Classification, Decision Trees, and a Generalization Theorem

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In **classification**, we are given a training set containing objects of two **classes** and want to learn a **classifier** to predict the class of an object outside the training set. This course will cover several techniques to perform classification effectively. We will start with one such technique: the **decision tree** method.

Classification

Let $A_1, ..., A_d$ be d **attributes**.

Define the **instance space** as $\mathcal{X} = dom(A_1) \times dom(A_2) \times ... \times dom(A_d)$ where $dom(A_i)$ represents the set of possible values on A_i.

Define the **label space** as $\mathcal{Y} = \{-1, 1\}$ (the elements in $\mathcal{Y}$ are called the **class labels**).

Each **instance-label pair** (a.k.a. **object**) is a pair $(\boldsymbol{x}, y)$ in $\mathcal{X} \times \mathcal{Y}$.

- Note that $\boldsymbol{x}$ is a vector; we use $\boldsymbol{x}[A_i]$ to represent the vector's value on A_i $(1 \leq i \leq d)$.

Denote by $\mathcal{D}$ a probabilistic distribution over $\mathcal{X} \times \mathcal{Y}$.

Classification

Goal: Given an object $(\boldsymbol{x}, y)$ drawn from $\mathcal{D}$, we want to predict its label y from its attribute values $\boldsymbol{x}[A_1], ..., \boldsymbol{x}[A_d]$.

We will find a function

$$h : \mathcal{X} \rightarrow \mathcal{Y}$$

which is referred to as a **classifier** (sometimes also called a **hypothesis**). Given an instance $\boldsymbol{x}$, we predict its label as $h(\boldsymbol{x})$.

The error of h on $\mathcal{D}$ — denoted as $err_{\mathcal{D}}(h)$ — is defined as:

$$err_{\mathcal{D}}(h) \quad = \quad \boldsymbol{Pr}_{(\boldsymbol{x},y)\sim\mathcal{D}}[h(\boldsymbol{x}) \neq y]$$

namely, if we draw an object $(\boldsymbol{x}, y)$ according to $\mathcal{D}$, what is the probability that h mis-predicts the label?

Classification

Ideally, we want to find an h to minimize $err_{\mathcal{D}}(h)$, but this in general is not possible without the precise information about $\mathcal{D}$.

Instead, we would like to learn a classifier h with small $err_{\mathcal{D}}(h)$ from a **training set** S where each object is drawn independently from $\mathcal{D}$.

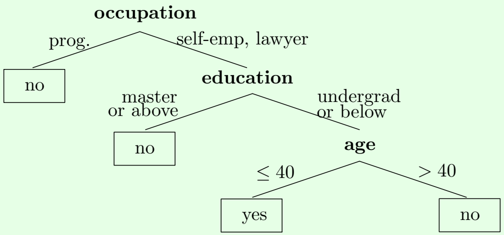
Example: Suppose that we have the following training set:

age	education	occupation	loan default
28	high school	self-employed	yes
32	master	programmer	no
33	undergrad	lawyer	yes
37	undergrad	programmer	no
40	undergrad	self-employed	yes
45	master	self-employed	no
48	high school	programmer	no
50	master	laywer	no
52	master	programmer	no
55	high school	self-employed	no

Now, given a new customer (50, high school, self-employed), how should we predict whether s/he would default?

The **decision tree method** represents a classifier h as a tree.

Example:



Given an instance (50, high school, self-employed), the above tree returns the class label "no" by descending a root-to-leaf path to the rightmost leaf.

Formally, a decision tree T is a binary tree where

- each leaf node carries a class label: yes or no (namely, 1 or -1);
- each internal node u has two child nodes, and carries a predicate P_u on an attribute A_u.

Given an instance $\boldsymbol{x}$, T predicts its label as follows:

1. $u \leftarrow$ the root of T.
2. If u is a leaf, return the class label associated with u.
3. If u is an internal node, check whether $\boldsymbol{x}[A_u]$ satisfies P_u:
    - if so, $u \leftarrow$ the left child of u;
    - otherwise, $u \leftarrow$ the right child of u.

Our objective is to produce a good decision tree from the training set S. Next, we will describe a simple algorithm called the **Hunt's algorithm** which achieves the purpose reasonably well in practice.

Given a node u in T, define $S(u)$ as follows:

- If u is the root of T, $S(u) = S$.
- Recursively, consider now u as an internal node whose $S(u)$ has been defined. Let v_1 and v_2 be the left and right child nodes of u, respectively.
    - $S(v_1)$ is the set of objects in $S(u)$ that satisfy $P(u)$;
    - $S(v_2) = S(u) \setminus S(v_1)$.

Think: What is $S(u)$ for each node u in the decision tree on Slide 7?

Hunt's Algorithm

The algorithm builds a decision tree T in a top-down and greedy manner. At each node u, it finds the "best" way to split $S(u)$ according to a certain quality metric.

algorithm Hunt(S)

```
/* $S$ is the training set; the function returns the root of a decision tree */
1.  if all the objects in $S$ belong to the same class
2.      return a leaf node with the value of this class
3.  if all the objects in $S$ have the same attribute values
4.      return a leaf node whose class label is the majority one in $S$
5.  find the "best" split attribute $A^*$ and predicate $P^*$ /* details next slide */
6.  $S_1 \leftarrow$ the set of objects in $S$ satisfying $P^*$; $S_2 \leftarrow S \setminus S_1$
7.  $u_1 \leftarrow$ Hunt($S_1$); $u_2 \leftarrow$ Hunt($S_2$)
8.  create a root $u$ with left child $u_1$ and right child $u_2$
9.  set $A_u \leftarrow A^*$ and $P_u \leftarrow P^*$
10. return $u$
```

Implementing Line 5 requires resolving the following issues:

1. What are the possible ways to perform a split?
2. How to evaluate the quality of a split?

We will provide a way to resolve these issues in the next few slides.

Candidate Split

A split concerns a single attribute A. We distinguish two types of A:

- **Ordinal**: there is an ordering on A.
- **Nominal**: no ordering makes sense on A.

Example: In the training set of Slide 6, age and education are ordinal attributes, whereas occupation is nominal.

Candidate Split

For an ordinal attribute A, a **candidate split** is a condition of the form $A \leq v$, where v is a value of A appearing in S.

For a nominal attribute A, a **candidate split** is a condition of the form $A \in S$, where S is a subset of the values of A appearing in S.

Example: In the training set of Slide 6, "age $\leq$ 40", "education $\leq$ undergrad", and "occupation $\in$ {self-employed, lawyer}" are all candidate split predicates.

Quality of a Split

Next, we tackle the second issue of Slide 11 by resorting to **GINI index**.

In general, let S be a set of objects whose class labels are known. Define:

$$\begin{aligned} n &= |S| \\ n_y &= \text{number of objects in } S \text{ with label yes} \\ p_y &= n_y / n \\ p_n &= 1 - p_y \end{aligned}$$

The GINI index of S is:

$$GINI(S) = 1 - (p_y^2 + p_n^2)$$

Quality of a Split

Example:

- If $p_y = 1$ and $p_n = 0$ (i.e., **maximum purity**), then $GINI(R) = 0$.
- If $p_y = 0.75$ and $p_n = 0.25$, then $GINI(R) = 0.375$.
- If $p_y = 0.5$ and $p_n = 0.5$ (i.e., **maximum impurity**), then $GINI(R) = 0.5$.

It is rudimentary to verify:

Lemma: $GINI(R)$ ranges from 0 to 0.5. It increases as $|p_y - p_n|$ decreases.

Quality of a Split

We are ready to resolve the second issue on Slide 11. Suppose that S has been split into S_1 and S_2. We define the **GINI index of the split** as

$$GINI_{split} = \frac{|S_1|}{|S|} GINI(S_1) + \frac{|S_2|}{|S|} GINI(S_2).$$

The **smaller** $GINI_{split}$ is, the **better** the split quality.

At this point, we have completed the description of Hunt's algorithm on Slide 10. An important issue has been left out: **overfitting**, i.e., although a tree may fit the training set well, its error on the distribution $\mathcal{D}$ is actually rather bad.

Next, we will discuss understand what causes overfitting and then fix the issue by modifying the algorithm slightly.

Let $\mathcal{P}$ be the set of people in the world. Given a random person, we want to predict whether s/he will commit a crime in her/his life.

Suppose that there are no attributes (i.e., $\mathcal{X} = \emptyset$). Given a training set $S \subseteq \mathcal{P}$, Hunt's algorithm returns a decision tree T that has only a single node (i.e., a leaf). Let c be the label at that leaf; note that T predicts the label of every person in $\mathcal{P}$ as c.

Which value of c is ideal for $\mathcal{P}$? This depends on how many people in $\mathcal{P}$ belong to the yes class. Specifically, let

$$\pi_y = \frac{\text{number of ``yes'' people in } \mathcal{P}}{|\mathcal{P}|}$$

$$\pi_n = \frac{\text{number of ``no'' people in } \mathcal{P}}{|\mathcal{P}|}$$

The optimal choice is to set c to yes if $\pi_y > \pi_n$, or to no otherwise.

Example: Suppose $\pi_y = 0.7$ and $\pi_n = 0.3$. If $c =$ yes, we err with probability 0.3; if $c =$ no, we err with probability 0.7.

However, π_y and π_n are unknown.

We rely on S to infer the relationship between π_y and π_n. If S has more yes objects, we "believe" $\pi_y > \pi_n$ and, hence, set c to yes; otherwise, we set c to no. This is precisely what Hunt's algorithm does.

To increase the confidence of our belief, we need S to be **sufficiently large**.

Without enough training data, you should not hope to build a reliable decision tree (lack of statistical significance).

As Hunt's algorithm builds a decision tree T, the $|S(u)|$ of the current node u continuously decreases as we go deeper. When $|S(u)|$ becomes too small, statistical significance is lost such that the subtree of u becomes unreliable: even though the subtree may fit the training set well, it does not accurately predict the label of an unknown object falling into the subtree. Therefore, **overfitting** occurs.

Hunt's Algorithm (Modified)

We now add a heuristic to the algorithm to alleviate overfitting.

```
algorithm Hunt($S$)
/* $S$ is the training set; the function returns the root of a decision tree */
1.  if all the objects in $S$ belong to the same class
2.      return a leaf node with the value of this class
3.  if (all the objects in $S$ have the same attribute values)
    or ($|S|$ is too small)
4.      return a leaf node whose class value is the majority one in $S$
5.  find the "best" split attribute $A^*$ and predicate $P^*$
6.  $S_1 \leftarrow$ the set of objects in $R$ satisfying $P^*$; $S_2 \leftarrow S \setminus S_1$
7.  $u_1 \leftarrow$ Hunt($R_1$); $u_2 \leftarrow$ Hunt($R_2$)
8.  create a root $u$ with left child $u_1$ and right child $u_2$
9.  set $A_u \leftarrow A^*$ and $P_u \leftarrow P^*$
10. return $u$
```

Next, we will provide a theoretical explanation about overfitting.

Given a classifier h, define its **error on S** — denote as $err_S(h)$ — to be:

$$err_S(h) = \frac{|\{(\boldsymbol{x}, y) \in S \mid h(\boldsymbol{x}) \neq y\}|}{|S|}.$$

namely, the percentage of objects in S whose labels are incorrectly predicted by h.

Remark:

- $err_S(h)$ is often called the **empirical error** of h.
- $err_{\mathcal{D}}(h)$ is often called the **generalization error** of h.

Generalization Theorem

Theorem: Let $\mathcal{H}$ be the set of classifiers that can possibly be returned. The following statement holds with probability at least $1 - \delta$ (where $0 < \delta \le 1$): for any $h \in \mathcal{H}$:

$$err_{\mathcal{D}}(h) \le err_S(h) + \sqrt{\frac{\ln(1/\delta) + \ln|H|}{2|S|}}.$$

Implications: we should

- look for a decision tree that is both accurate on the training set and small in size;
- increase the size of S as much as possible.

To prove the generalization theorem, we need:

Theorem (Hoeffding Bounds): Let $X_1, ..., X_n$ be independent Bernoulli random variables satisfying $\boldsymbol{Pr}[X_i = 1] = p$ for all $i \in [1, n]$. Set $s = \sum_{i=1}^{n} X_i$. Then, for any $0 \le \alpha \le 1$:

$$\begin{aligned} \boldsymbol{Pr}[s/n > p + \alpha] &\le e^{-2n\alpha^2} \\ \boldsymbol{Pr}[s/n < p - \alpha] &\le e^{-2n\alpha^2}. \end{aligned}$$

The proof of the theorem is not required in this course.

We will also need:

Lemma (Union Bound): Let $E_1, ..., E_n$ be n arbitrary events such that event E_i happens with probability p_i. Then,

$$\boldsymbol{Pr}[\text{at least one of } E_1,\ ...,\ E_n \text{ happens}] \quad \leq \quad \sum_{i=1}^{n} p_i.$$

The proof is rudimentary and left to you.

Proof of the Generalization Theorem

Fix any classifier $h \in \mathcal{H}$.

Let S be the training set; set $n = |S|$. For each $i \in [1, n]$, define $X_i = 1$ if the i-th object in S is incorrectly predicted by h, or 0 otherwise. Hence:

$$err_S(h) = \frac{1}{n} \sum_{i=1}^{n} X_i.$$

Proof of the Generalization Theorem

Since each object in S is drawn from $\mathcal{D}$ independently, for every $i \in [1, n]$:

$$\boldsymbol{Pr}[X_i = 1] = err_{\mathcal{D}}(h).$$

By the Hoeffding bounds, we have:

$$\boldsymbol{Pr}[err_S(h) < err_{\mathcal{D}}(h) - \alpha] \quad \leq \quad e^{-2n\alpha^2}$$

which is at most $\delta/|\mathcal{H}|$ by setting $e^{-2n\alpha^2} = \delta/|\mathcal{H}|$, namely

$$\alpha = \sqrt{\frac{\ln(1/\delta) + \ln|H|}{2n}}.$$

We say that h **fails** if $err_S(h) < err_{\mathcal{D}}(h) - \alpha$.

Proof of the Generalization Theorem

The above analysis shows that each classifier in $\mathcal{H}$ fails with probability at most $\delta/|\mathcal{H}|$. By the Union Bound, the probability that at least one classifier in $\mathcal{H}$ fails is at most δ. Hence, the probability that no classifiers fail is at least $1 - \delta$. $\square$

Our proof did not use any properties from decision trees. Indeed, the generalization theorem holds for any type of classifiers.