KD Trees

Cornell CS 4/5780, Spring 2023

Time Complexity of k-NN

Let's look at the time complexity of k-NN.
We are in a d-dimensional space.
To make it easier, let's assume we've already processed some number of inputs, and we want to know the time complexity of adding one more data point.
When training, k-NN simply memorizes the labels of each data point it sees.
This means adding one more data point is $O(d)$.
When testing, we need to compute the distance between our new data point and all of the data points we trained on.
If n is the number of data points we have trained on, then our time complexity for training is $O(dn)$.
Classifying one test input is also $O(dn)$.
To achieve the best accuracy we can, we would like our training data set to be very large ($n \gg 0$), but this will soon become a serious bottleneck during test time.
Goal: Can we make k-NN faster during testing? We can if we use clever data structures.

k-Dimensional Trees

The general idea of KD-trees is to partition the feature space.
We want discard lots of data points immediately because their partition is further away than our k closest neighbors.
We partition the following way:

1. Divide your data into two halves, e.g. left and right, along one feature.
2. For each training input, remember the half it lies in.

How can this partitioning speed up testing?
Let's think about it for the one neighbor case.

1. Identify which side the test point lies in, e.g. the right side.
2. Find the nearest neighbor x^R_{NN} of x_t in the same side. The R denotes that our nearest neighbor is also on the right side.
3. Compute the distance between x_y and the dividing "wall". Denote this as d_w. If $d_w > d(x_t, x^R_{\text{NN}})$ you are done, and we get a 2x speedup.

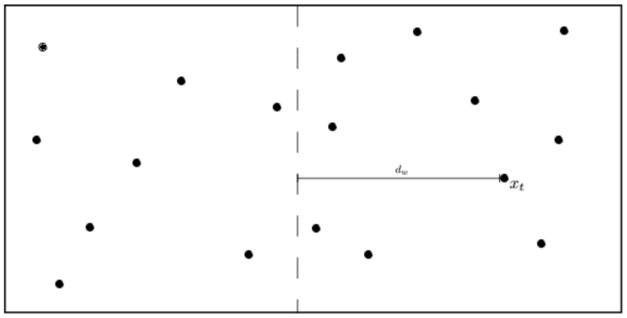


Fig: Partitioning the feature space.

In other words: if the distance to the partition is larger than the distance to our closest neighbor, we know that none of the data points *inside* that partition can be closer.
We can avoid computing the distance to any of the points in that entire partition.
We can prove this formally with the triangular inequality. (See Figure 2 for an illustration.)
Let $d(x_t, x)$ denote the distance between our test point x_t and a candidate x. We know that x lies on the other side of the wall, so this distance is dissected into two parts $d(x_t, x) = d_1 + d_2$, where d_1 is the part of the distance on $x_t's$ side of the wall and d_2 is the part of the distance on $x's$ side of the wall. Also let d_w denote the shortest distance from x_t to the wall. We know that $d_1 > d_w$ and therefore it follows that

$$d(x_t, x) = d_1 + d_2 \geq d_w + d_2 \geq d_w.$$

This implies that if d_w is already larger than the distance to the current best candidate point for the nearest neighbor, we can safely discard x as a candidate.

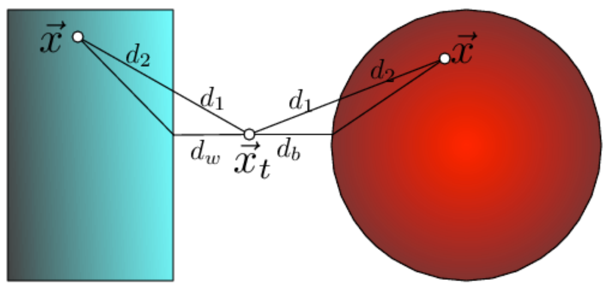


Fig 2: The bounding of the distance between $\vec{x}_t$ and $\vec{x}$ with KD-trees and Ball trees (here $\vec{x}$ is drawn twice, once for each setting). The distance can be dissected into two components $d(\vec{x}_t, \vec{x}) = d_1 + d_2$, where d_1 is the outside ball/box component and d_2 the component inside the ball/box. In both cases d_1 can be lower bounded by the distance to the wall, d_w, or ball, d_b, respectively i.e. $d(\vec{x}_t, \vec{x}) = d_1 + d_2 \geq d_w + d_2 \geq d_w$.

Quiz: Construct a case where this does not work.

KD-tree data structure

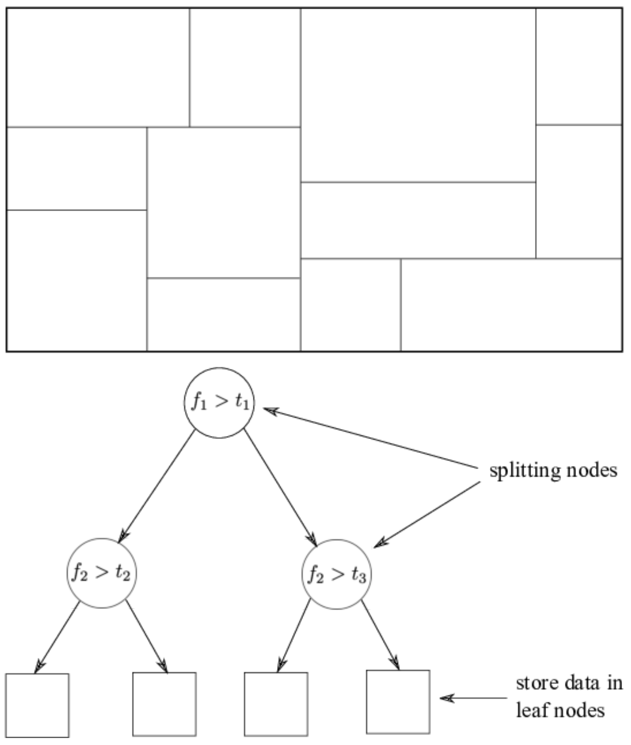


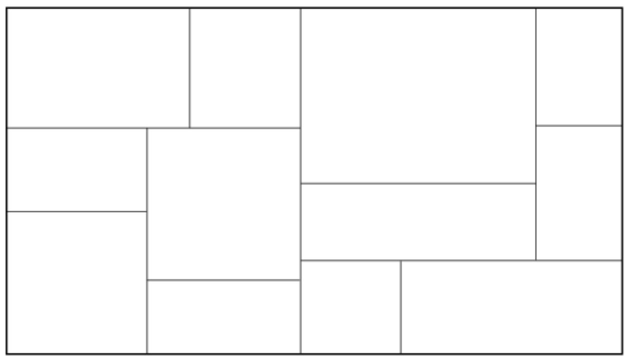
Fig: The partitioned feature space with corresponding KD-tree.

Tree Construction:

1. Split data recursively in half on exactly one feature.
2. Rotate through features.

When rotating through features, a good heuristic is to pick the feature with maximum variance.

Example:



Which partitions can be pruned?
Which must be searched and in what order?
Pros:

- Exact.
- Easy to build.

Cons:

- Curse of Dimensionality makes KD-Trees ineffective for higher number of dimensions.
- All splits are axis aligned.

Approximation: Limit search to m leafs only.

Ball-trees

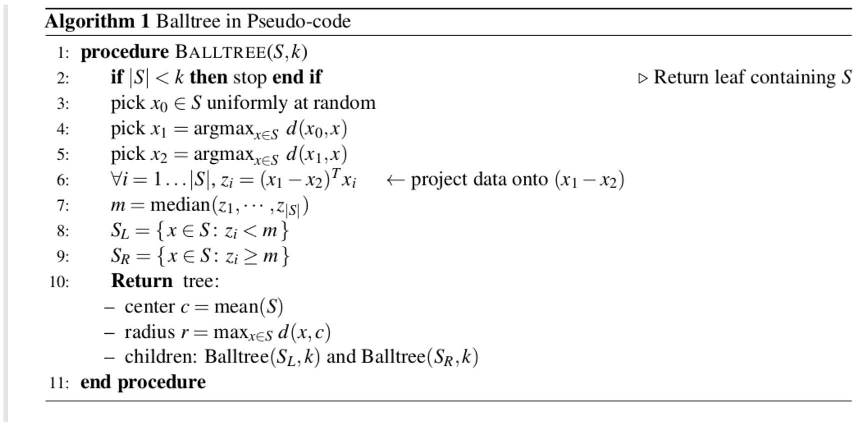
Similar to KD-trees, but instead of boxes use hyper-spheres (balls). (See Figure 2 for an illustration.)
As before we can dissect the distance and use the triangular inequality

$$d(x_t, x) = d_1 + d_2 \geq d_b + d_2 \geq d_b$$

If the distance to the ball, d_b, is larger than distance to the currently closest neighbor, we can safely ignore the ball and all points within.
The ball structure allows us to partition the data along an underlying manifold that our points are on, instead of repeatedly dissecting the entire feature space (as in KD-Trees).

Ball-tree Construction

Input: set S, $n = |S|$, k



Algorithm 1 Balltree in Pseudo-code

```
1:  procedure BALLTREE($S$,$k$)
2:      if $|S| < k$ then stop end if                     ▷ Return leaf containing $S$
3:      pick $x_0 \in S$ uniformly at random
4:      pick $x_1 = \text{argmax}_{x \in S}\ d(x_0, x)$
5:      pick $x_2 = \text{argmax}_{x \in S}\ d(x_1, x)$
6:      $\forall i = 1 \ldots |S|$, $z_i = (x_1 - x_2)^T x_i$    ← project data onto $(x_1 - x_2)$
7:      $m = \text{median}(z_1, \cdots, z_{|S|})$
8:      $S_L = \{x \in S : z_i < m\}$
9:      $S_R = \{x \in S : z_i \geq m\}$
10:     Return tree:
        – center $c = \text{mean}(S)$
        – radius $r = \max_{x \in S} d(x, c)$
        – children: Balltree($S_L$,$k$) and Balltree($S_R$,$k$)
11: end procedure
```

Note: Steps 3 & 4 pick the direction with a large spread ($x_1 - x_2$)

Ball-Tree Use

Same as KD-Trees
Slower than KD-Trees in low dimensions ($d \leq 3$) but a lot faster in high dimensions. Both are affected by the curse of dimensionality, but Ball-trees tend to still work if data exhibits local structure (e.g. lies on a low-dimensional manifold).

Summary

- k-NN is slow during testing because it does a lot of unecessary work.
- KD-trees partition the feature space so we can rule out whole partitions that are further away than our closest k neighbors. However, the splits are axis aligned which does not extend well to higher dimensions.
- Ball-trees partition the manifold the points are on, as opposed to the whole space. This allows it to perform much

better in higher dimensions.

Decision Trees

Cornell CS 4/5780

Spring 2023

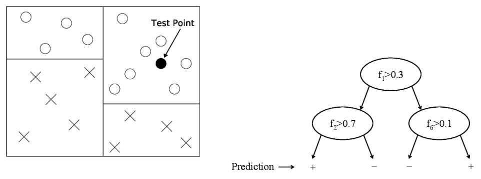
Motivation for Decision Trees

Let us return to the k-nearest neighbor classifier. In low dimensions it is actually quite powerful: It can learn non-linear decision boundaries and naturally can handle multi-class problems. There are however a few catches: kNN uses a lot of storage (as we are required to store the entire training data), the more training data we have the slower it becomes during testing (as we need to compute distances to all training inputs), and finally we need a good distance metric.

Most data that is interesting has some inherent structure. In the k-NN case we make the assumption that similar inputs have similar neighbors. This would imply that data points of various classes are not randomly sprinkled across the space, but instead appear in clusters of more or less homogeneous class assignments. Although there are efficient data structures enable faster nearest neighbor search, it is important to remember that the ultimate goal of the classifier is simply to give an accurate prediction. Imagine a binary classification problem with positive and negative class labels. If you knew that a test point falls into a cluster of 1 million points with all positive label, you would know that its neighbors will be positive even before you compute the distances to each one of these million distances. It is therefore sufficient to simply know that the test point is an area where all neighbors are positive, its exact identity is irrelevant.

Decision trees are exploiting exactly that. Here, we do not store the training data, instead we use the training data to build a tree structure that recursively divides the space into regions with similar labels. The root node of the tree represents the entire data set. This set is then split roughly in half along one dimension by a simple threshold t. All points that have a feature value $\geq t$ fall into the right child node, all the others into the left child node. The threshold t and the dimension are chosen so that the resulting child nodes are purer in terms of class membership. Ideally all positive points fall into one child node and all negative points in the other. If this is the case, the tree is done. If not, the leaf nodes are again split until eventually all leaves are pure (i.e. all its data points contain the same label) or cannot be split any further (in the rare case with two identical points of different labels).

Decision trees have several nice advantages over nearest neighbor algorithms: 1. once the tree is constructed, the training data does not need to be stored. Instead, we can simply store how many points of each label ended up in each leaf - typically these are pure so we just have to store the label of all points; 2. decision trees are very fast during test time, as test inputs simply need to traverse down the tree to a leaf - the prediction is the majority label of the leaf; 3. decision trees require no metric because the splits are based on feature thresholds and not distances.



Binary decision tree. Only labels are stored.

New goal: Build a tree that is:

1. Maximally compact
2. Only has pure leaves

Quiz: Is it always possible to find a consistent tree?
Yes, if and only if no two input vectors have identical features but different labels
Bad News! Finding a **minimum size** tree is NP-Hard!!
Good News: We can approximate it very effectively with a greedy strategy. We keep splitting the data to minimize an impurity function that measures label purity amongst the children.

Impurity Functions

Data: $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}, y_i \in \{1, \ldots, c\}$, where c is the number of classes

Gini impurity

Let $S_k \subseteq S$ where $S_k = \{(\mathbf{x}, y) \in S : y = k\}$ (all inputs with labels k)
$S = S_1 \cup \cdots \cup S_c$
Define:

$$p_k = \frac{|S_k|}{|S|} \leftarrow \text{fraction of inputs in } S \text{ with label } k$$

Note: This is different from Gini coefficient. See Gini impurity (not to be confused with the Gini Coefficient) of a leaf:

$$G(S) = \sum_{k=1}^{c} p_k(1 - p_k)$$

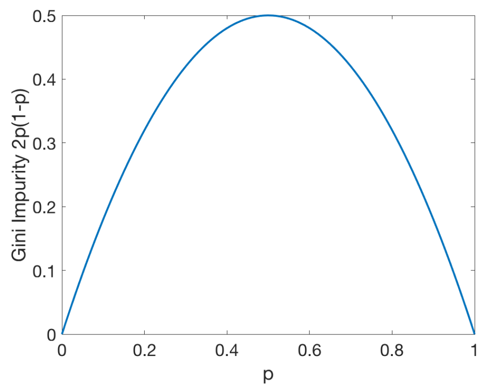


Fig: The Gini Impurity Function in the binary case reaches its maximum at $p = 0.5$.

Gini impurity of a tree:

$$G^T(S) = \frac{|S_L|}{|S|} G^T(S_L) + \frac{|S_R|}{|S|} G^T(S_R)$$

where:

- $(S = S_L \cup S_R)$
- $S_L \cap S_R = \varnothing$
- $\frac{|S_L|}{|S|} \leftarrow$ fraction of inputs in left substree
- $\frac{|S_R|}{|S|} \leftarrow$ fraction of inputs in right substree

Entropy

Let $p_1, \dots, p_k$ be defined as before. We know what we don't want (Uniform Distribution): $p_1 = p_2 = \cdots = p_c = \frac{1}{c}$ This is the worst case since each leaf is equally likely. Prediction is random guessing. Define the impurity as how close we are to uniform. Use KL-Divergence to compute "closeness"
Note: KL-Divergence is not a metric because it is not symmetric, i.e., $KL(p||q) \neq KL(q||p)$.
Let $q_1, \dots, q_c$ be the uniform label/distribution. i.e. $q_k = \frac{1}{c} \forall k$

$$KL(p||q) = \sum_{k=1}^{c} p_k \log\left(\frac{p_k}{q_k}\right) \geq 0 \leftarrow KL\text{-Divergence}$$

$$= \sum_k p_k \log(p_k) - p_k \log(q_k) \text{ where } q_k = \frac{1}{c}$$

$$= \sum_k p_k \log(p_k) + p_k \log(c)$$

$$= \sum_k p_k \log(p_k) + \log(c) \sum_k p_k \text{ where } \log(c) \leftarrow \text{constant}, \sum_k p_k = 1$$

$$\max_p KL(p||q) = \max_p \sum_k p_k \log(p_k)$$

$$= \min_p - \sum_k p_k \log(p_k)$$

$$= \min_p H(s) \leftarrow \text{Entropy}$$

Entropy over tree:

$$H(S) = p^L H(S^L) + p^R H(S^R)$$

$$p^L = \frac{|S^L|}{|S|}, p^R = \frac{|S^R|}{|S|}$$

ID3-Algorithm

Base Cases:

$$\text{ID3}(S): \begin{cases} \text{if } \exists \bar{y} \text{ s.t. } \forall (x,y) \in S, y = \bar{y} \Rightarrow \text{return leaf with label } \bar{y} \\ \text{if } \exists \bar{x} \text{ s.t. } \forall (x,y) \in S, x = \bar{x} \Rightarrow \text{return leaf with mode}(y : (x,y) \in S) \text{ or mean} \end{cases}$$

The Equation above indicates the ID3 algorithm stop under two cases. The first case is that all the data points in a subset of have the same label. If this happens, we should stop splitting the subset and create a leaf with label y. The other case is there are no more attributes could be used to split the subset. Then we create a leaf and label it with the most common y.

Try all features and all possible splits. Pick the split that minimizes impurity ($\text{e.g. } s > t$) where f ←feature and t ←threshold
Recursion:

$$\text{Define: } \begin{bmatrix} S^L = \{(x,y) \in S : x_f \leq t\} \\ S^R = \{(x,y) \in S : x_f > t\} \end{bmatrix}$$

Quiz: Why don't we stop if no split can improve impurity?
Example: **XOR**

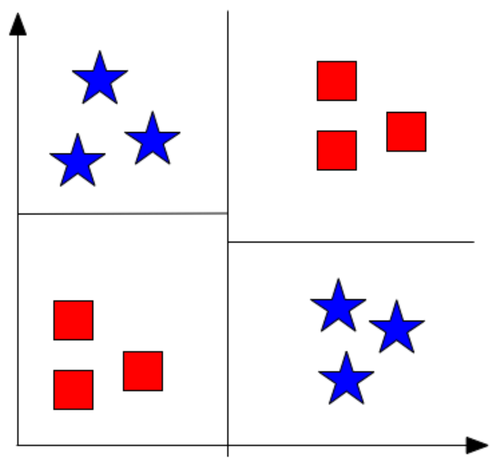


Fig 4: Example XOR

- First split does not improve impurity
- Decision trees are myopic

Regression Trees

CART: Classification and Regression Trees

Assume labels are continuous: $y_i \in \mathbb{R}$
Impurity: Squared Loss

$$L(S) = \frac{1}{|S|} \sum_{(x,y)\in S} (y - \bar{y}_S)^2 \leftarrow \text{Average squared difference from average label}$$

$$\text{where } \bar{y}_S = \frac{1}{|S|} \sum_{(x,y)\in S} y \leftarrow \text{Average label}$$

At leaves, predict $\bar{y}_S$. Finding best split only costs $O(n \log n)$.

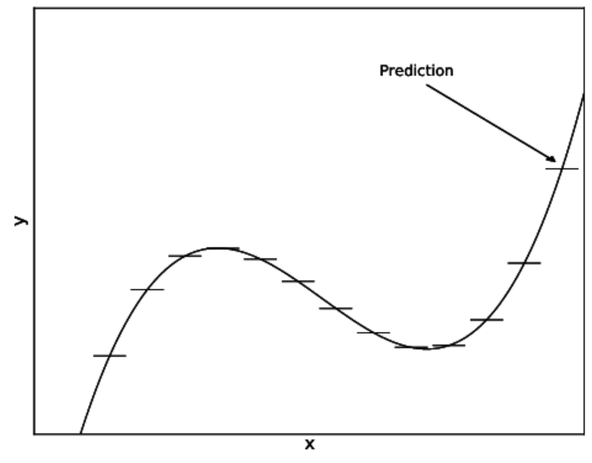


Fig: CART

CART summary:

- CART are very light weight classifiers
- Very fast during testing
- Usually not competitive in accuracy but can become very strong through bagging (Random Forests) and boosting (Gradient Boosted Trees)

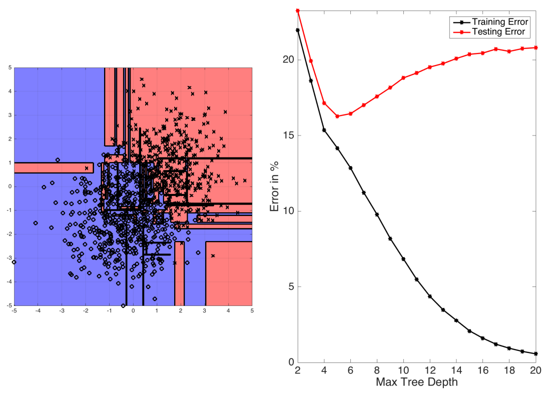


Fig: ID3-trees are prone to overfitting as the tree depth increases. The left plot shows the learned decision boundary of a binary data set drawn from two Gaussian distributions. The right plot shows the testing and training errors with increasing tree depth.

Parametric vs. Non-parametric algorithms

So far we have introduced a variety of algorithms. One can categorize these into different families, such as generative vs. discriminative, or probabilistic vs. non-probabilistic. Here we will introduce another one, *parametric* vs. *non-parametric*.

A *parametric* algorithm is one that has a constant set of parameters, which is independent of the number of training samples. You can think of it as the amount of much space you need to store the trained classifier. An examples for a parametric algorithm is the Perceptron algorithm, or logistic regression. Their parameters consist of $\mathbf{w}, b$, which define the separating hyperplane. The dimension of $\mathbf{w}$ depends of the dimension of the training data, but not on how many training samples you use for training.

In contrast, the number of parameters of a *non-parametric* algorithm scales as a function of the training samples. An example of a non-parametric algorithm is the k-Nearest Neighbors classifier. Here, during "training" we store the entire training data -- so the parameters that we learn are identical to the training set and the number of parameters (/the storage we require) grows linearly with the training set size.

An interesting edge case is kernel-SVM. Here it depends very much which kernel we are using. E.g. linear SVMs are parametric (for the same reason as the Perceptron or logistic regression). So if the kernel is linear the algorithm is clearly parametric. However, if we use an RBF kernel then we cannot represent the classifier of a hyper-plane of finite dimensions. Instead we have to store the support vectors and their corresponding dual variables α_i -- the number of which is a function of the data set size (and complexity). Hence, the kernel-SVM with an RBF kernel is non-parametric. A strange in-between case is the polynomial kernel. It represents a hyper-plane in an extremely high but still finite-dimensional space. So technically one could represent any solution of an SVM with a polynomial kernel as a hyperplane in an extremely high dimensional space with a fixed number of parameters, and the algorithm is therefore (technically) parametric. However, in practice this is not practical. Instead, it is almost always more economical to store the support vectors and their corresponding dual variables (just like with the RBF kernel). It therefore is technically parametric but for all means and purposes behaves like a non-parametric algorithm.

Decision Trees are also an interesting case. If they are trained to full depth they are non-parametric, as the depth of a decision tree scales as a function of the training data (in practice $O(\log_2(n))$). If we however limit the tree depth by a maximum value they become parametric (as an upper bound of the model size is now known prior to observing the training data).