

# Machine Learning I

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# Ordering

## Contents.

- ▶ This part of the course is about the problem of learning to order a finite set.
- ▶ This problem is introduced as an **unsupervised learning** problem w.r.t. **constrained data**.

## Ordering

**Definition.** A strict order on  $A$  is a binary relation  $< \subseteq A \times A$  with the following properties:

$$\forall a \in A: \quad \neg a < a \quad (1)$$

$$\forall \{a, b\} \in \binom{A}{2}: \quad a < b \text{ xor } b < a \quad (2)$$

$$\forall \{a, b, c\} \in \binom{A}{3}: \quad a < b \wedge b < c \Rightarrow a < c \quad (3)$$

**Lemma.** The strict orders on  $A$  are characterized by the bijections  $\alpha : \{0, \dots, |A| - 1\} \rightarrow A$ .

*Proof.* For any such bijection, consider the order  $<_{\alpha}$  such that

$$\forall a, b \in A: \quad a < b \Leftrightarrow \alpha^{-1}(a) < \alpha^{-1}(b) . \quad (4)$$

**Lemma.** The strict orders on  $A$  are characterized by those  $y : \{(a, b) \in A \times A \mid a \neq b\} \rightarrow \{0, 1\}$  that satisfy the following conditions:

$$\forall a \in A \forall b \in A \setminus \{a\}: \quad y_{ab} + y_{ba} = 1 \quad (5)$$

$$\forall a \in A \forall b \in A \setminus \{a\} \forall c \in A \setminus \{a, b\}: \quad y_{ab} + y_{bc} - 1 \leq y_{ac} \quad (6)$$

## Ordering

We reduce the problem of learning and inferring orders to the problem of learning and inferring decisions, by defining **constrained data**  $(S, X, x, Y)$  with

$$S = \{(a, b) \in A \times A \mid a \neq b\} \quad (7)$$

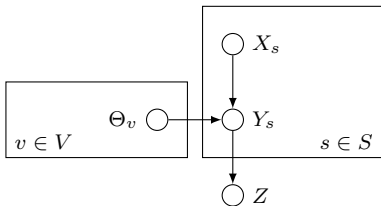
$$\mathcal{Y} = \left\{ y \in \{0, 1\}^S \mid \begin{array}{l} \forall a \in A \forall b \in A \setminus \{a\}: \quad y_{ab} + y_{ba} = 1 \\ \forall a \in A \forall b \in A \setminus \{a\} \forall c \in A \setminus \{a, b\}: \\ \quad y_{ab} + y_{bc} - 1 \leq y_{ac} \end{array} \right\} \quad (8)$$

We consider a finite, non-empty set  $V$ , called a set of **features**, and the **feature 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

$$\forall \theta \in \Theta \forall \hat{x} \in \mathbb{R}^V: \quad f_{\theta}(\hat{x}) = \sum_{v \in V} \theta_v \hat{x}_v = \langle \theta, \hat{x} \rangle . \quad (9)$$

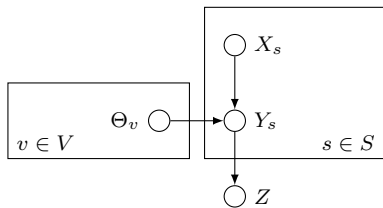
## Ordering



Probabilistic model:

- ▶ 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 **feature vector** of  $s$ .
- ▶ For any  $(a, b) = s \in S$ , let  $Y_s$  be a random variable whose value is a binary number  $y_s \in \{0, 1\}$ , called the **decision** placing  $a$  before  $b$ .
- ▶ For any  $v \in V$ , let  $\Theta_v$  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 ordering, we are interested in  $\mathcal{Z} = \mathcal{Y}$ , the set of characteristic functions of strict orders on  $A$ .

## Ordering



Probabilistic model: We assume the factorization

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

## Ordering

► Supervised learning:

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

## Ordering

► Inference:

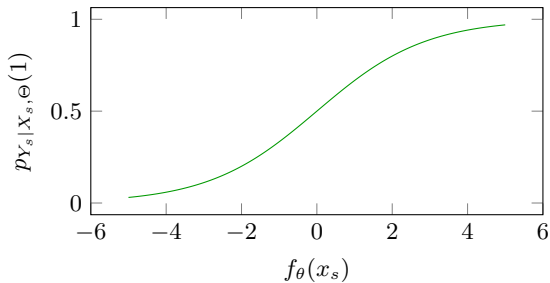
$$\begin{aligned} P(Y | X, Z, \theta) &= \frac{P(X, Y, Z, \Theta)}{P(X, Z, \Theta)} \\ &= \frac{P(Z | Y) P(Y | X, \Theta) P(X) P(\Theta)}{P(X, Z, \Theta)} \\ &\propto P(Z | Y) P(Y | X, \Theta) \\ &= P(Z | Y) \prod_{s \in S} P(Y_s | X_s, \Theta) \end{aligned}$$



## Ordering

### ► Sigmoid distribution

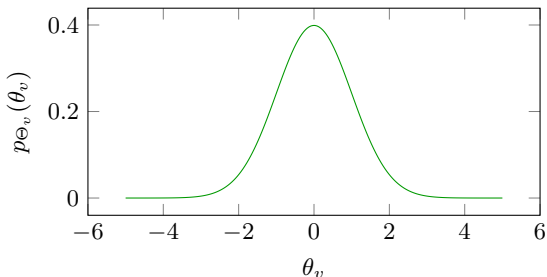
$$\forall s \in S: \quad p_{Y_s|X_s, \Theta}(1) = \frac{1}{1 + 2^{-f_{\theta}(x_s)}} \quad (10)$$



## Ordering

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

$$\forall v \in V : \quad p_{\Theta_v}(\theta_v) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\theta_v^2/2\sigma^2} \quad (11)$$



► **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  $p_{\mathcal{Z}|Y}(\mathcal{Z}, y)$  is non-zero iff the labeling  $y: S \rightarrow \{0, 1\}$  defines an order on  $A$ .

## Ordering

**Lemma.** Estimating maximally probable parameters  $\theta$ , given features  $x$  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.

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

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

## Ordering

**Lemma.** Estimating maximally probable decisions  $y$ , given features  $x$ , given the set of feasible decisions  $\mathcal{Y}$ , and given parameters  $\theta$ , i.e.,

$$\operatorname{argmax}_{y \in \{0,1\}^S} p_{Y|X,Z,\Theta}(y, x, \mathcal{Y}, \theta) \quad (12)$$

assumes the form of the **linear ordering problem**:

$$\operatorname{argmin}_{y: S \rightarrow \{0,1\}} \sum_{s \in S} (-\langle \theta, x_s \rangle) y_s \quad (13)$$

$$\text{subject to } \forall a \in A \forall b \in A \setminus \{a\}: y_{ab} + y_{ba} = 1 \quad (14)$$

$$\forall a \in A \forall b \in A \setminus \{a\} \forall c \in A \setminus \{a, b\}: \\ y_{ab} + y_{bc} - 1 \leq y_{ac} \quad (15)$$

**Theorem.** The linear ordering problem is NP-hard.

The linear ordering problem has been studied intensively. A comprehensive survey is by Martí and Reinelt (2011). Pioneering research is by Grötschel (1984).

We define two **local search algorithms** for the linear ordering problem.

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

$$\forall s \in S: \quad c_s = -\langle \theta, x_s \rangle \quad (16)$$

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

$$\forall y \in \{0, 1\}^S: \quad \varphi(y) = \sum_{s \in S} c_s y_s \quad (17)$$

### Greedy transposition algorithm:

- ▶ The greedy transposition algorithm starts from any initial strict order.
- ▶ It searches for strict orders with lower objective value by swapping pairs of elements

**Definition.** For any bijection  $\alpha : \{0, \dots, |A| - 1\} \rightarrow A$  and any  $j, k \in \{0, \dots, |A| - 1\}$ , let  $\text{transpose}_{jk}[\alpha]$  the bijection obtained from  $\alpha$  by swapping  $\alpha_j$  and  $\alpha_k$ , i.e.

$$\forall l \in \{0, \dots, |A| - 1\}: \quad \text{transpose}_{jk}[\alpha](l) = \begin{cases} \alpha_k & \text{if } l = j \\ \alpha_j & \text{if } l = k \\ \alpha_l & \text{otherwise} \end{cases} . \quad (18)$$

## Ordering

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$\alpha' = \text{greedy-transposition}(\alpha)$

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choose  $(j, k) \in \underset{0 \leq j' < k' < |A|}{\text{argmin}} \varphi(y^{\text{transpose}_{j'k'}[\alpha]}) - \varphi(y^\alpha)$

if  $\varphi(y^{\text{transpose}_{jk}[\alpha]}) - \varphi(y^\alpha) < 0$

$\alpha' := \text{greedy-transposition}(\text{transpose}_{jk}[\alpha])$

else

$\alpha' := \alpha$

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## Greedy transposition using the technique of Kernighan and Lin (1970)

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 $\alpha' = \text{greedy-transposition-kl}(\alpha)$ 


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 $\alpha^0 := \alpha$  $\delta_0 := 0$  $J_0 := \{0, \dots, |A| - 1\}$  $t := 0$ 

repeat

(build sequence of swaps)

choose  $(j, k) \in \operatorname{argmin}_{\{(j', k') \in J_t^2 \mid j' < k'\}} \varphi(y^{\text{transpose}_{j' k'}[\alpha^t]}) - \varphi(y^{\alpha^t})$

 $\alpha^{t+1} := \text{transpose}_{jk}[\alpha^t]$  $\delta_{t+1} := \varphi(y^{\alpha^{t+1}}) - \varphi(y^{\alpha^t}) < 0$  $J_{t+1} := J_t \setminus \{j, k\}$  $t := t + 1$ (move  $\alpha_j$  and  $\alpha_k$  only once)until  $|J_t| < 2$ 
 $\hat{t} := \min_{t' \in \{0, \dots, |A|\}} \operatorname{argmin}_{\tau=0}^{t'} \delta_\tau$ 

(choose sub-sequence)

if  $\sum_{\tau=0}^{\hat{t}} \delta_\tau < 0$  $\alpha' := \text{greedy-transposition-kl}(\alpha^{\hat{t}})$ 

(recurse)

else

 $\alpha' := \alpha$ 

(terminate)

### Summary.

- ▶ Learning and inferring orders on a finite set  $A$  is an unsupervised learning problem w.r.t. constrained data whose feasible labelings characterize the strict orders on  $A$ .
- ▶ The supervised learning problem can assume the form of  $l_2$ -regularized logistic regression where samples are pairs  $(a, b) \in A^2$  such that  $a \neq b$  and decisions indicate whether  $a < b$ .
- ▶ The inference problem assumes the form of the NP-hard linear ordering problem
- ▶ Local search algorithms for tackling this problem are greedy transposition and greedy transposition using the technique of Kernighan and Lin.