Machine Learning I

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Contents.

- ▶ This part of the course introduces the problem of classifying data w.r.t. any given finite number of classes.
- ► This problem is introduced as an unsupervised learning problem w.r.t. constrained data whose feasible labelings are characteristic functions of maps.

We consider

- ightharpoonup A finite, non-empty set A whose elements we seek to classify
- ightharpoonup A finite, non-empty set B of class labels

Learning to classify the elements of A into classes labeled by the elements of B consists in learning a $\operatorname{map} \varphi: A \to B$ that assigns to every element $a \in A$ precisely one class label $\varphi(a) \in B$.

Maps $\varphi \colon A \to B$ are precisely those subsets of $\varphi \subseteq A \times B$ that satisfy

$$\forall a \in A \ \exists b \in B : \quad (a, b) \in \varphi \tag{1}$$

$$\forall a \in A \ \forall b, b' \in B : \ (a, b) \in \varphi \ \land \ (a, b') \in \varphi \ \Rightarrow \ b = b' \ .$$
 (2)

They are characterized by those functions $y: A \times B \rightarrow \{0,1\}$ that satisfy

$$\forall a \in A: \quad \sum_{b \in R} y_{ab} = 1 . \tag{3}$$

We reduce the problem of learning and inferring maps to the problem of learning and inferring decisions, by defining **constrained data** (S,X,x,\mathcal{Y}) with

$$S = A \times B \tag{4}$$

$$\mathcal{Y} = \left\{ y \in \{0, 1\}^S \ \middle| \ \forall a \in A \colon \sum_{b \in B} y_{ab} = 1 \right\} . \tag{5}$$

More specifically, we consider

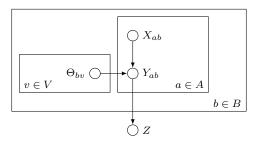
- \blacktriangleright a finite, non-empty set V, called a set of attributes
- ▶ the attribute space $X = B \times \mathbb{R}^V$ such that, for any $(a,b) \in A \times B$, the class label b is the first attribute of (a,b), i.e.:

$$\forall a \in A \ \forall b \in B \ \exists \hat{x} \in \mathbb{R}^V : \quad x_{ab} = (b, \hat{x})$$
 (6)

Familiy of functions

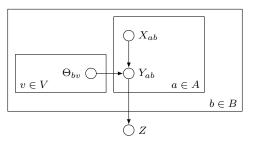
We consider **linear functions** with a separate set of coefficients for every class label. Specifically, we consider $\Theta = \mathbb{R}^{B \times V}$ and $f: \Theta \to \mathbb{R}^X$ such that

$$\forall \theta \in \Theta \ \forall b \in B \ \forall \hat{x} \in \mathbb{R}^V : \quad f_{\theta}((b, \hat{x})) = \sum_{v \in V} \theta_{bv} \ \hat{x}_v = \langle \theta_{b\cdot}, \hat{x} \rangle \ .$$
 (7)



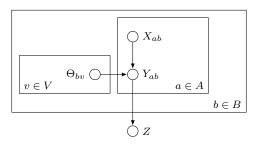
Random Variables

- ▶ For any $(a,b) \in A \times B$, let X_{ab} be a random variable whose value is a vector $x_{ab} \in B \times \mathbb{R}^V$, the **attribute vector** of (a,b).
- ▶ For any $(a,b) \in A \times B$, let Y_{ab} be a random variable whose value is a binary number $y_{ab} \in \{0,1\}$, called the **decision** of classifying a as b
- ▶ For any $b \in B$ and any $v \in V$, let Θ_{bv} be a random variable whose value is a real number $\theta_{bv} \in \mathbb{R}$, a **parameter** of the function we seek to learn



Random Variables

▶ Let Z be a random variable whose value is a subset $\mathcal{Z} \subseteq \{0,1\}^{A \times B}$ called the set of **feasible decisions**. For multiple label classification, we are interested in $\mathcal{Z} = \mathcal{Y}$, the set of the characteristic functions of all maps from A to B.



Factorization

$$P(X, Y, Z, \Theta) = P(Z \mid Y) \prod_{(a,b) \in A \times B} P(Y_{ab} \mid X_{ab}, \Theta) \prod_{(b,v) \in B \times V} P(\Theta_{bv}) \prod_{(a,b) \in A \times B} P(X_{ab})$$

Factorization

Supervised learning:

$$\begin{split} P(\Theta \mid X, Y, Z) &= \frac{P(X, Y, Z, \Theta)}{P(X, Y, Z)} \\ &= \frac{P(Z \mid Y) P(Y \mid X, \Theta) P(X) P(\Theta)}{P(Z \mid X, Y) P(X, Y)} \\ &= \frac{P(Z \mid Y) P(Y \mid X, \Theta) P(X) P(\Theta)}{P(Z \mid Y) P(X, Y)} \\ &= \frac{P(Y \mid X, \Theta) P(X) P(\Theta)}{P(X, Y)} \\ &\propto P(Y \mid X, \Theta) P(\Theta) \\ &= \prod_{(a, b) \in A \times B} P(Y_{ab} \mid X_{ab}, \Theta) \prod_{(b, v) \in B \times V} P(\Theta_{bv}) \end{split}$$

Factorization

► Inference:

$$P(Y \mid X, Z, \theta) = \frac{P(X, Y, Z, \Theta)}{P(X, Z, \Theta)}$$

$$= \frac{P(Z \mid Y) P(Y \mid X, \Theta) P(X) P(\Theta)}{P(X, Z, \Theta)}$$

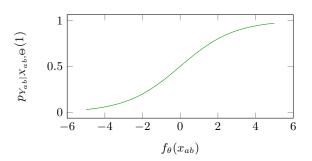
$$\propto P(Z \mid Y) P(Y \mid X, \Theta)$$

$$= P(Z \mid Y) \prod_{(a,b) \in A \times B} P(Y_{ab} \mid X_{ab}, \Theta)$$

Distributions

► Logistic distribution

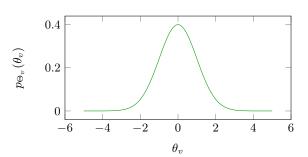
$$\forall a \in A \ \forall b \in B: \qquad p_{Y_{ab}|X_{ab},\Theta}(1) = \frac{1}{1 + 2^{-f_{\theta}(x_{ab})}}$$
 (8)



Distributions

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

$$\forall b \in B \ \forall v \in V: \qquad p_{\Theta_{bv}}(\theta_{bv}) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\theta_{bv}^2/2\sigma^2} \tag{9}$$



Distributions

► Uniform distribution on a subset

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

Note that $p_{Z|Y}(\mathcal{Y},y)$ is non-zero iff the relation $y^{-1}(1) \subseteq A \times B$ is a map.

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

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

separates into |B| independent $l_2\text{-regularized}$ logistic regression problems, each w.r.t. parameters in $\mathbb{R}^V.$

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

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

$$= \underset{\theta \in \mathbb{R}^{B \times V}}{\operatorname{argmin}} \quad \sum_{(a,b) \in A \times B} \left(-y_{ab} f_{\theta}(x_{ab}) + \log\left(1 + 2^{f_{\theta}(x_{ab})}\right) \right) + \frac{\log e}{2\sigma^{2}} \|\theta\|_{2}^{2} .$$

Consider the unique $x':A\times B\to\mathbb{R}^V$ such that, for any $(a,b)\in A\times B$, we have $x_{ab}=(b,x'_{ab})$. Now:

$$\begin{split} & \min_{\theta \in \mathbb{R}^{B \times V}} \sum_{(a,b) \in A \times B} \left(-y_{ab} \langle \theta_b, x'_{ab} \rangle + \log \left(1 + 2^{\langle \theta_b, x'_{ab} \rangle} \right) \right) + \frac{\log e}{2\sigma^2} \|\theta\|_2^2 \\ &= \min_{\theta \in \mathbb{R}^{B \times V}} \sum_{b \in B} \left(\sum_{a \in A} \left(-y_{ab} \langle \theta_b, x'_{ab} \rangle + \log \left(1 + 2^{\langle \theta_b, x'_{ab} \rangle} \right) \right) + \frac{\log e}{2\sigma^2} \|\theta_b\|_2^2 \right) \\ &= \sum_{b \in B} \min_{\theta_b, \in \mathbb{R}^V} \left(\sum_{a \in A} \left(-y_{ab} \langle \theta_b, x'_{ab} \rangle + \log \left(1 + 2^{\langle \theta_b, x'_{ab} \rangle} \right) \right) + \frac{\log e}{2\sigma^2} \|\theta_b\|_2^2 \right) \end{split}.$$

Lemma. For any constrained data as defined above, any $\theta \in \mathbb{R}^{B \times V}$ and any $\hat{y}: A \times B \to \{0,1\}$, \hat{y} is a solution to the inference problem

$$\min_{y \in \mathcal{Y}} \sum_{(a,b) \in A \times B} L(f_{\theta}(x_{ab}), y_{ab}) \tag{10}$$

iff there exists an $\varphi:A\to B$ such that

$$\forall a \in A \colon \quad \varphi(a) \in \max_{b \in B} \langle \theta_b, x'_{ab} \rangle \tag{11}$$

and

$$\forall (a,b) \in A \times B : \quad \hat{y}_{ab} = 1 \iff \varphi(a) = b . \tag{12}$$

Proof.

$$\begin{split} &\sum_{(a,b)\in A\times B} L(f_{\theta}(x_{ab}),y_{ab}) \\ &= \sum_{(a,b)\in A\times B} \left(L(f_{\theta}(x_{ab}),1)\,y_{ab} + L(f_{\theta}(x_{ab}),0)\,(1-y_{ab})\right) \\ &= \sum_{(a,b)\in A\times B} \left(L(f_{\theta}(x_{ab}),1) - L(f_{\theta}(x_{ab}),0)\right)y_{ab} + \text{const.} \\ &= \sum_{(a,b)\in A\times B} \left(-f_{\theta}(x_{ab})\right)y_{ab} \\ &= \sum_{(a,b)\in A\times B} \left(-\langle \theta_b, x'_{ab}\rangle\right)y_{ab} \\ &= \sum_{a\in A} \sum_{b\in B} \left(-\langle \theta_b, x'_{ab}\rangle\right)y_{ab} \end{split}$$

Summary.

- Classification can be cast as an unsupervised learning problem w.r.t. constrained data defined such that the feasible labelings are characteristic functions of maps.
- ▶ In the special case of supervised learning and the logistic loss function, this problem separates into as many independent independent logistic regression problems as there are classes. This is commonly called one-versus-rest learning.