Machine Learning I

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Contents. This part of the course is about a special case of supervised learning: the supervised learning of binary decision trees.

- We state the problem by defining labeled data, a family of functions, a regularizer and a loss function
- We prove that the problem is hard to solve (technically: NP-hard), by relating it to the exact cover by 3-sets problem.

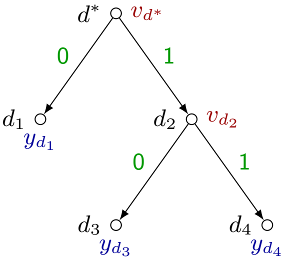
Data

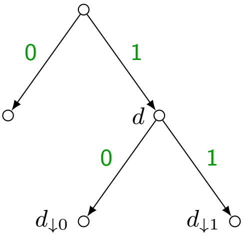
We consider binary attributes. More specifically, we consider some finite, non-empty set V, called the set of attributes, and labeled data $T = (S, X, x, y)$ such that $X = \{0,1\}^V$.

Hence, $x\colon S \to \{0,1\}^V$ and $y\colon S \to \{0,1\}$.

Definition. A tuple $(V, Y, D, D', d^*, E, \delta, v, y)$ is called a V-variate Y-valued **binary decision tree** (BDT) iff the following conditions hold:

1. $V \neq \emptyset$ is finite (set of **variables**)
2. $Y \neq \emptyset$ is finite (set of **values**)
3. $(D \cup D', E)$ is a finite, non-empty directed binary tree with root d^*
4. every $d \in D'$ is a leaf
5. $\delta\colon E \to \{0, 1\}$
6. every $d \in D$ has precisely two out-edges, $e = (d, d'), e' = (d, d'')$, such that $\delta(e) = 0$ and $\delta(e') = 1$
7. $v\colon D \to V$
8. $y\colon D' \to Y$





Definition. For any BDT $(V, Y, D, D', d^*, E, \delta, v, y)$, any $d \in D$ and any $j \in \{0, 1\}$, we let $d_{\downarrow j} \in D \cup D'$ the unique node such that $e = (d, d_{\downarrow j}) \in E$ and $\delta(e) = j$.

Definition. For any BDT $\theta = (V, Y, D, D', d^*, E, \delta, v, y)$ and any $d \in D \cup D'$, the tuple $\theta[d] = (V, Y, D_2, D_2', d, E', \delta', v', y')$ is called the **binary decision subtree** of θ rooted at d iff

- $(D_2 \cup D_2', E')$ is the subtree of $(D \cup D', E)$ rooted at d
- δ', v' and y' are the restrictions of δ, v and y to the subsets D_2, D_2' and E'

Lemma. For any BDT $\theta = (V, Y, D, D', d^*, E, \delta, v, y)$ and any $d \in D \cup D'$, the binary decision subtree $\theta[d]$ is itself a V-variate Y-valued BDT.

Definition. For any BDT $\theta = (V, Y, D, D', d^*, E, \delta, v, y)$, the function defined by θ is the $f_\theta : \{0,1\}^V \to Y$ such that $\forall x \in \{0,1\}^V$:

$$f_\theta(x) = \begin{cases} y(d^*) & \text{if } D = \emptyset \\ f_{\theta[d^*_{\downarrow 0}]}(x) & \text{if } D \neq \emptyset \wedge x_{v(d^*)} = 0 \\ f_{\theta[d^*_{\downarrow 1}]}(x) & \text{if } D \neq \emptyset \wedge x_{v(d^*)} = 1 \end{cases}$$

$$= \begin{cases} y(d^*) & \text{if } D = \emptyset \\ (1 - x_{v(d^*)}) f_{\theta[d^*_{\downarrow 0}]}(x) + x_{v(d^*)} f_{\theta[d^*_{\downarrow 1}]}(x) & \text{otherwise} \end{cases}$$

Note. The set Θ of V-variate $Y = \{0,1\}$-valued BDTs can be identified with a subset of V-variate DNFs.

Regularization

In order to quantify the complexity of BDTs, we consider the following regularizer.

Definition. For any BDT $\theta = (V, Y, D, D', d^*, E, \delta, v, y)$, the **depth** of θ is the $R(\theta) \in \mathbb{N}$ such that

$$R(\theta) = \begin{cases} 0 & \text{if } D = \emptyset \\ 1 + \max\{R(\theta[d^*_{\downarrow 0}]), R(\theta[d^*_{\downarrow 1}])\} & \text{otherwise} \end{cases} . \qquad (1)$$

Loss function

We consider the **0/1-loss** L, i.e.

$$\forall r \in \mathbb{R}\ \forall \hat{y} \in \{0,1\}\colon \quad L(r,\hat{y}) = \begin{cases} 0 & r = \hat{y} \\ 1 & \text{otherwise} \end{cases} . \tag{2}$$

Definition. For any $\lambda \in \mathbb{R}_0^+$, the instance of the **supervised learning problem of BDTs** with respect to T, L, R and λ has the form

$$\min_{\theta \in \Theta} \quad \lambda R(\theta) + \frac{1}{|S|} \sum_{s \in S} L(f_\theta(x_s), y_s) \tag{3}$$

Definition. For any $m \in \mathbb{N}$, the **bounded depth BDT problem** w.r.t. T and m is to decide whether there exists a BDT $\theta = (V, Y, D, D', d^*, E, \delta, v, y')$ such that

$$R(\theta) \leq m \tag{4}$$

$$\forall s \in S\colon \quad f_\theta(x_s) = y_s \quad . \tag{5}$$

Next, we will reduce the hard-to-solve (technically: NP-hard) exact cover by 3-sets problem to the bounded depth BDT problem, thereby showing that the latter problem is hard to solve (NP-hard) as well. The reduction is by Haussler (1988).

Definition. For any set S, a cover Σ of S is called **exact** iff the elements of Σ are pairwise disjoint.

Definition. Let S be any set, and let $\emptyset \notin \Sigma \subseteq 2^S$.

Deciding whether there exists a $\Sigma' \subseteq \Sigma$ such that Σ' is an exact cover of S is called the instance of the **exact cover problem** w.r.t. S and Σ.

Additionally, if $|S|$ is an integer multiple of three and any $U \in \Sigma$ is such that $|U| = 3$, the instance of the exact cover problem w.r.t. S and Σ is also called the instance of the **exact cover by 3-sets problem** with respect to S and Σ.

Proof. For any instance (S', Σ) of the exact cover by 3-sets problem and the $n \in \mathbb{N}$ such that $|S'| = 3n$, we construct the instance of the m-bounded depth BDT problem such that

- $V = \Sigma$
- $S = S' \mathbin{\dot\cup} \{0\}$
- $x : S \to \{0,1\}^\Sigma$ such that $x_0 = 0$ and

$$\forall s \in S' \; \forall \sigma \in \Sigma\colon \quad x_s(\sigma) = \begin{cases} 1 & \text{if } s \in \sigma \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

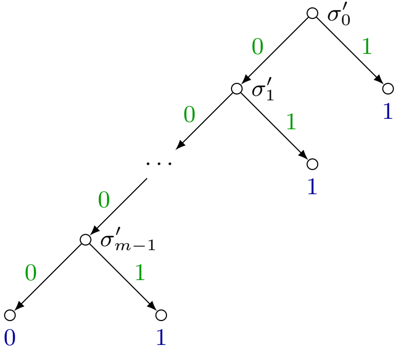
- $y : S \to \{0,1\}$ such that $y_0 = 0$ and $\forall s \in S'\colon y_s = 1$.
- $m = n$

We show that the instance the exact cover problem has a solution iff the instance of the bounded depth BDT problem has a solution.

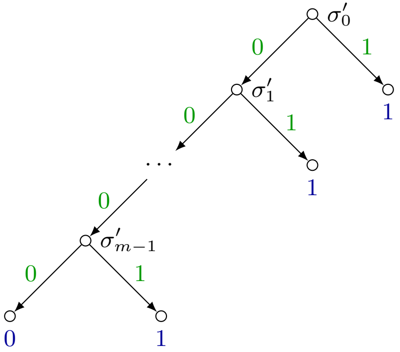
($\Rightarrow$) Let $\Sigma' \subseteq \Sigma$ a solution to the instance of the exact cover problem.

Consider any order on Σ' and the bijection $\sigma' : [n] \to \Sigma'$ induced by this order.

We show that the BDT θ depicted below solves the instance of the bounded depth BDT problem.



Deciding with Binary Decision Trees



The BDT satisfies $R(\theta) = m$.

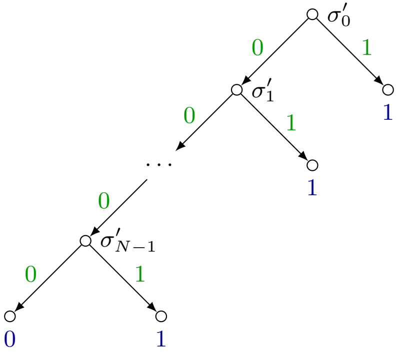
The BDT decides the labeled data correctly because

- $f_\theta(x_0) = 0 = y_0$
- At each of the m interior nodes, three additional elements of S' are mapped to 1. Thus, all $3m$ many elements $s \in S'$ are mapped to 1. That is $\forall s \in S' \colon f_\theta(x_s) = 1 = y_s$.

($\Leftarrow$) Let $\theta = (V, Y, D, D', d^*, E, \delta, \sigma, y')$ a BDT that solves the instance of the bounded depth BDT problem.

W.l.o.g., we assume, for any interior node $d \in D$, that $d_{\downarrow 1}$ is a leaf and $y'(d_{\downarrow 1}) = 1$.

Hence, θ is of the form depicted below.



Therefore:

$$\forall x \in X\colon \quad f_\theta(x) = \begin{cases} 1 & \text{if } \exists j \in [N]\colon x(\sigma_j) = 1 \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

Thus,

$$\forall s \in S\colon \quad f_\theta(x_s) = \begin{cases} 1 & \text{if } \exists j \in [N]\colon s \in \sigma_j \\ 0 & \text{otherwise} \end{cases} , \tag{8}$$

by definition of x in (6).

Consequently,

$$\bigcup_{j=0}^{N-1} \sigma_j = S' , \tag{9}$$

by definition of y such that $\forall s \in S'\colon y_s = 1$.

Moreover, $N = m$, because

$$3m = |S'| \overset{(9)}{=} \left| \bigcup_{j=0}^{N-1} \sigma_j \right| \leq \sum_{j=0}^{N-1} |\sigma_j| = \sum_{j=0}^{N-1} 3 = 3N \overset{(4)}{\leq} 3m \ .$$

Therefore:

$$\forall \{j, l\} \in \tbinom{[N]}{2} : \quad \sigma_k \cap \sigma_l = \emptyset \tag{10}$$

Thus,

$$\bigcup_{j=0}^{N-1} \sigma_j$$

is a solution to the instance of the exact cover by 3-sets problem defined by (S', Σ), by (9) and (10).

□

Summary:

- BDTs can be identified with a subset of DNFs.
- Supervised learning of BDTs is hard. More specifically, the NP-hard exact cover by 3-sets problem is reducible to the bounded depth BDT problem by construction of Haussler data.

Further reading: Readers who are not familiar with the exact cover by 3-sets problem or the set cover problem will find proofs of their NP-hardness in Appendicies A.1–A.4 of the lecture notes.