Applied Machine Learning

Decision Trees

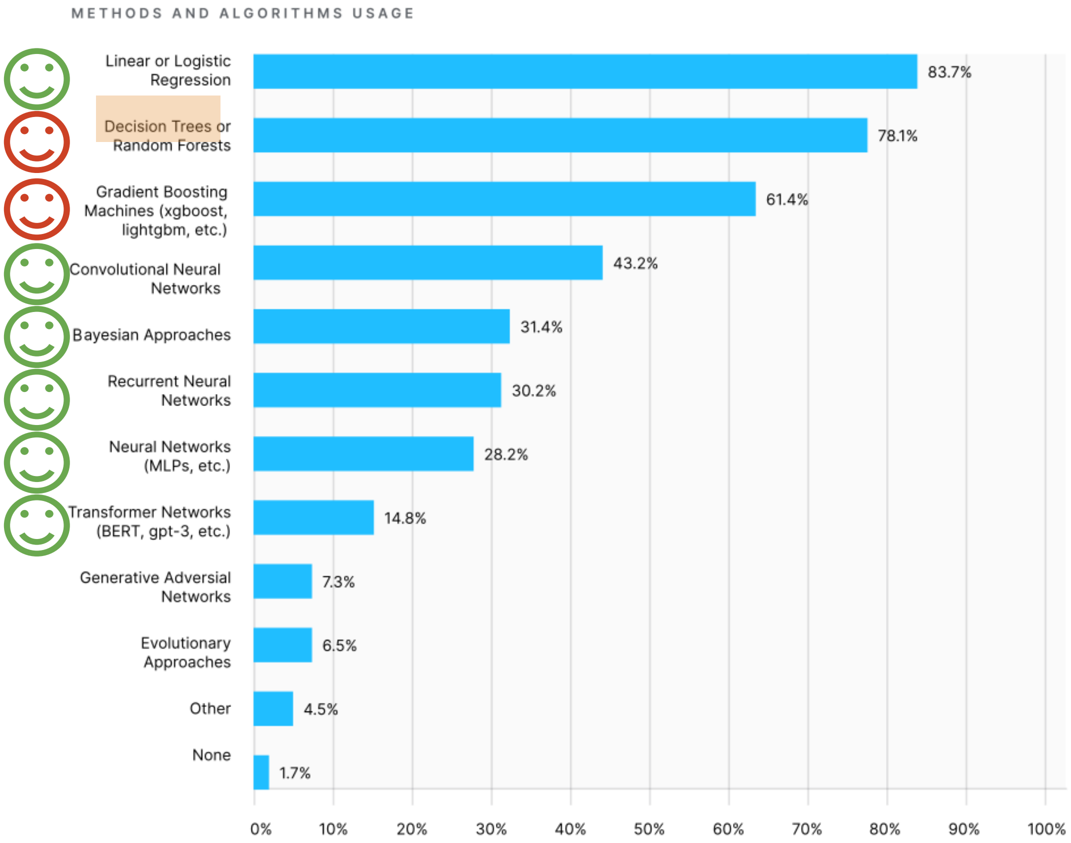
Isabeau Prémont-Schwarz

McGill School of Computer Science

Motivation

What we have left to cover for this course:

- Classification and regression trees
- Linear support vector machines
- Bagging & boosting
- Unsupervised learning
- Dimensionality reduction



from 2020 Kaggle's survey on the state of Machine Learning and Data Science, you can read the full version here

Learning objectives

Decision trees:

- how does it model the data?
- how to specify the best model using a cost function
- how the cost function is optimized

Decision trees: motivation

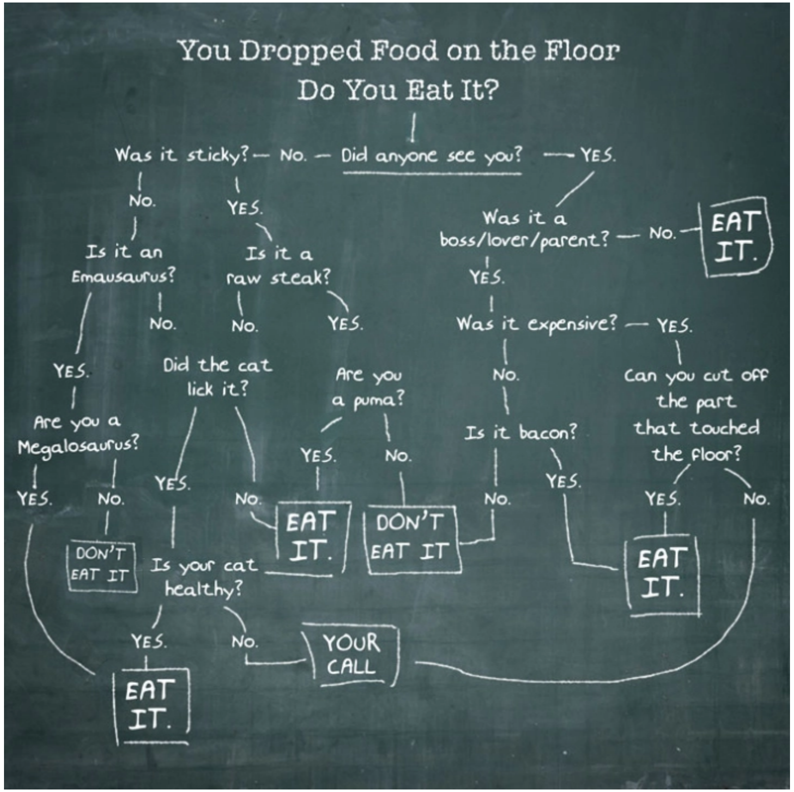


image credit:https://mymodernmet.com/the-30second-rule-a-decision/

pros.

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

cons.

- they could easily overfit and are unstable to small changes in input data

Notation overview

	<tumorsize,	texture,	perimeter>	,	<cancer>	
$x^{(1)}$	<18.2,	27.6,	117.5>	,	< No >	$y^{(1)}$
$x^{(2)}$	<17.9,	10.3,	122.8>	,	< No >	$y^{(2)}$
$x^{(3)}$	<20.2,	14.3,	111.2>	,	< Yes >	$y^{(3)}$
$\vdots$		$\vdots$				$\vdots$
$x^{(N)}$	<15.5,	15.2,	135.5>	,	< No >	$y^{(N)}$

Our datasets consists of N pairs of input vector and corresponding target or label

$$\mathcal{D} = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$$

we use N to denote the size of the dataset and n for indexing a pair of input, label

x, y denote an input and label pair where

x is a *D*-dimensional vector: $x = [x_1, x_2, \ldots, x_D]$

we use D to denote the number of *features* (dimensionality of the input space)

$y \in \{1, \ldots, C\}$ for classification problems, we use C for number of classes

$x_d^{(n)}$ — $n \in [1 \ldots N]$ indexes an instance, row index, e.g. which patient
$d \in [1 \ldots D]$ indexes a feature, column index, e.g. which measurement

e.g. $x_2^{(3)}$

Decision trees: idea

- divide the input space into regions $\mathbb{R}_1, \ldots, \mathbb{R}_K$ using a tree structure
- assign a prediction **label** to each region

for classification this is the class label

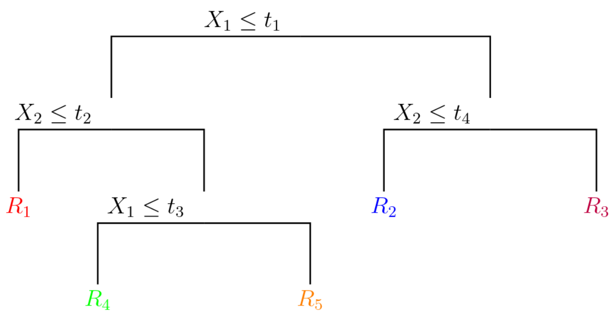
for regression, this is a real scalar or vector

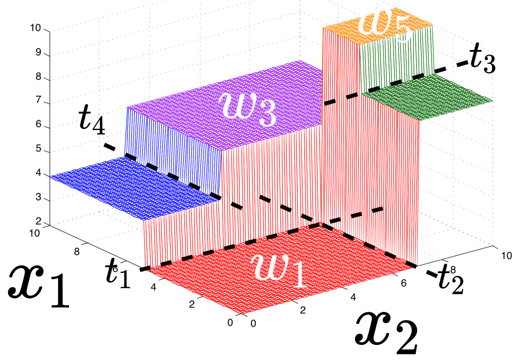
$$f(x) = \sum_k w_k \mathbb{I}(x \in \mathbb{R}_k)$$

how to build the regions and the tree?

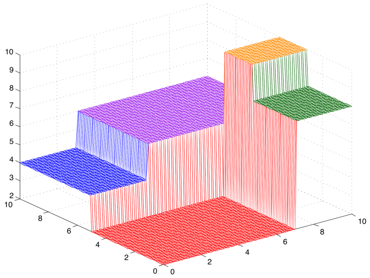
split regions successively based on the value of a single variable called test

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





Prediction per region



What constant w_k should we use for prediction in each region $\mathbb{R}_k$?

Classification

count the frequency of classes per region, predict the most frequent label or return probability $w_k = \mathrm{mode}(y^{(n)} | x^{(n)} \in \mathbb{R}_k)$

Regression

use the mean value of training data-points in that region $w_k = \mathrm{mean}(y^{(n)} | x^{(n)} \in \mathbb{R}_k)$

example: predicting survival in titanic

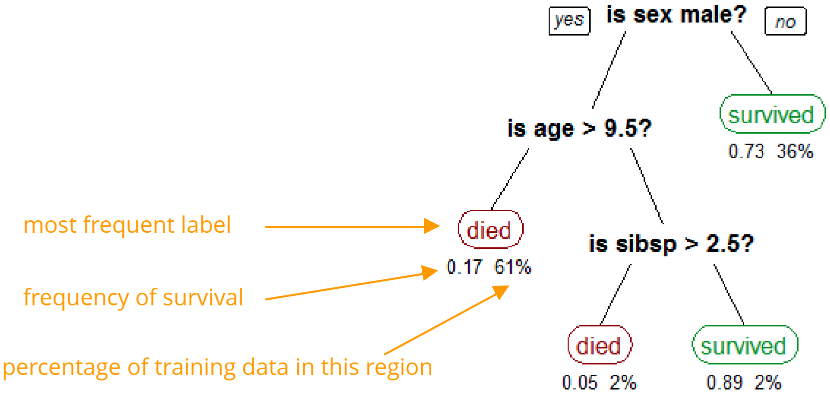
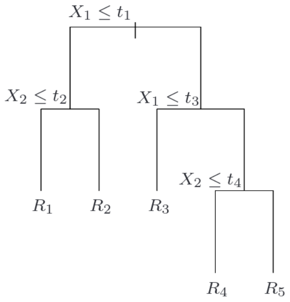
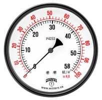


figure from wiki

Possible tests



next questions: what are all the possible tests? which test do we choose next?



Continuous features

all the values that appear in the dataset can be used to split

♣♦♥♠

Categorical features

if a feature can take C values $x_i \in \{1, \ldots, C\}$

convert that feature into C binary features **(one-hot coding)** $x_{i,1}, \ldots, x_{i,C} \in \{0, 1\}$

split based on the value of a binary feature

alternatives:

- **multi-way** split: can lead to regions with few datapoints
- binary splits that produce balanced subsets

Food Name	Categorical #	Calories
Apple	1	95
Chicken	2	231
Broccoli	3	50

Apple	Chicken	Broccoli	Calories
1	0	0	95
0	1	0	231
0	0	1	50

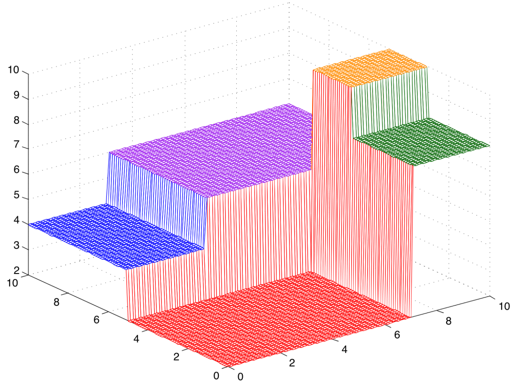
one-hot example from here

Cost function

find a **decision tree** minimizing the following cost function, this cost function specifies "what is a good decision or regression tree?"

Similar to other ML algorithms minimize a cost function or maximize an objective function

regression cost first calculate cost per region $\mathbb{R}_k$



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

mean squared error (MSE)

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

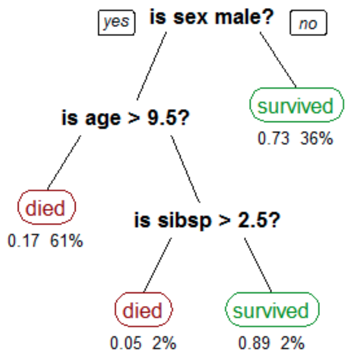
number of instances in region k — truth — prediction

total cost is the normalized sum over all regions $\text{cost}(\mathcal{D}) = \sum_k \frac{N_k}{N} \text{cost}(\mathbb{R}_k, \mathcal{D})$

Cost function

find a **decision tree** minimizing the following cost function, this cost function specifies "what is a good decision or regression tree?"

classification cost again, calculate the cost per region $\mathbb{R}_k$



for each region we predict the most frequent label $w_k = \mathrm{mode}(y^{(n)} | x^{(n)} \in \mathbb{R}_k)$

misclassification rate

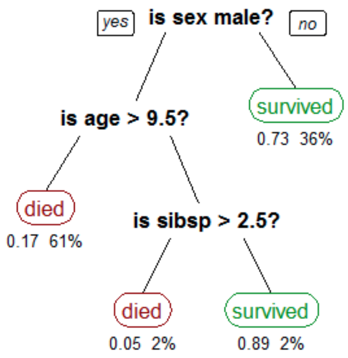
$$\mathrm{cost}(\mathbb{R}_k, \mathcal{D}) = \frac{1}{N_k} \sum_{x^{(n)} \in \mathbb{R}_k} \mathbb{I}(y^{(n)} \neq w_k)$$

number of instances in region k   truth   prediction

total cost is the normalized sum $\mathrm{cost}(\mathcal{D}) = \sum_k \frac{N_k}{N} \mathrm{cost}(\mathbb{R}_k, \mathcal{D})$

Cost function

find a **decision tree** minimizing the following cost function, this cost function specifies "what is a good decision or regression tree?"



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

problem

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

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

example use features such as height, eye color etc, to make perfect prediction on training data

solution find a decision tree with at most **K tests** minimizing the cost function

K tests = K internal node in our binary tree = K+1 leaves (regions)

Search space

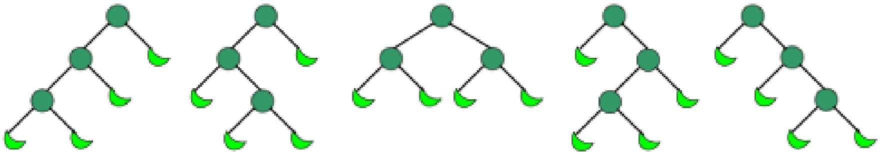
K+1 regions

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

the number of full binary trees with K+1 leaves (regions $\mathbb{R}_k$) is the ***Catalan number*** $\frac{1}{K+1}\binom{2K}{K}$

exponential in K

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

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

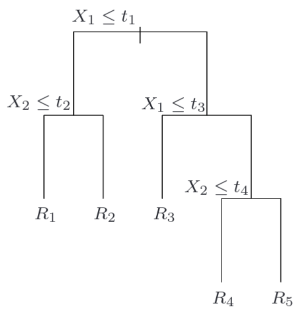
Greedy heuristic

finding the optimal tree is too difficult, instead use a greedy heuristic to find a good tree

recursively split the regions based on a greedy choice of the next test

end the recursion if not worth-splitting

```
function fit-tree(ℝnode , 𝒟 ,depth)

    ℝleft, ℝright = greedy-test (ℝnode , 𝒟 )

    if not worth-splitting(depth, ℝleft, ℝright )
          return ℝnode
    else
        left-set = fit-tree( ℝleft , 𝒟, depth+1)
        right-set = fit-tree(ℝright , 𝒟, depth+1)
        return {left-set, right-set}
```



$\{\{\mathbb{R}_1, \mathbb{R}_2\}, \{\mathbb{R}_3, \{\mathbb{R}_4, \mathbb{R}_5\}\}$

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 lowest overall cost

```
function greedy-test ( ℝnode , 𝒟 )
    best-cost = inf
    for each feature d ∈ {1,...,D} and each possible test
        split ℝnode into ℝleft, ℝright based on the test
        split-cost = (Nleft/Nnode) cost(ℝleft, 𝒟) + (Nright/Nnode) cost(ℝright, 𝒟)
        if split-cost < best-cost:
            best-cost = split-cost
            ℝ*left = ℝleft
            ℝ*right = ℝright
return ℝ*left, ℝ*right
```

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

Stopping the recursion

`worth-splitting` subroutine

if we stop when $\mathbb{R}_{\text{node}}$ has zero cost, we may overfit

heuristics for stopping the splitting:

- reached a desired depth
- number of examples in $\mathbb{R}_{\text{left}}$ 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

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

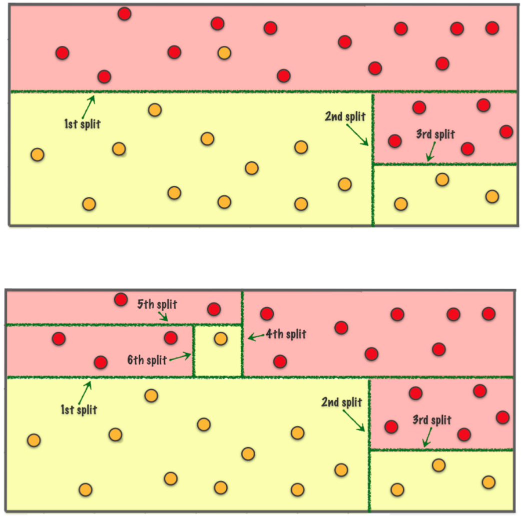


image credit: https://alanjeffares.wordpress.com/tutorials/decision-tree/

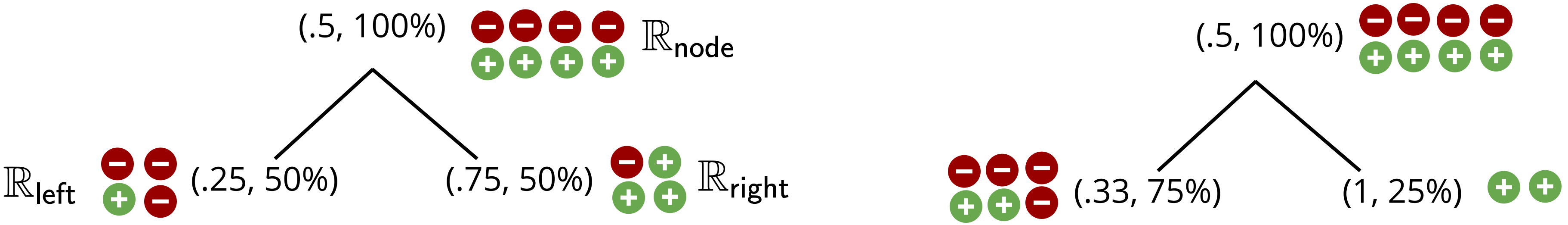
revisiting the classification cost

ideally we want to optimize the misclassification rate

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

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

example both splits have the same misclassification rate (2/8) $\mathrm{cost}(\mathcal{D}) = \frac{1}{N} \sum_k \sum_{x^{(n)} \in \mathbb{R}_k} \mathbb{I}(y^{(n)} \neq w_k)$



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

idea: use a measure for homogeneity of labels in regions

Entropy: a measure of the *unpredictability*

The most basic concept in the field of **Information Theory**

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

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

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

averaged on all its possible outcomes

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

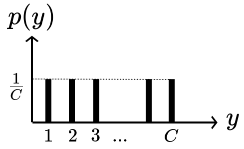
$I(y=c) = \log(\frac{1}{p(y=c)}) = -log(p(y=c))$

zero information if p(c)=1

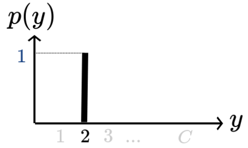
less probable events are more informative $p(c) < p(c') \Rightarrow -\log p(c) > -\log p(c')$

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

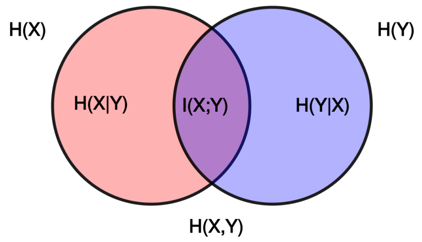
a uniform distribution has the highest entropy $H(y) = -\sum_{c=1}^{C} \frac{1}{C} \log \frac{1}{C} = \log C$



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



Mutual information



for two random variables t, y, their **mutual information** is

the amount of information t conveys about y

change in the entropy of y after observing the value of t

how much knowing t reduces uncertainty about y

$$I(t, y) = H(y) - H(y|t)$$

conditional entropy $\sum_{l=1}^{L} p(t = l) H(x|t = l)$ uncertainty we have in y after seeing t

$$= \sum_l \sum_c p(y = c, t = l) \log \frac{p(y=c,t=l)}{p(y=c)p(t=l)}$$

this is symmetric wrt y and t

$$= H(t) - H(t|y) = I(y, t)$$

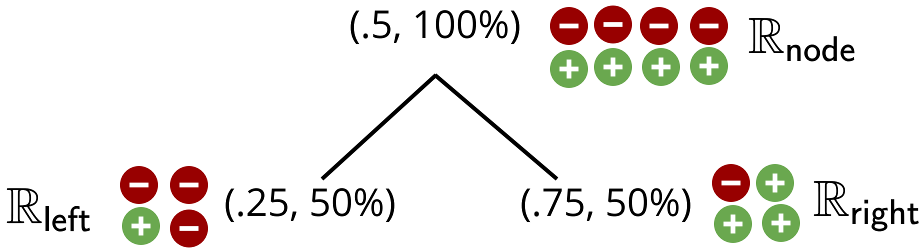
mutual information is always positive and zero only if y and t are independent

Classification cost: example

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

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

the most probable class $w_k = \arg\max_c p_k(c)$



$p(y=+) = \frac{1}{4}, p(y=-) = \frac{3}{4}$ $\quad$ $p(y=+) = \frac{3}{4}, p(y=-) = \frac{1}{4}$

$w_k = -$ $\quad$ $w_k = +$

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

$\mathrm{cost}(\mathcal{D}) = \sum_k \frac{N_k}{N} \mathrm{cost}(\mathbb{R}_k, \mathcal{D})$

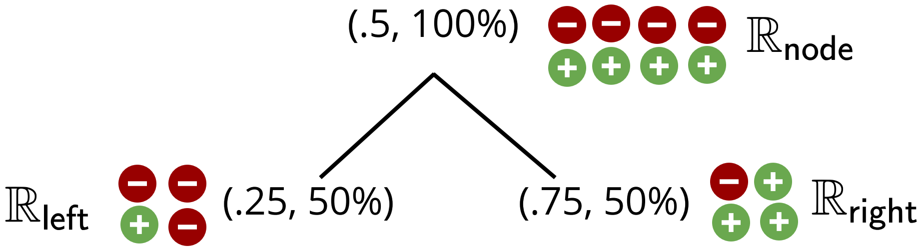
Entropy for classification cost: example

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

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 $\text{cost}(\mathbb{R}_k, \mathcal{D}) = H(y) = -\sum_{c=1}^{C} p(y=c) \log p(y=c)$ choose the split with the lowest entropy



$p(y=+) = \frac{1}{4}, p(y=-) = \frac{3}{4}$

misclassification cost

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

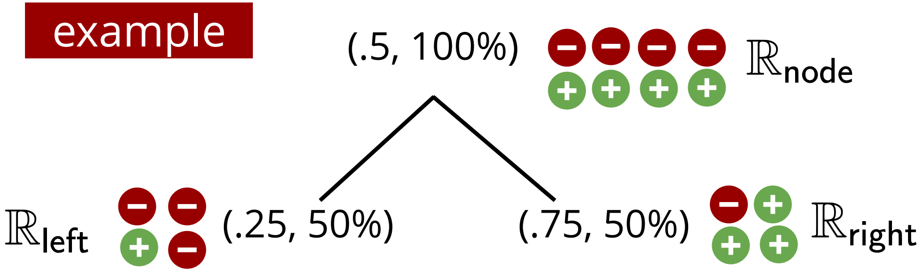
entropy cost

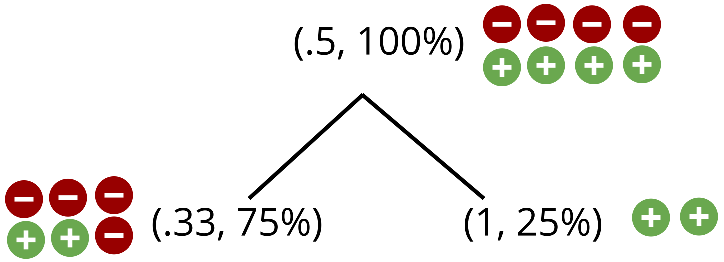
$$\boxed{\frac{4}{8}\left(-\frac{1}{4}\log\left(\frac{1}{4}\right) - \frac{3}{4}\log\left(\frac{3}{4}\right)\right)} + \frac{4}{8}\left(-\frac{1}{4}\log\left(\frac{1}{4}\right) - \frac{3}{4}\log\left(\frac{3}{4}\right)\right)$$

$\text{cost}(\mathcal{D}) = \sum_k \frac{N_k}{N} \text{cost}(\mathbb{R}_k, \mathcal{D})$

Entropy for classification cost: example

example





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)

$$\tfrac{4}{8}\Big(-\tfrac{1}{4}\log(\tfrac{1}{4})-\tfrac{3}{4}\log(\tfrac{3}{4})\Big)+\tfrac{4}{8}\Big(-\tfrac{1}{4}\log(\tfrac{1}{4})-\tfrac{3}{4}\log(\tfrac{3}{4})\Big)\approx .81$$

$$\tfrac{6}{8}\Big(-\tfrac{1}{3}\log(\tfrac{1}{3})-\tfrac{2}{3}\log(\tfrac{2}{3})\Big)+\tfrac{2}{8}\cdot 0\approx .68$$

lower cost split

Entropy for classification cost

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

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

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

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

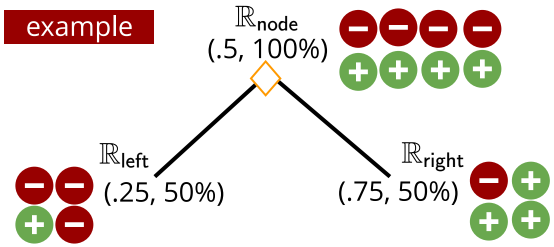
$$= H(y) - \Big(p(x_d \geq t) H(y | x_d \geq t) + p(x_d < t) H(y | x_d < t) \Big) = I(y, x > t)$$

$$I(t, y) = H(y) - H(y|t)$$

$$\sum_{l=1}^{L} p(t=l) H(y|t=l)$$

this means by using entropy as our cost, we are choosing the test which is **maximally informative** about labels

example



$$I(y, \diamond) = H(y) - \Big(p(\diamond) H(y|\diamond) + p(!\diamond) H(y|!\diamond) \Big)$$

$$= 1 - 0.81$$

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

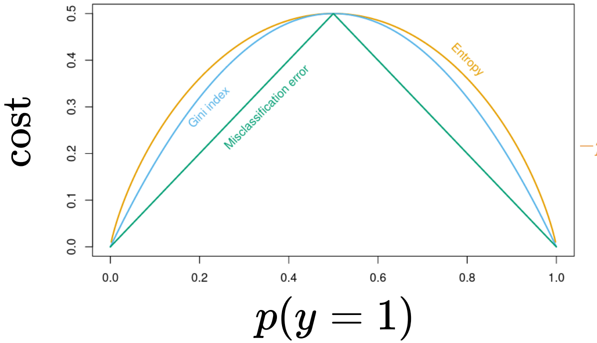
Gini index it is the expected error rate

$$\text{cost}(\mathbb{R}_k, \mathcal{D}) = \sum_{c=1}^{C} p(c)(1 - p(c))$$

probability of class c probability of error

$$= \sum_{c=1}^{C} p(c) - \sum_{c=1}^{C} p(c)^2 = 1 - \sum_{c=1}^{C} p(c)^2$$

comparison of costs of a node when we have 2 classes



C=2

$1 - max(p, 1 - p)$

$-p \log p - (1 - p)log(1 - p)$

$2p(1 - p)$

entropy & gini very similar and both favour pure nodes

Building the Tree

Naive Algorithm:

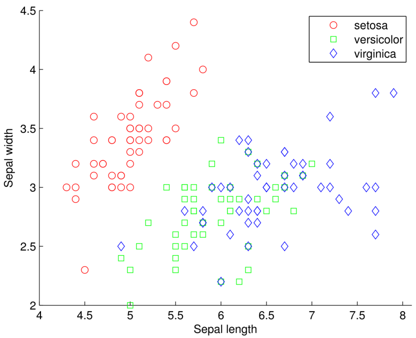
Just do a for loop over all possible questions (exhaustive search).

```
def find_root_question(features, values):
  best_tree = None
  best_loss = np.infty
  for f in features:
      prev_v = None
      for v in sort(values[f]):
          if prev_v is None:
              continue
          split = (v + prev)/2
          tree = Tree(f, split)
          tree_loss = loss(Tree)
          if tree_loss < best_loss:
              best_tree = tree
              best_loss = tree_loss
          prev_v = v

def add_question(tree, features, values):
  best_tree = None
  best_loss = np.infty
  for leaf in tree.leaves():
    for f in features:
        prev_v = None
        for v in sort(values[f]):
            if prev_v is None:
                continue
            split = (v + prev)/2
            test_tree = tree.add_question(leaf, feature, split)
            tree_loss = loss(Tree)
            if tree_loss < best_loss:
                best_tree = tree
                best_loss = tree_loss

            prev_v = v
```

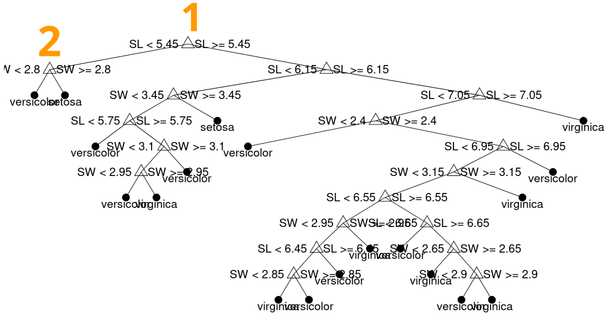
Decision tree

decision tree for Iris dataset

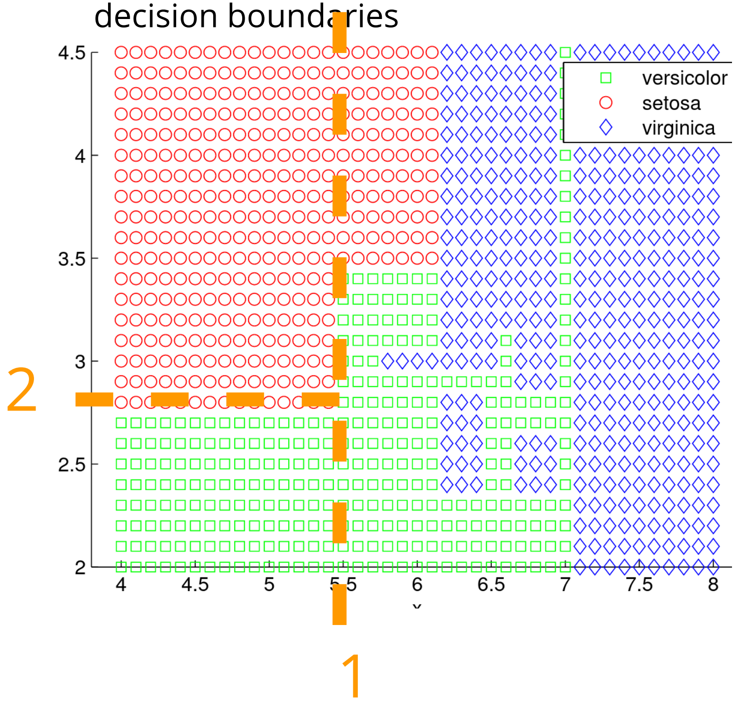
dataset (D=2)



decision tree



decision boundaries



decision boundaries suggest overfitting

confirmed using a validation set

training accuracy ~ 85%
validation accuracy ~ 70%

Decision tree: 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)

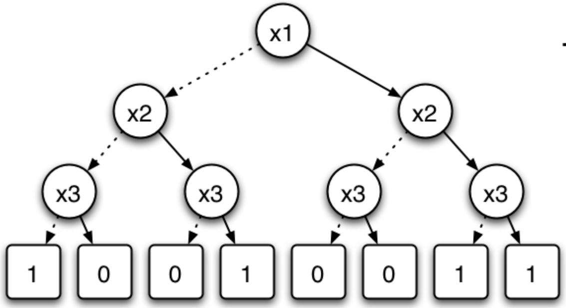


image from: https://www.wikiwand.com/en/Binary_decision_diagram

x1	x2	x3	*f*
0	0	0	1
0	0	1	0
0	1	0	0
0	1	1	1
1	0	0	0
1	0	1	0
1	1	0	1
1	1	1	1

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

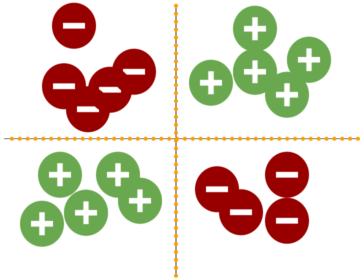
decision tree can perfectly fit our training data

How to solve the problem of overfitting in large decision trees?

idea 1. grow a small tree

☹ problem: substantial reduction in cost may happen after a few steps

by stopping early we cannot know this



example cost drops after the second node

Decision tree: overfitting & pruning

idea 2. grow a large tree and then prune it

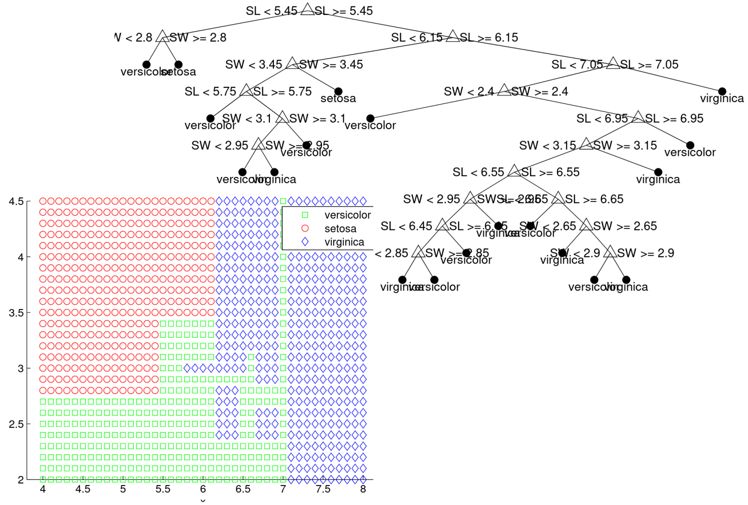
greedily turn an internal node into a leaf node
choice is based on the lowest increase in the cost
repeat this until left with the root node

pick the best among the above models using a validation set

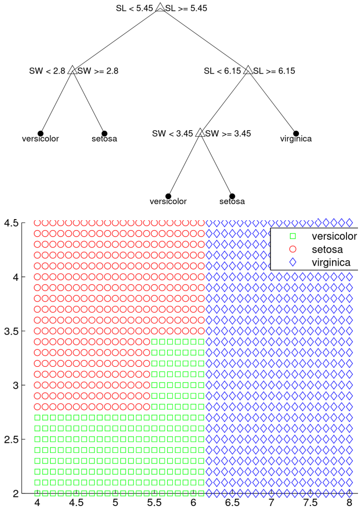
idea 3. random forests (later!)

example

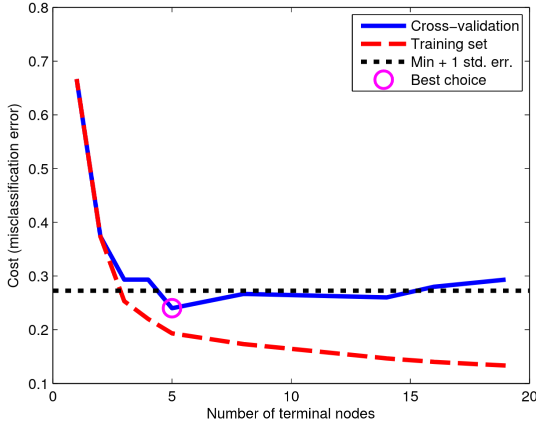
before pruning



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
- there are variations on decision tree heuristics
  - what we discussed in called *Classification and Regression Trees (CART)*
- Compared to KNN, robust to scaling and noise, fast predictions, more interpretable