

Applied Machine Learning

Decision Trees

Siamak Ravanbakhsh

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Learning objectives

decision trees:

- model
- cost function
- how it is optimized

how to grow a tree and why you should prune it!

Adaptive bases

so far we assume a fixed set of bases in $f(x) = \sum_d w_d \phi_d(x)$

several methods can be classified as *learning these bases adaptively*

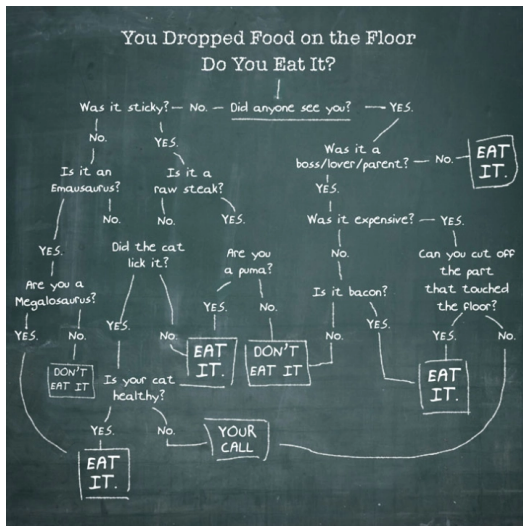
$$f(x) = \sum_d w_d \phi_d(x; v_d)$$

each basis has its own parameters

- decision trees
- generalized additive models
- boosting
- neural networks



Decision trees: motivation



pros.

decision trees are interpretable!
they are not very sensitive to outliers
do not need data normalization

cons.

they could easily overfit and they are unstable

- pruning
- random forests

Small bias, large variance

image credit: <https://mymodernmet.com/the-30second-rule-a-decision/>

Decision trees: idea

divide the input space into regions and learn one function per region

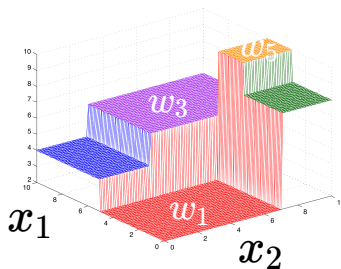
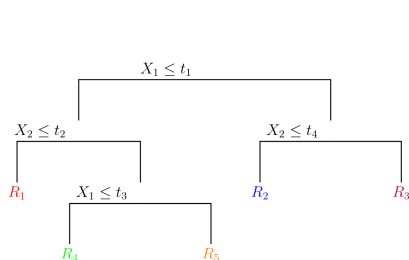
$$f(x) = \sum_k w_k \mathbb{I}(x \in \mathbb{R}_k)$$

the regions are learned adaptively

more sophisticated prediction per region is also possible (e.g., one linear model per region)

split regions successively based on the value of a single variable called **test**

each region is a set of conditions $\mathbb{R}_2 = \{x_1 \leq t_1, x_2 \leq t_4\}$



Prediction per region

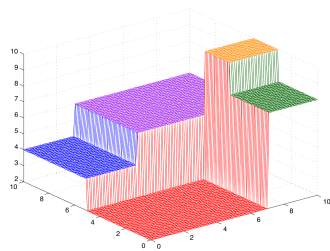
suppose we have identified the regions \mathbb{R}_k

what constant w_k to use for prediction in each region?

for regression

use the **mean value** of training data-points in that region

$$w_k = \text{mean}(y^{(n)} | x^{(n)} \in \mathbb{R}_k)$$



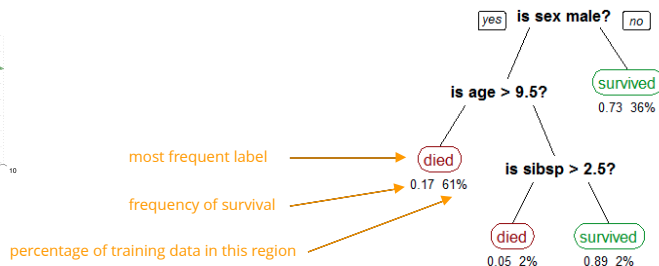
for classification

count the frequency of classes per region

predict the **most frequent label** $w_k = \text{mode}(y^{(n)} | x^{(n)} \in \mathbb{R}_k)$

or return probability

example: predicting survival in titanic



Feature types

given a feature what are the possible tests



continuous features - e.g., age, height, GDP

all the values that appear in the dataset can be used to split $\mathbb{S}_d = \{s_{d,n} = x_d^{(n)}\}$
 one set of possible splits for each feature d
 each split is asking $x_d > s_{d,n}$?



ordinal features - e.g., grade, rating $x_d \in \{1, \dots, C\}$

we can split any any value so $\mathbb{S}_d = \{s_{d,1} = 1, \dots, s_{d,C} = C\}$
 each split is asking $x_d > s_{d,c}$?



categorical features -
 - types, classes and categories



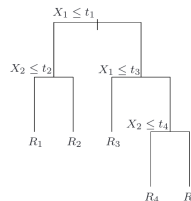
multi-way split

problem:

it could lead to sparse subsets

data fragmentation: some splits may have few/no datapoints

$$x_d = \begin{Bmatrix} \spadesuit ? \\ \heartsuit ? \\ \clubsuit ? \\ \spadesuit ? \end{Bmatrix}$$



binary split

assume C binary features (one-hot coding)

instead of $x_d \in \{1, \dots, C\}$ we have

$$\begin{cases} x_{d,1} \in \{0, 1\} \\ x_{d,2} \in \{0, 1\} \\ \vdots \\ x_{d,C} \in \{0, 1\} \end{cases} \quad \begin{cases} \spadesuit \heartsuit \clubsuit \spadesuit & x_{d,2} \stackrel{?}{=} 0 \\ \spadesuit \heartsuit \spadesuit \spadesuit & x_{d,2} \stackrel{?}{=} 1 \end{cases}$$

alternative: binary splits that produce balanced subsets

Cost function

objective: find a decision tree minimizing the **cost function**

regression cost

for predicting constant $w_k \in \mathbb{R}$

cost per region (mean squared error - MSE)

$$\text{cost}(\mathbb{R}_k, \mathcal{D}) = \frac{1}{N_k} \sum_{x^{(n)} \in \mathbb{R}_k} (y^{(n)} - w_k)^2$$

number of instances in region k

mean($y^{(n)} | x^{(n)} \in \mathbb{R}_k$)

total cost in both cases is the normalized sum $\sum_k \frac{N_k}{N} \text{cost}(\mathbb{R}_k, \mathcal{D})$

it is sometimes possible to build a tree with **zero cost**:

build a large tree with each instance having its own region (*overfitting!*)

new objective: find a decision tree with **K tests** minimizing the cost function

classification cost

for predicting constant class $w_k \in \{1, \dots, C\}$

cost per region (misclassification rate)

$$\text{cost}(\mathbb{R}_k, \mathcal{D}) = \frac{1}{N_k} \sum_{x^{(n)} \in \mathbb{R}_k} \mathbb{I}(y^{(n)} \neq w_k)$$

mode($y^{(n)} | x^{(n)} \in \mathbb{R}_k$)

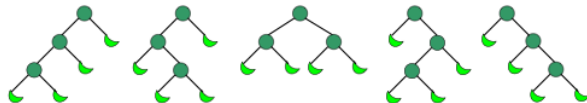
Search space

objective: find a decision tree with K tests minimizing the cost function
alternatively, find the smallest tree (K) that classifies all examples correctly

assuming D features how many different partitions of size $K+1$?

the number of full binary trees with $K+1$ leaves (regions \mathbb{R}_k) is the **Catalan number**

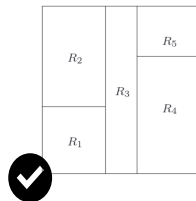
1, 1, 2, 5, 14, 42, 132, 429, 1430, 4862, 16796, 58786, 208012, 742900, 2674440, 9694845, 35357670, 129644790, 477638700, 1767263190, 6564120420, 24466267020, 91482563640, 343059613650, 1289904147324, 4861946401452



we also have a choice of feature x_d for each of K internal node D^K

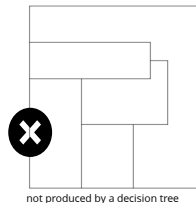
moreover, for each feature different choices of splitting $x_d \in \mathbb{S}_d$

bottom line: finding optimal decision tree is an **NP-hard** combinatorial optimization problem



$$\frac{1}{K+1} \binom{2K}{K}$$

exponential in K



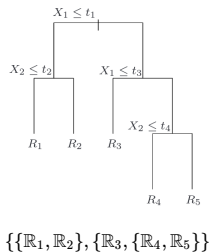
Greedy heuristic

recursively split the regions based on a **greedy choice of the next test**
end the recursion if not **worth-splitting**

```
function fit-tree( $\mathbb{R}_{\text{node}}$ ,  $\mathcal{D}$ , depth)

     $\mathbb{R}_{\text{left}}, \mathbb{R}_{\text{right}}$  = greedy-test ( $\mathbb{R}_{\text{node}}$ ,  $\mathcal{D}$  )
    if not worth-splitting(depth,  $\mathbb{R}_{\text{left}}$ ,  $\mathbb{R}_{\text{right}}$  )
        return  $\mathbb{R}_{\text{node}}$ 
    else
        left-set = fit-tree( $\mathbb{R}_{\text{left}}$ ,  $\mathcal{D}$ , depth+1)
        right-set = fit-tree( $\mathbb{R}_{\text{right}}$ ,  $\mathcal{D}$ , depth+1)
        return {left-set, right-set}
```

final decision tree in the form of nested list of regions



Choosing tests

the split is greedy because it looks one step ahead
this may not lead to the the lowest overall cost

```
function greedy-test ( $\mathbb{R}_{\text{node}}, \mathcal{D}$ )
```

```
    best-cost = inf
```

```
    for  $d \in \{1, \dots, D\}, x_d \in \mathbb{S}_d$ 
```

```
         $\mathbb{R}_{\text{left}} = \mathbb{R}_k \cup \{s_{d,n} < x_d\}$ 
```

```
         $\mathbb{R}_{\text{right}} = \mathbb{R}_k \cup \{s_{d,n} \geq x_d\}$ 
```

```
        split-cost =  $\frac{N_{\text{left}}}{N_{\text{node}}}$  cost( $\mathbb{R}_{\text{left}}, \mathcal{D}$ ) +  $\frac{N_{\text{right}}}{N_{\text{node}}}$  cost( $\mathbb{R}_{\text{right}}, \mathcal{D}$ )
```

```
        if split-cost < best-cost:
```

```
            best-cost = split-cost
```

```
             $\mathbb{R}_{\text{left}}^* = \mathbb{R}_{\text{left}}$ 
```

```
             $\mathbb{R}_{\text{right}}^* = \mathbb{R}_{\text{right}}$ 
```

```
    return  $\mathbb{R}_{\text{left}}^*, \mathbb{R}_{\text{right}}^*$ 
```

→ creating new regions

→ evaluate their cost

normalized.

→ return the split with the lowest greedy cost

Stopping the recursion

worth-splitting subroutine

if we stop when \mathbb{R}_{node} has zero cost, we may overfit
heuristics for stopping the splitting:

- reached a desired depth
- number of examples in \mathbb{R}_{left} or $\mathbb{R}_{\text{right}}$ is too small
- w_k is a good approximation, the cost is small enough
- reduction in cost by splitting is small

$$\text{cost}(\mathbb{R}_{\text{node}}, \mathcal{D}) = \left(\frac{N_{\text{left}}}{N_{\text{node}}} \text{cost}(\mathbb{R}_{\text{left}}, \mathcal{D}) + \frac{N_{\text{right}}}{N_{\text{node}}} \text{cost}(\mathbb{R}_{\text{right}}, \mathcal{D}) \right)$$

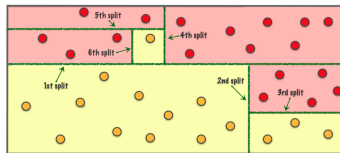
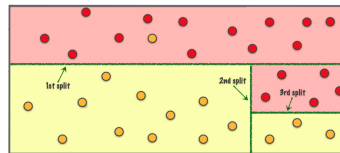


image credit: <https://alanjeffares.wordpress.com/tutorials/decision-tree/>

revisiting the classification cost

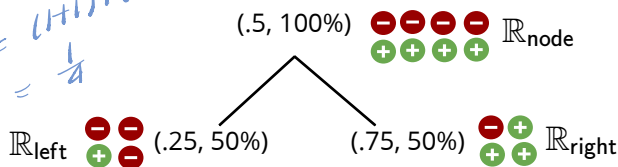
ideally we want to optimize the 0-1 loss (misclassification rate)

$$\text{cost}(\mathbb{R}_k, \mathcal{D}) = \frac{1}{N_k} \sum_{x^{(n)} \in \mathbb{R}_k} \mathbb{I}(y^{(n)} \neq w_k)$$

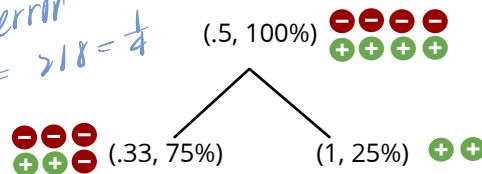
this may not be the optimal cost for *each step of greedy heuristic*

example both splits have the same misclassification rate (2/8)

error = $\frac{1+1}{8} = \frac{1}{4}$



error = $\frac{2}{8} = \frac{1}{4}$



however the second split *may be* preferable because one region does not need further splitting

use a measure for homogeneity of labels in regions

Entropy

entropy is the **expected amount of information** in observing a random variable y

note that it is common to use capital letters for random variables (here for consistency we use lower-case)

*always
positive*

$$H(y) = - \sum_{c=1}^C p(y=c) \log p(y=c)$$

$-\log p(y=c)$ is the amount of **information** in observing c

zero information of $p(c)=1$

less probable events are more informative $p(c) < p(c') \Rightarrow -\log p(c) > -\log p(c')$

information from two independent events is additive $-\log(p(c)q(d)) = -\log p(c) - \log q(d)$

a uniform distribution has the highest entropy $H(y) = - \sum_{c=1}^C \frac{1}{C} \log \frac{1}{C} = \log C$

a deterministic random variable has the lowest entropy $H(y) = -1 \log(1) = 0$

Mutual information

for two random variables t, y

mutual information is the amount of information \mathbf{t} conveys about \mathbf{y}
change in the entropy of \mathbf{y} after observing the value of \mathbf{t}

$$\begin{aligned} I(t, y) &= H(y) - H(y|t) \\ &\quad \text{conditional entropy } \sum_{l=1}^L p(t=l) H(y|t=l) \\ &= \sum_l \sum_c p(y=c, t=l) \log \frac{p(y=c, t=l)}{p(y=c)p(t=l)} \quad \text{this is symmetric wrt } \mathbf{y} \text{ and } \mathbf{t} \\ &= H(t) - H(t|y) = I(y, t) \end{aligned}$$

it is always positive and zero only if \mathbf{y} and \mathbf{t} are independent

try to prove these properties



Entropy for classification cost

we care about the distribution of labels $p_k(y = c) = \frac{\sum_{x^{(n)} \in \mathbb{R}_k} \mathbb{I}(y^{(n)} = c)}{N_k}$

misclassification cost $\text{cost}(\mathbb{R}_k, \mathcal{D}) = \frac{1}{N_k} \sum_{x^{(n)} \in \mathbb{R}_k} \mathbb{I}(y^{(n)} \neq w_k) = 1 - p_k(w_k)$
the most probable class $w_k = \arg \max_c p_k(c)$

entropy cost $\text{cost}(\mathbb{R}_k, \mathcal{D}) = H(y)$ choose the split with the lowest entropy

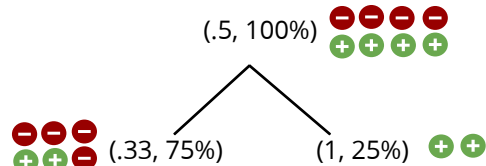
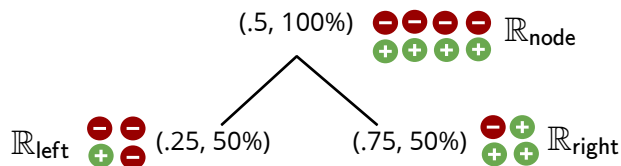
change in the cost becomes the mutual information between the test and labels

$$\begin{aligned} \text{cost}(\mathbb{R}_{\text{node}}, \mathcal{D}) &= \left(\frac{N_{\text{left}}}{N_{\text{node}}} \text{cost}(\mathbb{R}_{\text{left}}, \mathcal{D}) + \frac{N_{\text{right}}}{N_{\text{node}}} \text{cost}(\mathbb{R}_{\text{right}}, \mathcal{D}) \right) \\ &= H(y) - \left(p(x_d \geq s_{d,n}) H(p(y|x_d \geq s_{d,n})) + p(x_d < s_{d,n}) H(p(y|x_d < s_{d,n})) \right) = I(y, x > s_{d,n}) \end{aligned}$$

choosing the test which is **maximally informative** about labels

example

Entropy for classification cost



misclassification cost

$$\frac{4}{8} \cdot \frac{1}{4} + \frac{4}{8} \cdot \frac{1}{4} = \frac{1}{4}$$

the same costs

$$\frac{6}{8} \cdot \frac{1}{3} + \frac{2}{8} \cdot \frac{0}{2} = \frac{1}{4}$$

entropy cost (using base 2 logarithm)

$$\frac{4}{8} \left(-\frac{1}{4} \log\left(\frac{1}{4}\right) - \frac{3}{4} \log\left(\frac{3}{4}\right) \right) + \frac{4}{8} \left(-\frac{1}{4} \log\left(\frac{1}{4}\right) - \frac{3}{4} \log\left(\frac{3}{4}\right) \right) \approx .81$$



$$\frac{6}{8} \left(-\frac{1}{3} \log\left(\frac{1}{3}\right) - \frac{2}{3} \log\left(\frac{2}{3}\right) \right) + \frac{2}{8} \cdot 0 \approx .68$$

lower cost split

Gini index

another cost for selecting the *test* in classification

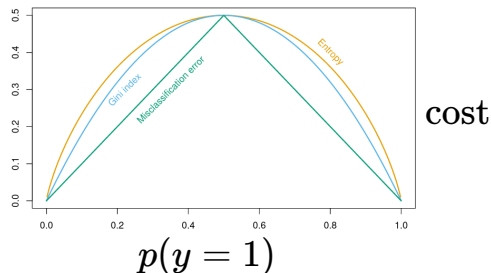
misclassification (error) rate $\text{cost}(\mathbb{R}_k, \mathcal{D}) = \frac{1}{N_k} \sum_{x^{(n)} \in \mathbb{R}_k} \mathbb{I}(y^{(n)} \neq w_k) = 1 - p(w_k)$

entropy $\text{cost}(\mathbb{R}_k, \mathcal{D}) = H(y)$

Gini index it is the expected error rate

$$\begin{aligned} \text{cost}(\mathbb{R}_k, \mathcal{D}) &= \sum_{c=1}^C \underbrace{p(c)}_{\text{probability of class } c} \underbrace{(1 - p(c))}_{\text{probability of error}} \\ &= \sum_{c=1}^C p(c) - \sum_{c=1}^C p(c)^2 = 1 - \sum_{c=1}^C p(c)^2 \end{aligned}$$

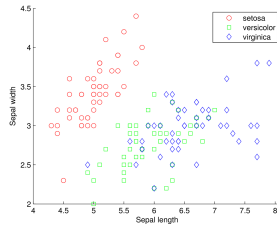
comparison of costs of a node when we have 2 classes



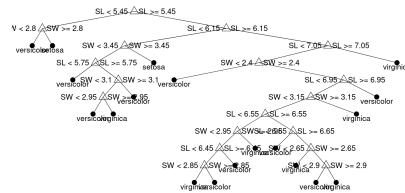
Example

decision tree for Iris dataset

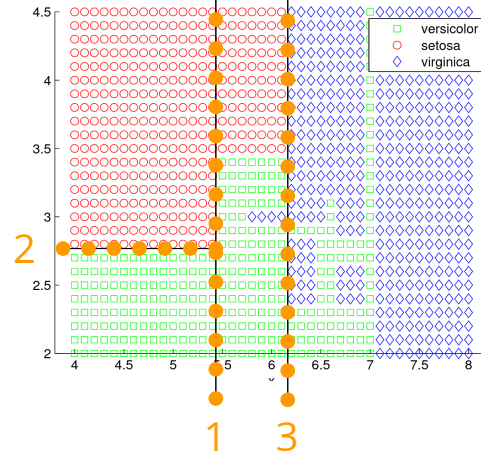
dataset (D=2)



decision tree



decision boundaries



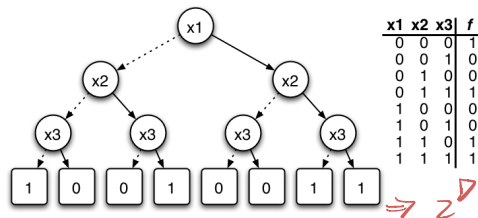
decision boundaries suggest overfitting
confirmed using a validation set

training accuracy ~ 85%
(Cross) validation accuracy ~ 70%

Overfitting

a decision tree can fit any Boolean function (binary classification with binary features)

example: of decision tree representation of a boolean function (D=3)



there are 2^{2^D} such functions, why?

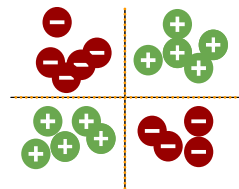
large decision trees have a high variance - low bias (low training error, high test error)

idea 1. grow a small tree



substantial reduction in cost may happen after a few steps
by stopping early we cannot know this

doesn't improve at first ^ node.



example

cost drops after the second node

Pruning

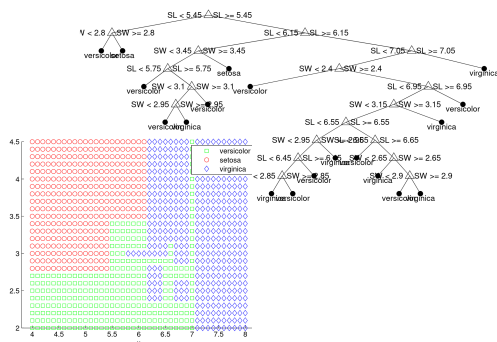
idea 2. grow a large tree and then prune it
greedily turn an internal node into a leaf node
choice is based on the lowest increase in the cost
repeat this until left with the root node

idea 3. random forests (later!)

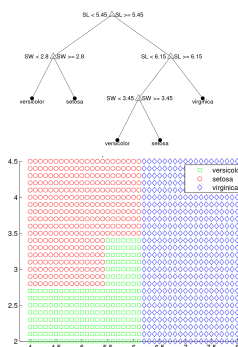
pick the best among the above models using using a validation set

example

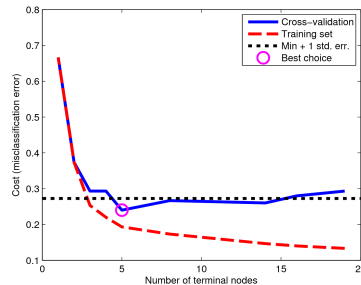
before pruning



after pruning



cross-validation is used to pick the best size



Summary

- model: divide the input into axis-aligned regions
- cost: for regression and classification
- optimization:
 - NP-hard
 - use greedy heuristic
- adjust the cost for the heuristic
 - using entropy (relation to mutual information maximization)
 - using Gini index
- decision trees are unstable (have high variance)
 - use pruning to avoid overfitting
- there are variations on decision tree heuristics
 - what we discussed in called *Classification and Regression Trees (CART)*