April 11, 2018

CS 361: Probability & Statistics

Classification

Classifier evaluation

After we've trained a classifier we have a nice machine that can look at new data and hopefully accurately apply class labels. There are many other design considerations besides accuracy that we may want to take into account

How long does a classifier take to train?

How long does it take to make a prediction?

Is the classifier interpretable? Does looking at the resulting classifier tell us anything interesting about our data?

Among others

Multi-class classification

We have considered the Perceptron and SVM classifiers which are binary classifiers

However, we can use binary classifiers to handle multiple classes in a couple of different ways

In the **all vs all** approach, we would train a classifier for each pair of potential class labels. For instance if we were trying to train a classifier that analyzed radiology images and made a diagnosis of healthy, benign tumor, malignant tumor, in the all vs all approach we would train a classifier for healthy vs benign, healthy vs malignant, and benign vs malignant. We then run all of the classifiers and see which class label wins the most 1vs1 competitions

Multi-class classification

Another approach for using binary classifiers to handle multiple classes is the **one-vs-all** approach

In this case we train a classifier for each label separately. For example we would train a healthy vs non-healthy, benign vs non-benign, and malignant vs non-malignant classifier. To classify a new example, we show it to each of the classifiers and record the score. We output the class label which had the highest score

All vs all requires training O(N^2) classifiers, whereas one vs all requires O(N). In practice both methods work fairly well

Class confusion matrices

A tool for evaluating multi-class (including binary) classifiers

	Predict 0	Predict 1	Predict 2	Predict 3	Predict 4	Class error
True 0	151	7	2	3	1	7.9%
True 1	32	5	9	9	0	91%
True 2	10	9	7	9	1	81%
True 3	6	13	9	5	2	86%
True 4	2	3	2	6	0	100%

Normalization

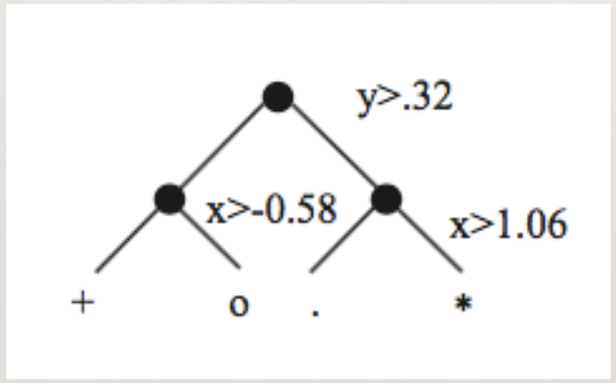
For the classifiers we have learned so far, there is one caveat worth commenting on

It is usually a good idea to normalize your data—make sure each dimension has 0 mean and variance of 1—before feeding it into an SVM or perceptron

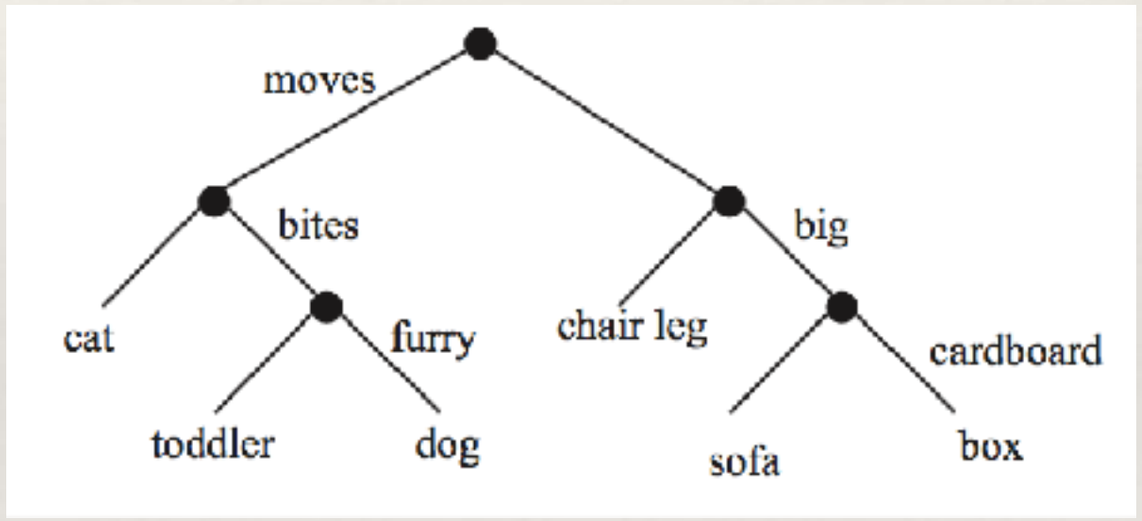
Due to the loss function, a feature with a much larger variance than the others will have a larger effect on the resulting classifier than the other features

Decision trees

Examples



(0, 0)
(2,1)



Decision trees

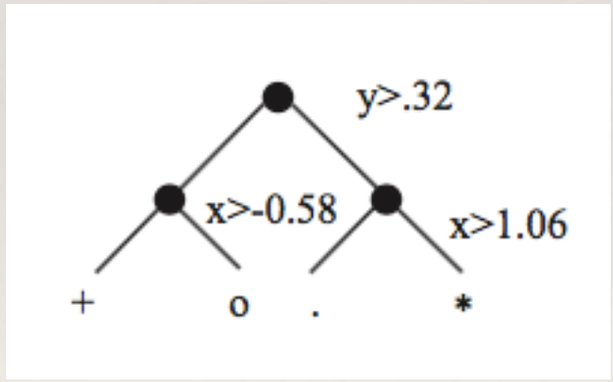
A decision tree is a type of classifier that operates as follows

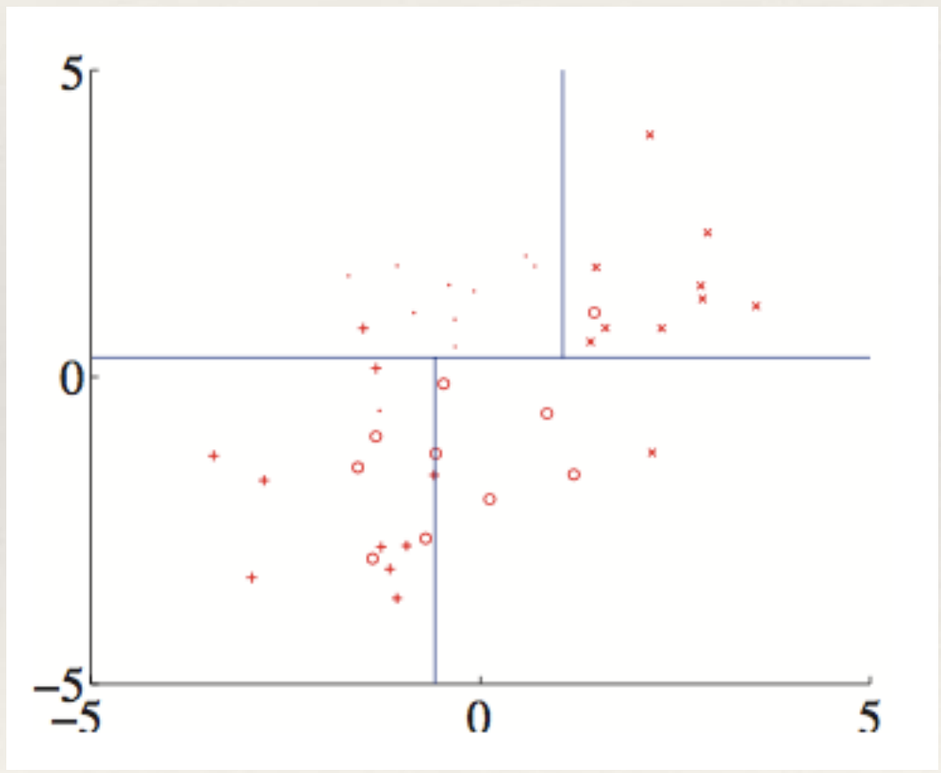
Each internal node of the tree corresponds to a single dimension of the data and a binary **split** for that dimension, i.e. a set of values for the dimension which points to the left child and the remainder of values which point to the right child

To classify a new data item, you start at the root node. Being an internal (non-leaf) node, the root will refer to one of the dimensions of the data item. Depending on the split, the data item will next visit the left or right child

Continue to traverse the tree according to dimensions and splits until reaching a leaf. Each leaf in the tree gives a class label

The decision surface





How to make a decision tree from training data

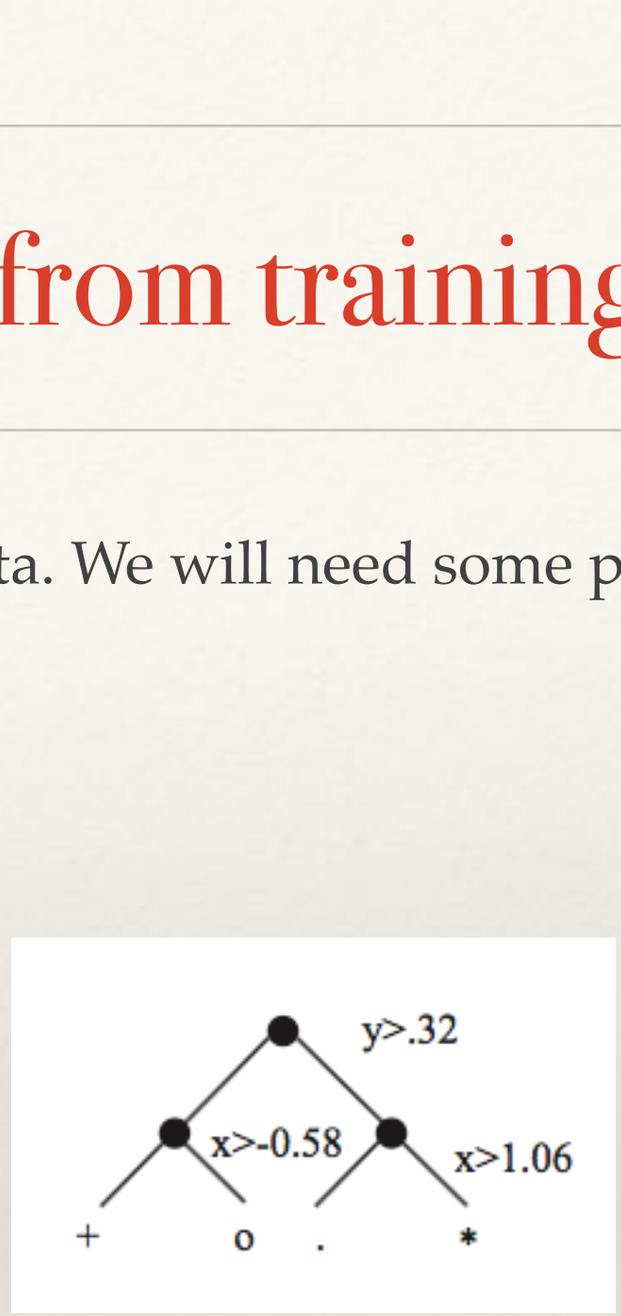
We will recursively build our tree using the training data. We will need some principles in order to

Decide which dimension to split on

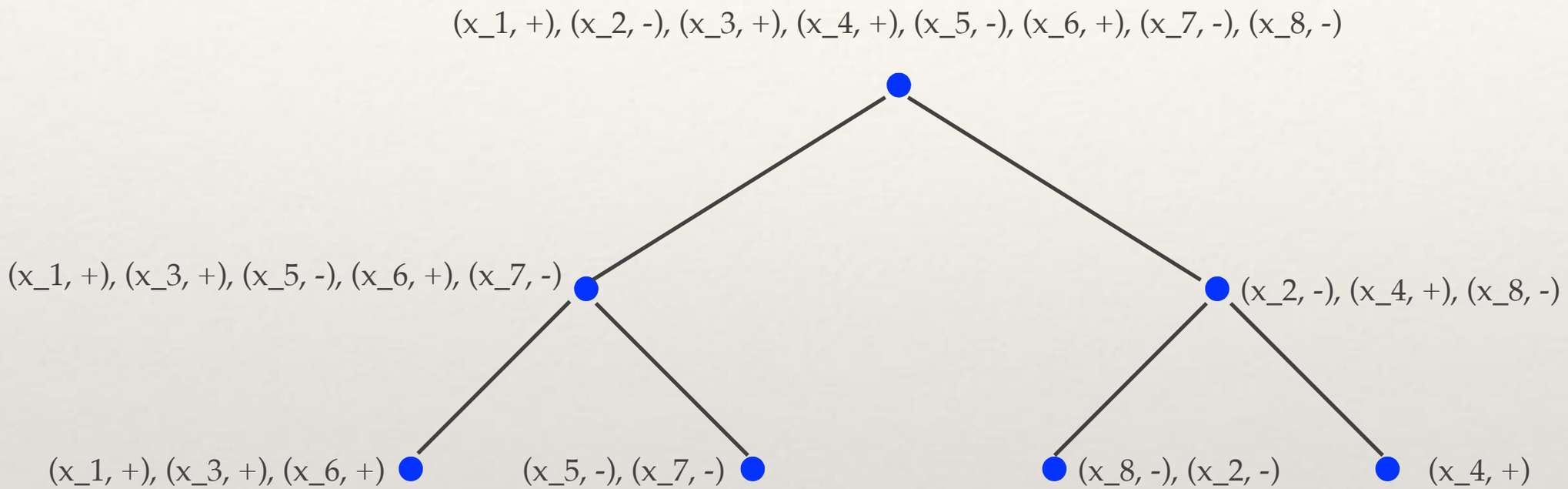
Decide how to split the dimension

Decide how deep to make the tree
or equivalently when to end
recursion

Decide which labels to put on the leaves



Recursively splitting the data



What kind of splits

We want to split the data in some informative way

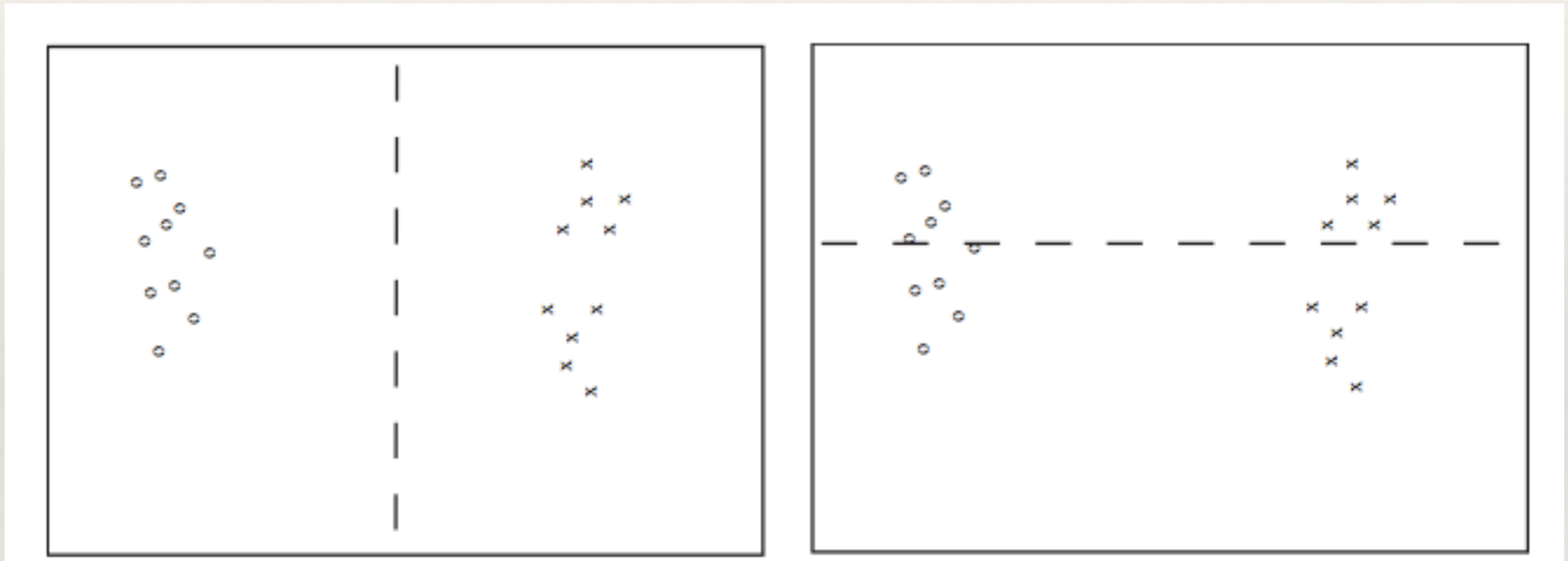
Suppose this was our entire training data set

X1	X2	Class
0	0	-1
0	8.5	-1
0.5	3.25	-1
1.2	-1.5	-1
2.5	5	-1
3.75	1	1
4	1.5	1
4.5	4.5	1
4	3.25	1
5.25	5.5	1

Why is X1>3 a great split? Why is X2 > 3 not as good?

What kind of split

In general we would like it if whatever the "class balance" at the node is (say it starts out 50-50 class 1 and class -1) is more imbalanced in the children



Informative split

Less informative split

Entropy

It turns out that a good way to measure this "class imbalance" feature of a dataset comes to us from communication theory or information theory

Suppose we had four classes: A, B, C, and D

One way to encode those classes, for communication over a network for example, would be A=00, B=01, C=10, D=11. If we did this, it would take on average, indeed in every case, 2 bits to communicate the class label

The idea with entropy is that if we have some class imbalance, say $P(A) = 1/2$, $P(B) = 1/4$, $P(C) = 1/8$, $P(D) = 1/8$, maybe there is a better encoding we can use

Entropy

If we had classes with frequencies given by P(A) = 1/2, P(B) = 1/4, P(C) = 1/8, P(D) = 1/8

Then if we used the following encoding scheme

A	0
B	10
C	110
D	111

The expected number of bits to communicate a class label is given by

$$(1/2)(1) + (1/4)(2) + (1/8)(3) + (1/8)(3)$$

Which is 1.75 bits

Entropy

The **entropy** of a probability distribution or a dataset is the smallest number of bits on average you would need to identify an item sampled from a distribution. It can be thought of as measuring the degree of uncertainty of the distribution. We can use this to evaluate the splits we are considering for our data

This quantity is large when the probability distribution is close to uniform and small when one class is very likely while the others are unlikely. The entropy is denoted with an H and is given by the following formula

$$-\sum_i p(i) \log_2 p(i)$$

Where the $p(i)$ are the probability of class i which in this case is just the relative frequency of the class

Example

Calculate the entropy for this dataset

$$-\sum_i p(i)\log_2 p(i)$$

X1	X2	Class
0	0	-1
0	8.5	-1
0.5	3.25	-1
1.2	-1.5	-1
2.5	5	-1
3.75	1	1
4	1.5	1
4.5	4.5	1
4	3.25	1
5.25	5.5	1

We get

$$-5/10\log(5/10) - 5/10\log(5/10) = 1$$

Split evaluation

Let H(P) be the entropy of all the training data. In order to evaluate a potential split at the root node of the tree, we want to compute the difference between the entropy of the whole dataset and the subsets of the data that would wind up in the left and right children after the split, which we will call H(P_l) and H(P_r) respectively.

The average entropy after the split between the left and right subtrees will be

$$\frac{N(\mathcal{P}_l)}{N(\mathcal{P})}H(\mathcal{P}_l) + \frac{N(\mathcal{P}_r)}{N(\mathcal{P})}H(\mathcal{P}_r)$$

The proportion of the dataset that goes left times the entropy of the left child plus the proportion that goes right times the entropy of the right child

Information gain

This difference between the entropy or average number of bits needed before and after a split is called the **information gain** of the split. We would like to choose the split with the largest information gain

$$I(\mathcal{P}_l, \mathcal{P}_r; \mathcal{P}) = H(\mathcal{P}) - \left(\frac{N(\mathcal{P}_l)}{N(\mathcal{P})} H(\mathcal{P}_l) + \frac{N(\mathcal{P}_r)}{N(\mathcal{P})} H(\mathcal{P}_r) \right)$$

Example

For the training set below, evaluate the information gain of the split x2>1

X1	X2	Class
0	0	-1
0	8.5	-1
0.5	3.25	-1
1.2	-1.5	-1
2.5	5	-1
3.75	1	1
4	1.5	1
4.5	4.5	1
4	3.25	1
5.25	5.5	1

From our prior example we know that the entropy of the whole dataset is $H(P) = 1$

For this split, data items {2, 3, 5, 7, 8, 9, 10} go to the right subtree and items {1, 4, 6} go to the left

Example

Let's say that data items {2, 3, 5, 7, 8, 9, 10} go to the right and items {1, 4, 6} go to the left

X1	X2	Class
0	0	-1
0	8.5	-1
0.5	3.25	-1
1.2	-1.5	-1
2.5	5	-1
3.75	1	1
4	1.5	1
4.5	4.5	1
4	3.25	1
5.25	5.5	1

$$-\sum_i p(i)\log_2 p(i)$$

$$I(\mathcal{P}_l, \mathcal{P}_r; \mathcal{P}) = H(\mathcal{P}) - \left(\frac{N(\mathcal{P}_l)}{N(\mathcal{P})}H(\mathcal{P}_l) + \frac{N(\mathcal{P}_r)}{N(\mathcal{P})}H(\mathcal{P}_r)\right)$$

What is H(P_r)?

$$-3/7 \log(3/7) - 4/7 \log(4/7) = 0.985$$

Example

Let's say that data items {2, 3, 5, 7, 8, 9, 10} go to the right and items {1, 4, 6} go to the left

X1	X2	Class
0	0	-1
0	8.5	-1
0.5	3.25	-1
1.2	-1.5	-1
2.5	5	-1
3.75	1	1
4	1.5	1
4.5	4.5	1
4	3.25	1
5.25	5.5	1

$$-\sum_i p(i) \log_2 p(i)$$

$$I(\mathcal{P}_l, \mathcal{P}_r; \mathcal{P}) = H(\mathcal{P}) - \left(\frac{N(\mathcal{P}_l)}{N(\mathcal{P})} H(\mathcal{P}_l) + \frac{N(\mathcal{P}_r)}{N(\mathcal{P})} H(\mathcal{P}_r)\right)$$

What is H(P_l)?

$$-2/3 \log(2/3) - 1/3 \log(1/3) = 0.918$$

Example

$$I(\mathcal{P}_l, \mathcal{P}_r; \mathcal{P}) = H(\mathcal{P}) - \left(\frac{N(\mathcal{P}_l)}{N(\mathcal{P})} H(\mathcal{P}_l) + \frac{N(\mathcal{P}_r)}{N(\mathcal{P})} H(\mathcal{P}_r) \right)$$

So we had H(P) = 1, H(P_l) = 0.918, H(P_r) = 0.985, N(P_l) = 3, N(P_r) = 7, N(P)=10

Giving an information gain of 0.0351

Choosing a split in practice

In practice the way we will choose **which feature** to split on will be by looking at a random subset of the features. For each node in the tree, we will choose m of the dimensions of the data at random and then evaluate each as a candidate for the split for that node

We will choose m = square root of d

Then for each of our m features we will compute the **best split** for that feature. And we will choose to split on the feature whose best split gives the greatest information gain

Evaluating an ordinal feature

If the feature we are trying to evaluate is continuous or otherwise ordinal we can sort the data according to that feature and consider N-1 potential splits by evaluating the information gain of splitting on the halfway point between each consecutive pair of points, i.e.

$$\frac{x_i + x_{i+1}}{2}$$

For example if our data in a given dimension $x^{(j)}$ was {1, 3, 6, 8} we would evaluate the information gain for $x^{(j)} > 2$, $x^{(j)} > 4.5$, and $x^{(j)} > 7$

Evaluating a categorical feature

As an example suppose we wish to evaluate a categorical variable for splitting and the variable can take on values of {rain, sunny, windy, cloudy, snow}.

However we decide to split this variable, we will have a rule where some subset of the values of that feature will go left and some will go right.

We probably don't want to exhaustively evaluate every possible split for a given categorical variable since there are an exponential number of ways to split the set into two subsets

Evaluating a categorical feature

One trick we can do is look at each valid value for the feature and just flip a coin to say whether data with that value goes left or right. In order to give the feature a good evaluation, we will want to repeat this some number of times and keep the split that gives the best information gain

We would then evaluate the information gain if we did that split and repeat the process a few times in order to find a good split for the categorical variable in question

We would flip coins for each value and, for example, might conclude that data items with {rain, snow} go left and items with {sunny, windy, cloudy} go right

Tree depth

So when do we stop splitting?

If all of the data in a node has the same class label, there is no need to continue splitting. So we could adopt the strategy of continuing to split until each item in the training set is unambiguously classified by the tree.

Alternatively, we can specify a maximum depth for the tree ahead of time. We can use a validation set in order to test out various depths to see which one seems to work best

Prediction

If we do happen to stop creating nodes after a depth threshold we will have a situation in which the leaves of the tree may not be unanimous

If this is the case we will do the obvious thing of outputting the class label that has a majority in the leaf, flipping a coin in the case of ties

Forests

The approach to constructing a tree we have just outlined won't find the "best possible" tree for the data. At each node we have only looked at a random subset of the features. If we looked at every feature we would very often get a decision tree that predicts the training data with higher accuracy

It turns out that decision trees can fit training data really well (even data that's not linearly separable—recall the decision surface). So well in fact that overfitting can become a problem and generalization to unseen test data can suffer

It also turns out that a very effective strategy in both theory and practice is to train a number of slightly different decent classifiers and combine them together to make one really good classifier

Forests

A decision forest is when we train many distinct decision trees on the same training dataset, using randomization to get different trees

To make a prediction with a decision forest, we present the data item to all of the trees and predict the class label that gets the most votes

An alternative and even more effective way to predict is to give each tree not just one vote. In particular, if a tree reaches a leaf with p training data instances that vote for its majority class, then that tree will cast p votes for that class instead of just one

Nearest neighbors

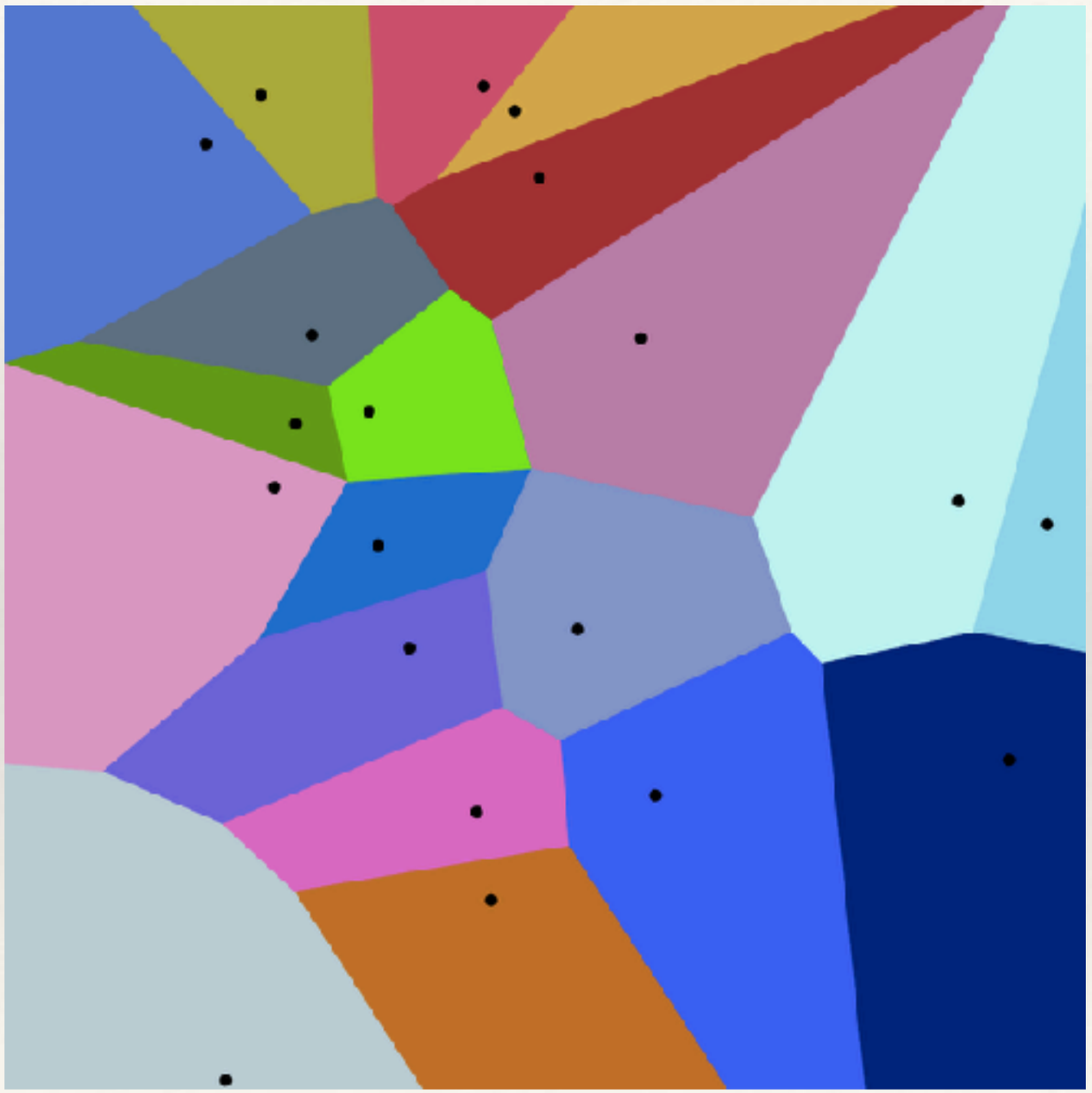
Closeness and labels

We've made the argument a few times so far that if two points are close to one another, we expect them to have the same label much of the time

Of course, we could have two points that are close and on opposite sides of a decision boundary, but we expect that for most pairs of points that are near one another, their labels will be the same

Our prediction function for our next classifier will find the closest point in the training set to the query point and predict the label associated with that item of training data

The decision surface



k-nearest neighbors, etc.

Rather than just use one neighbor for the classification, we might use *k*. This is the most common implementation of nearest neighbors and is called k-nearest neighbors

Furthermore, we might only output a label if at least *l* of these *k* can agree on a common label. This is maybe less common and is called a (*k,l)*-nearest neighbor classifier

Training and other practical issues

"Training" then for this classifier is just any pre-processing we do that makes looking up near neighbors easier

Of course, one of the things we are going to need to make this work at all is a notion of "distance" between points. There are many potential choices we could use depending on the nature of our data and our assumptions about it

If our dimensions have wildly different scales, this might be problematic. We may wish to standardize our data in each dimension prior to inserting it into the search data structure