost by joining pairs of **neighboring (!)** components recursively.
- ▶ As components can only grow and the number of components decreases by one in every step, one typically starts from the finest decomposition Π_0 of A into one-elementary components.

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- ▶ For any decomposition Π of a graph $G = (A, E)$, we define

$$\mathcal{E}_\Pi = \{\{B, C\} \in \binom{\Pi}{2} \mid \exists b \in B \exists c \in C: \{b, c\} \in E\} . \quad (12)$$

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- ▶ For any decomposition Π of $G = (A, E)$ and any $\{B, C\} \in \mathcal{E}_\Pi$, let $\text{join}_{BC}[\Pi]$ be the decomposition of G obtained by joining the sets B and C in Π , i.e.

$$\text{join}_{BC}[\Pi] = (\Pi \setminus \{B, C\}) \cup \{B \cup C\} . \quad (13)$$

Clustering

$\Pi' = \text{greedy-joining}(\Pi)$

choose $\{B, C\} \in \underset{\{B', C'\} \in \mathcal{E}_\Pi}{\text{argmin}} \varphi(y^{\text{join}_{B'C'}[\Pi]}) - \varphi(y^\Pi)$

if $\varphi(y^{\text{join}_{BC}[\Pi]}) - \varphi(y^\Pi) < 0$

$\Pi' := \text{greedy-joining}(\text{join}_{BC}[\Pi])$

else

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- ▶ It searches for decompositions with lower cost by recursively moving individual nodes from one component to a **neighboring!** component, possibly a new one.
- ▶ When a **cut node** is moved out of a component or a node is moved to a new component, the number of components increases. When the last element is moved out of a component, the number of components decreases.

Clustering

Definition. For any graph $G = (A, E)$ and any decomposition Π of G , the decomposition Π is called **coarsest** iff, for every $U \in \Pi$, the component $(U, E \cap \binom{U}{2})$ induced by U is maximal.

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Lemma. For any graph G , the coarsest decomposition is unique. We denote it by Π_G^* .

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Lemma. For any graph G , the coarsest decomposition is unique. We denote it by Π_G^* .

Definition. For any graph $G = (A, E)$, any decomposition Π of A and any $a \in A$, choose U_a to be the unique $U_a \in \Pi$ such that $a \in U_a$, and let

$$\mathcal{N}_a = \{\emptyset\} \cup \{W \in \Pi \mid a \notin W \wedge \exists w \in W : \{a, w\} \in E\} \quad (14)$$

$$G_a = \left(U_a \setminus \{a\}, E \cap \binom{U_a \setminus \{a\}}{2} \right) \quad (15)$$

For any $U \in \mathcal{N}_a$, let $\text{move}_{aU}[\Pi]$ the decomposition of A obtained by moving the node a to the set U , i.e.

$$\text{move}_{aU}[\Pi] = \Pi \setminus \{U_a, U\} \cup \{U \cup \{a\}\} \cup \Pi_{G_a}^* . \quad (16)$$

Clustering

$\Pi' = \text{greedy-moving}(\Pi)$

choose $(a, U) \in \underset{a' \in A, U' \in \mathcal{N}_{a'}}{\text{argmin}} \varphi(y^{\text{move}_{a'U'}[\Pi]}) - \varphi(y^\Pi)$

if $\varphi(y^{\text{move}_{aU}[\Pi]}) - \varphi(y^\Pi) < 0$

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A generalization of this algorithm by means of the technique of Kernighan and Lin (1970) is analogous to the greedy moving algorithm for the set partition problem.

Clustering

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- ▶ The supervised learning problem can assume the form of l_2 -regularized logistic regression where samples are pairs of neighboring nodes and decisions indicate whether these nodes are in the same or distinct components
- ▶ The inference problem assumes the form of the NP-hard minimum cost multicut problem
- ▶ Local search algorithms for tackling this problem are greedy joining, greedy moving, and greedy moving using the technique of Kernighan and Lin.