

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

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

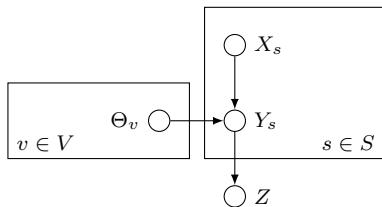
$$\mathcal{Y} = \left\{ y \in \{0, 1\}^S \mid \begin{aligned} &\forall a \in A \forall b \in A \setminus \{a\}: \quad y_{ab} + y_{ba} = 1 \\ &\forall a \in A \forall b \in A \setminus \{a\} \forall c \in A \setminus \{a, b\}: \\ &\quad y_{ab} + y_{bc} - 1 \leq y_{ac} \end{aligned} \right\} \quad (8)$$

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

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

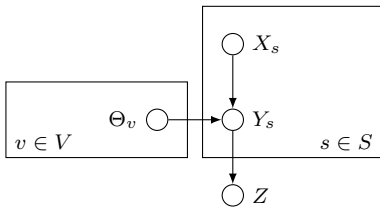
Ordering



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 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 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

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

► 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

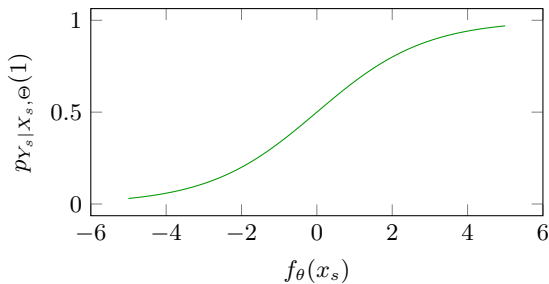
► Inference:

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

Ordering

► Sigmoid distribution

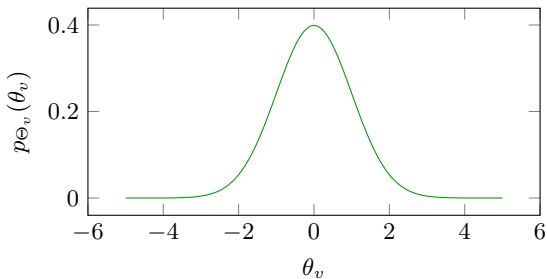
$$\forall s \in S: \quad p_{Y_s|X_s, \Theta}(1) = \frac{1}{1 + 2^{-f_{\theta}(x_s)}} \quad (10)$$



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

Lemma. Estimating maximally probable parameters θ , 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 θ , 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**:

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

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

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

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 α by swapping α_j and α_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

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

$$\text{choose } (j, k) \in \underset{0 \leq j' < k' < |A|}{\operatorname{argmin}} \varphi(y^{\text{transpose}_{j'k'}[\alpha]}) - \varphi(y^\alpha)$$
$$\text{if } \varphi(y^{\text{transpose}_{jk}[\alpha]}) - \varphi(y^\alpha) < 0$$
$$\alpha' := \text{greedy-transposition}(\text{transpose}_{jk}[\alpha])$$
$$\text{else}$$
$$\alpha' := \alpha$$

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

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

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

repeat

(build sequence of swaps)

$$\text{choose } (j, k) \in \underset{\{(j', k') \in J_t^2 \mid j' < k'\}}{\text{argmin}} \varphi(y^{\text{transpose}_{j'k'}[\alpha^t]}) - \varphi(y^{\alpha^t})$$
 $\alpha^{t+1} := \text{transpose}_{jk}[\alpha^t]$
 $\delta_{t+1} := \varphi(y^{\alpha^{t+1}}) - \varphi(y^{\alpha^t}) < 0$
 $J_{t+1} := J_t \setminus \{j, k\}$

 (move α_j and α_k only once)

 $t := t + 1$

 until $|J_t| < 2$

$$\hat{t} := \min_{t' \in \{0, \dots, |A|\}} \underset{\tau=0}{\text{argmin}} \sum_{\tau=0}^{t'} \delta_\tau$$

(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.