ECE901 Spring 2007 Statistical Learning Theory **Instructor: R. Nowak**

Lecture 11: Decision Trees

1 Minimum Complexity Penalized Function

Recall the basic results of the last lectures: let $\mathcal{X}$ and $\mathcal{Y}$ denote the input and output spaces respectively. Let $X \in \mathcal{X}$ and $Y \in \mathcal{X}$ be random variables with unknown joint probability distribution P_{XY}. We would like to use X to "predict" Y. Consider a loss function $0 \leq \ell(y_1, y_2) \leq 1, \ \forall y_1, y_2 \in \mathcal{Y}$. This function is used to measure the accuracy of our prediction. Let $\mathcal{F}$ be a collection of candidate functions (models), $f : \mathcal{X} \to \mathcal{Y}$. The expected risk we incur is given by $R(f) \equiv E_{XY}[\ell(f(X), Y)]$. We have access only to a number of i.i.d. samples, $\{X_i, Y_i\}_{i=1}^n$. These allow us to compute the empirical risk $\widehat{R}_n(f) \equiv \frac{1}{n}\sum_{i=1}^n \ell(f(X_i), Y_i)$.

Assume in the following that $\mathcal{F}$ is countable. Assign a positive number $c(f)$ to each $f \in \mathcal{F}$ such that $\sum_{f\in\mathcal{F}} 2^{-c(f)} \leq 1$. If we use a prefix code to describe each element of $\mathcal{F}$ and define $c(f)$ to be the codeword length (in bits) for each $f \in \mathcal{F}$, the last inequality is automatically satisfied.

We define the *minimum complexity penalized estimator* as

$$\widehat{f}_n \equiv \arg\min_{f\in\mathcal{F}} \left\{ \widehat{R}_n(f) + \sqrt{\frac{c(f)\log 2 + \frac{1}{2}\log n}{2n}} \right\}.$$

As we showed previously we have the bound

$$E[R(\widehat{f}_n)] \leq \min_{f\in\mathcal{F}} \left\{ R(f) + \sqrt{\frac{c(f)\log 2 + \frac{1}{2}\log n}{2n}} + \frac{1}{\sqrt{n}} \right\}.$$

The performance (risk) of $\widehat{f}_n$ is on average better than

$$R(f_n^*) + \sqrt{\frac{c(f_n^*)\log 2 + \frac{1}{2}\log n}{2n}} + \frac{1}{\sqrt{n}},$$

where

$$f_n^* = \arg\min_{f\in\mathcal{F}} \left\{ R(f) + \sqrt{\frac{c(f)\log 2 + \frac{1}{2}\log n}{2n}} \right\}.$$

If it happens that the optimal function, that is

$$f^* = \arg \min_{f \text{ measurable}} R(f),$$

is close to an $f \in \mathcal{F}$ with a small $c(f)$, then $\widehat{f}_n$ will perform almost as well as the optimal function.

Example 1 *Suppose $f^* \in \mathcal{F}$, then*

$$E[R(\widehat{f}_n)] \leq R(f^*) + \sqrt{\frac{c(f^*)\log 2 + \frac{1}{2}\log n}{2n}} + \frac{1}{\sqrt{n}}.$$

Furthermore if $c(f^*) = O(\log n)$ *then*

$$E[R(\widehat{f}_n)] \leq R(f^*) + O\left(\sqrt{\frac{\log n}{n}}\right),$$

that is, only within a small $O\left(\sqrt{\frac{\log n}{n}}\right)$ *offset of the optimal risk.*

In general, we can also bound the excess risk $E[R(\widehat{f}_n)] - R^*$, where R^* is the Bayes risk,

$$R^* = \inf_{f \text{ measurable}} R(f).$$

By subtracting R^* (a constant) from both sides of the inequality

$$E[R(\widehat{f}_n)] \leq \min_{f \in \mathcal{F}} \left\{ R(f) + \sqrt{\frac{c(f)\log 2 + \frac{1}{2}\log n}{2n}} + \frac{1}{\sqrt{n}} \right\}$$

we obtain

$$E[R(\widehat{f}_n)] - R^* \leq \min_{f \in \mathcal{F}} \left\{ R(f) - R^* + \sqrt{\frac{c(f)\log 2 + \frac{1}{2}\log n}{2n}} + \frac{1}{\sqrt{n}} \right\}.$$

Note that two terms in this upper bound: $R(f) - R^*$ is a bound on the approximation error of a model f, and remainder is a bound on the estimation error associated with f. Thus, we see that complexity regularization automatically optimizes a balance between approximation and estimation errors. In other words, complexity regularization is *adaptive* to the unknown tradeoff between approximation and estimation.

2 Classification

Consider the particularization of the above to a classification scenario. Let $\mathcal{X} = [0,1]^d$, $\mathcal{Y} = \{0,1\}$ and $\ell(\widehat{y}, y) \equiv \mathbf{1}_{\{\widehat{y} \neq y\}}$. Then $R(f) = E_{XY}[\mathbf{1}_{\{f(X) \neq Y\}}] = P(f(X) \neq Y)$. The Bayes risk is given by

$$R^* = \inf_{f \text{ measurable}} R(f).$$

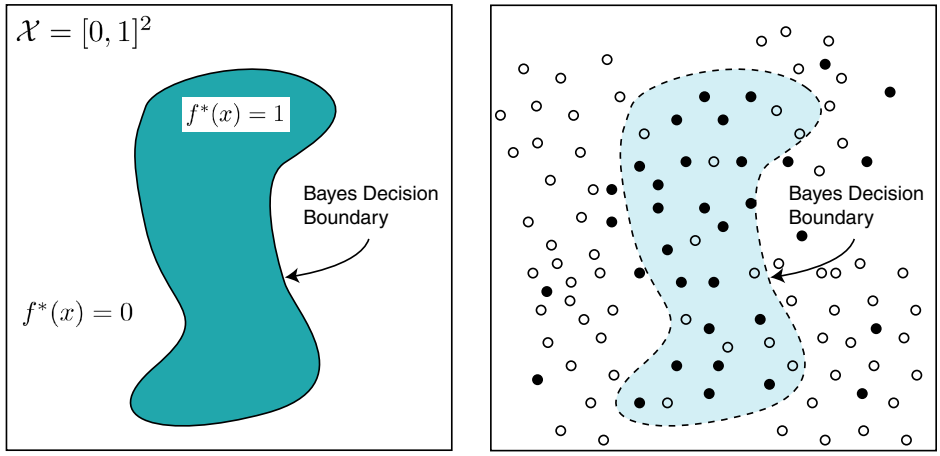
As it was observed before, the Bayes classifier (*i.e.,* a classifier that achieves the Bayes risk) is given by

$$f^*(x) = \begin{cases} 1, & P(Y=1|X=x) \geq \frac{1}{2} \\ 0, & P(Y=1|X=x) < \frac{1}{2} \end{cases}.$$

This classifier can be expressed in a different way. Consider the set $G^* = \{x : \ P(Y=1|X=x) \geq 1/2\}$. The Bayes classifier can written as $f^*(x) = \mathbf{1}_{\{x \in G^*\}}$. Therefore the classifier is characterized entirely by the set G^*, if $X \in G^*$ then the "best" guess is that Y is one, and vice-versa. The boundary of this set corresponds to the points where the decision is harder. The boundary of G^* is called the *Bayes Decision Boundary.* In Figure 1(a) this concept is illustrated. If $\eta(x) = P(Y=1|X=x)$ is a continuous function then the Bayes decision boundary is simply given by $\{x : \ P(Y=1|X=x) = 1/2\}$. Clearly the structure of the decision boundary provides important information on the difficulty of the problem.

2.1 Empirical Classifier Design

Given n i.i.d. training pairs, $\{X_i, Y_i\}_{i=1}^n$, we want to construct a classifier $\widehat{f}_n$ that performs well on average, *i.e.,* we want $E[R(\widehat{f}_n)]$ as close to R^* as possible. In Figure 1(b) an example of the i.i.d. training pairs is depicted.



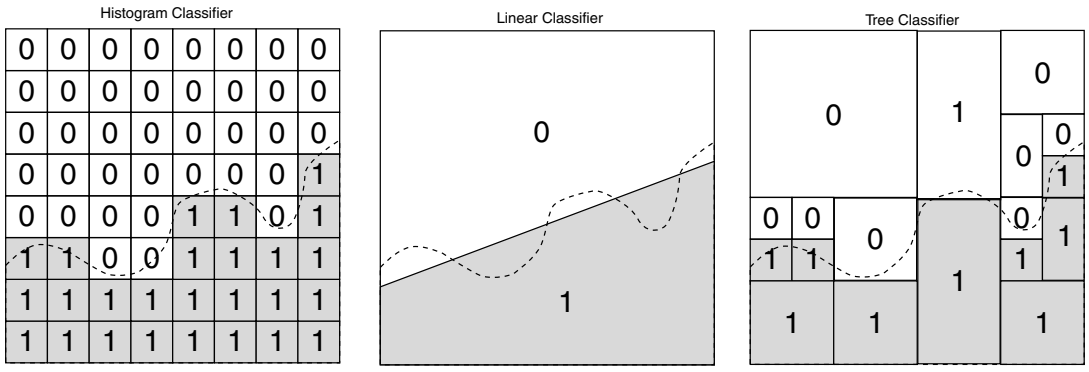
(a) (b)

Figure 1: (a) The Bayes classifier and the Bayes decision boundary ; (b) Example of the i.i.d. training pairs.

The construction of a classifier boils down to the estimation of the Bayes decision boundary. The histogram rule, discussed in a previous lecture, approaches the problem by subdividing the feature space into small boxes and taking a majority vote of the training data in each box. A typical result is depicted in Figure 2(a).

The main problem with the histogram rule is that it is solving a more complicated problem than it is actually necessary. We do not need to determine the correct label for each individual box directly (the histogram rule is essentially estimating $\eta(x)$). In principle we only need to locate the decision boundary and assign the correct label on either side (notice that the accuracy of a majority vote over a region increases with the size of the region). The next example illustrates this.

Example 2 (Three Different Classifiers) *The pictures below correspond to the approximation of the Bayes classifier by three different classifiers:*



(a) (b) (c)

Figure 2: (a) Histogram classifier ; (b) Linear classifier; (c)Decision tree.

The linear classifier and the tree classifier (to be defined formally later) both attack the problem of finding the boundary more directly than the histogram classifier, and therefore they tend to produce much better results in theory and practice. In the following we will demonstrate this for decision trees.

3 Decision Trees

Decision trees are constructed by a two-step process:

1. Tree growing
2. Tree pruning

The basic idea is to first grow a very large, complicated tree classifier, that explains the the training data very accurately, but has poor generalization characteristics, and then prune this tree, to avoid overfitting.

3.1 Growing Trees

The growing process is based on recursively subudividing the feature space. Usually the subdivisions are splits of existing regions into two smaller regions (*i.e.,* binary splits) and usually the splits are perpendicular to one of the feature axes. An example of such construction is depicted in Figure 3.

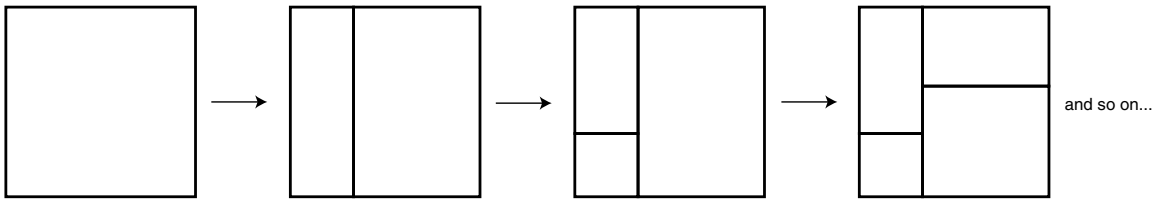


Figure 3: Growing a recursive binary tree ($\mathcal{X} = [0,1]^2$).

Often the splitting process is based on the training dat, and is designed to separate data with different labels as much as possible. It such constructions, the "splits," and hence the tree-structure itself, are data dependent. Alternatively, the splitting and subdivision could be independent from the training data. The latter approach is the one we are going to investigate in detail, and we will consider Dyadic Decision Trees and Recursive Dyadic Partitions (depicted in Figure 4) in particular.

Until now we have been referring to trees, but did not made clear how do trees relate to partitions. It turns out that any decision tree can be associated with a partition of the input space $\mathcal{X}$ and vice-versa. In particular, a Recursive Dyadic Partition (RDP) can be associated with a (binary) tree. In fact, this is the most efficient way of describing a RDP. In Figure 4 we illustrate the procedure. Each leaf of the tree corresponds to an cell of the partition. The nodes in the tree correspond to the various partition cells that are generated through in the construction of the tree. The orientation of the dyadic split alternates between the levels of the tree (for the example of Figure 4, at the root level the split is done in the horizontal axis, at the level below that (the level of nodes 2 and 3) the split is done in the vertical axis, and so on...). The tree is called dyadic because the splits of cells are always at the midpoint along one coordinate axis, and consequently the sidelengths of all cells are dyadic (i.e., powers of 2).

In the following we are going to consider the 2-dimensional case, but all the results can be easily generalized for the d-dimensional case ($d \geq 2$), provided the dyadic tree construction is defined properly. Consider a recursive dyadic partition of the feature space into k boxes of equal size. Associated with this partition is a tree T. Minimizing the empirical risk with respect to this partition produces the histogram classifier with k equal-sized cells. Consider also all the possible partitions corresponding to pruned versions of the tree T. Minimizing the empirical risk with respect to those other partitions results in other classifiers (dyadic decision trees) that are fundamentally different than the histogram rule we analyzed earlier.

3.2 Pruning

Let $\mathcal{F}$ be the collection of all possible dyadic decision trees corresponding to recursive dyadic partitions of the feature space. Each such tree can be prefix encoded with a bit-string proportional to the number of leafs

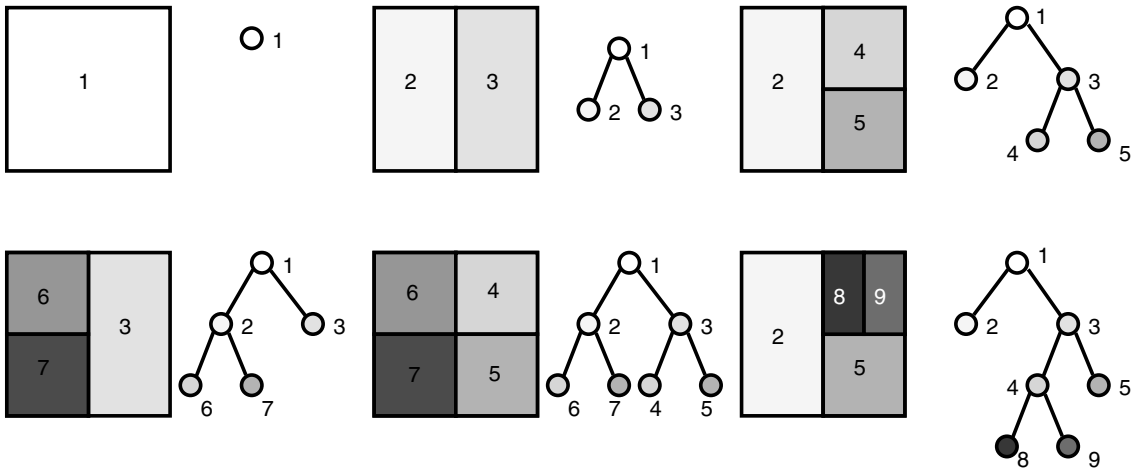


Figure 4: Example of Recursive Dyadic Partition (RDP) growing ($\mathcal{X} = [0,1]^2$).

in the tree as follows; encode the structure of the tree in a top-down fashion: (i) assign a zero at each branch node and a one at each leaf node (terminal node) (ii) read the code in a breadth-first fashion, top-down, left-right. Figure 5 exemplifies this coding strategy. Notice that, since we are considering binary trees, the total number of nodes is twice the number of leafs minus one, that is, if the number of leafs in the tree is k then the number of nodes is $2k-1$. Therefore to encode a tree with k leafs we need $2k-1$ bits.

Since we want to use the partition associated with this tree for classification we need to assign a decision label (either zero or one) to each leaf. Hence, to encode a decision tree in this fashion we need $3k-1$ bits, where k is the number of leafs. For a tree with k leafs the first $2k-1$ bits of the codeword encode the tree structure, and the remaining k bits encode the classification labels. This is easily shown to be a prefix code, therefore we can use this under our classification scenario.

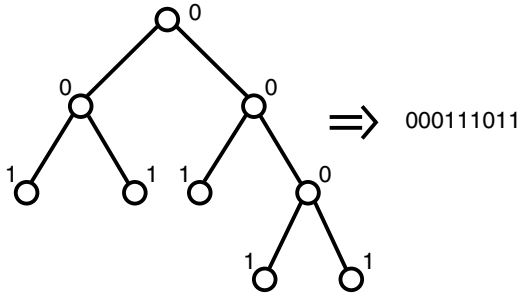


Figure 5: Illustration of the tree coding technique: example of a tree and corresponding prefix code.

Let

$$\widehat{f}_n^* = \arg\min_{f \in \mathcal{F}} \left\{ \widehat{R}_n(f) + \sqrt{\frac{(3k-1)\log 2 + \frac{1}{2}\log n}{2n}} \right\}.$$

This optimization can be solved through a bottom-up pruning process (starting from a very large initial tree T_0) in $O(|T_0|^2)$ operations, where $|T_0|$ is the number of leafs in the initial tree. The complexity regularization theorem tells us that

$$E[R(\widehat{f}_n)] \leq \min_{f \in \mathcal{F}} \left\{ R(f) + \sqrt{\frac{(3k-1)\log 2 + \frac{1}{2}\log n}{2n}} \right\} + \frac{1}{\sqrt{n}}. \tag{1}$$

4 Comparison between Histogram Classifiers and Classification Trees

In the following we will illustrate the idea behind complexity regularization by applying the basic theorem to histogram classifiers and decision trees (using our setup above).

Consider the classification setup described in Section 2, with $\mathcal{X} = [0,1]^2$.

4.1 Histogram Risk Bound

Recall the setup and results of a previous lecture[1]. Let

$$\mathcal{F}_k^H = \{\text{histogram rules with } k^2 \text{ cells}\}.$$

Then $|\mathcal{F}_k^H| = 2^{k^2}$. Let $\mathcal{F}^H = \bigcup_{k\geq 1} \mathcal{F}_k^H$. We can encode each element f of $\mathcal{F}^H$ with $c_H(f) = k + k^2$ bits, where the first k bits indicate the smallest k such that $f \in \mathcal{F}_k^H$ and the following k^2 bits encode the labels of each bin. This is a prefix encoding of all the elements in $\mathcal{F}^H$.

We define our estimator as

$$\widehat{f}_n^H = \widehat{f}_n^{(\widehat{k})},$$

where

$$\widehat{f}_n^{(k)} = \arg\min_{f\in\mathcal{F}_k^H} \widehat{R}_n(f),$$

and

$$\widehat{k} = \arg\min_{k\geq 1} \left\{ \widehat{R}_n(\widehat{f}_n^{(k)}) + \sqrt{\frac{(k+k^2)\log 2 + \frac{1}{2}\log n}{2n}} \right\}.$$

Therefore $\widehat{f}_n^H$ minimizes

$$\widehat{R}_n(f) + \sqrt{\frac{c_H(f)\log 2 + \frac{1}{2}\log n}{2n}},$$

over all $f \in \mathcal{F}^H$. We showed before that

$$E[R(\widehat{f}_n^H)] - R^* \leq \min_{f\in\mathcal{F}^H} \left\{ R(f) - R^* + \sqrt{\frac{c_H(f)\log 2 + \frac{1}{2}\log n}{2n}} \right\} + \frac{1}{\sqrt{n}}.$$

To proceed with our analysis we need to make some assumptions on the intrinsic difficulty of the problem. We will assume that the Bayes decision boundary is a "well-behaved" 1-dimensional set, in the sense that it has box-counting dimension one (see Appendix A). This implies that, for an histogram with k^2 cells, the Bayes decision boundary intersects less than Ck cells, where C is a constant that does not depend on k. Furthermore we assume that the marginal distribution of X satisfies $P_X(A) \leq K|A|$, for any measurable subset $A \subseteq [0,1]^2$. This means that the samples collected do not accumulate anywhere in the unit square.

Under the above assumptions we can conclude that

$$\min_{f\in\mathcal{F}_k^H} R(f) - R^* \;\leq\; \frac{K}{k^2}Ck = \frac{CK}{k}.$$

Therefore

$$E[R(\widehat{f}_n^H)] - R^* \;\leq\; CK/k + \sqrt{\frac{(k+k^2)\log 2 + \frac{1}{2}\log n}{2n}} + \frac{1}{\sqrt{n}}.$$

We can balance the terms in the right side of the above expression using $k = n^{1/4}$ (for n large) therefore

$$E[R(\widehat{f}_n^H)] - R^* \;=\; O(n^{-1/4}), \quad \text{as } n \to \infty.$$

[1]The description here is slightly different than the one in the previous lecture.

4.2 Risk Bounds for Dyadic Decision Trees

Now let's consider the dyadic decision trees, under the assumptions above, and contrast these with the histogram classifier. Let

$$\mathcal{F}_k^T = \{\text{dyadic decision trees with } k \text{ leafs}\}.$$

Let $\mathcal{F}^T = \bigcup_{k\geq 1} \mathcal{F}_k^T$. We can prefix encode each element f of $\mathcal{F}^T$ with $c_T(f) = 3k - 1$ bits, as described before. Let

$$\widehat{f}_n^T = \widehat{f}_n^{(\widehat{k})},$$

where

$$\widehat{f}_n^{(k)} = \arg\min_{f\in\mathcal{F}_k^T} \widehat{R}_n(f),$$

and

$$\widehat{k} = \arg\min_{k\geq 1} \left\{ \widehat{R}_n(\widehat{f}_n^{(k)}) + \sqrt{\frac{(3k-1)\log 2 + \frac{1}{2}\log n}{2n}} \right\}.$$

Hence $\widehat{f}_n^T$ minimizes

$$\widehat{R}_n(f) + \sqrt{\frac{c_T(f)\log 2 + \frac{1}{2}\log n}{2n}},$$

over all $f \in \mathcal{F}^T$. In fact, the optimization

$$\min_{f\in\mathcal{F}^T} \left\{ R_n(f) + \sqrt{\frac{c_T(f)\log 2 + \frac{1}{2}\log n}{2n}} \right\},$$

can be performed using a simple bottom up tree-pruning algorithm in $O(n^2)$ time[2]. Moreover

$$E[R(\widehat{f}_n^T)] - R^* \;\leq\; \min_{f\in\mathcal{F}^T} \left\{ R(f) - R^* + \sqrt{\frac{c_T(f)\log 2 + \frac{1}{2}\log n}{2n}} \right\} + \frac{1}{\sqrt{n}}.$$

If the Bayes decision boundary is a 1-dimensional set, as in Section 4.1, there exists a tree with at most $8Ck$ leafs such that the boundary is contained in at most Ck squares, each of volume $1/k^2$. To see this, start with a tree yielding the histogram partition with k^2 boxes (*i.e.,* the tree partitioning the unit square into k^2 equal sized squares). Now prune all the nodes that do not intersect the boundary. In Figure 6 we illustrate the procedure. If one carefully bounds the number of leafs required at each level, then it can be shown that the total number of leafs is at most $8Ck$. We conclude then that there exists a tree with at most $8Ck$ leafs that has the same risk as a histogram with k^2 cells. Therefore, using equation (1) we have

$$E[R(\widehat{f}_n^T)] - R^* \;\leq\; CK/k + \sqrt{\frac{(3(8Ck)-1)\log 2 + \frac{1}{2}\log n}{2n}} + \frac{1}{\sqrt{n}}.$$

We can balance the terms in the right side of the above expression using $k = n^{1/3}$ (for n large) therefore

$$E[R(\widehat{f}_n^T)] - R^* \;=\; O(n^{-1/3}), \quad \text{as } n \to \infty.$$

[2]C. Scott, "Tree pruning with subadditive penalties," IEEE Transactions on Signal Processing, vol. 53, no. 12, pp. 4518-4525, Dec. 2005.

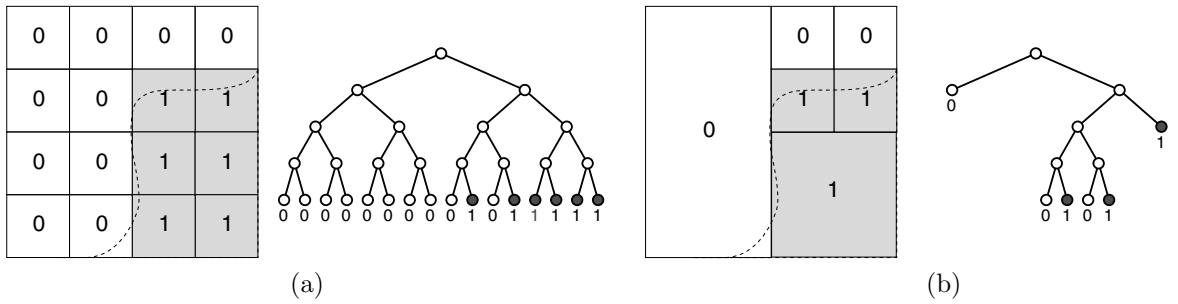


Figure 6: Illustration of the tree pruning procedure: (a) Histogram classification rule, for a partition with 16 cells, and corresponding binary tree representation (with 16 leafs). (b) Pruned version of the histogram tree, yielding exactly the same classification rule, but now requiring only 6 leafs. (*Note:* The trees where constructed using the procedure of Figure 4)

5 Final Comments

Trees generally work much better than histogram classifiers. This is essentially because they provide much more efficient ways of approximating the Bayes decision boundary (as we saw in our example, under reasonable assumptions on the Bayes boundary, a tree encoded with $O(k)$ bits can describe the same classifier as an histogram that requires $O(k^2)$ bits).

The dyadic decision trees studied here are different than classical tree rules, such as `CART` (Breiman et al., 1984) or `C4.5` (Quinlan, 1993). Those techniques select a tree according to

$$\widehat{k} = \arg\min_{k \geq 1} \left\{ \widehat{R}_n(\widehat{f}_n^{(k)}) + \alpha k \right\},$$

for some $\alpha > 0$ whereas in the analysis above the penalty was roughly

$$\widehat{k} = \arg\min_{k \geq 1} \left\{ \widehat{R}_n(\widehat{f}_n^{(k)}) + \alpha \sqrt{k} \right\},$$

for $\alpha \approx \sqrt{\frac{3 \log 2}{2n}}$. The square root penalty is essential for the risk bound. No such bound exists for `CART` or `C4.5`, except under very restrictive assumptions. Moreover, recent experimental work has shown that the square root penalty often performs better in practice. Finally, recent results show that a slightly tighter bounding procedure for the estimation error can be used to show that dyadic decision trees (with a slightly different pruning procedure) achieve a rate of

$$E[R(\widehat{f}_n^T)] - R^* \;=\; O(n^{-1/2}), \quad \text{as } n \to \infty,$$

which turns out to be the minimax optimal rate (i.e., under the boundary assumptions above, no method can achieve a faster rate of convergence to the Bayes error) .

A Box Counting Dimension

The notion of dimension of a sets arises in many aspects of mathematics, and it is particularly relevant to the study of fractals (that besides some important applications make really cool t-shirts). The dimension somehow indicates how we should measure the complexity of a set (length, area, volume, etc...). The box-counting dimension is a simple measure of the dimension of a set. The main idea is to cover the set with boxes with sidelength r. Let $N(r)$ denote the smallest number of such boxes, then the box counting dimension is defined as

$$\lim_{r \to 0} \frac{\log N(r)}{-\log r}.$$

Although the boxes considered above do not need to be aligned on a rectangular grid (and can in fact overlap) we can usually consider them over a grid and obtain an upper bound on the box-counting dimension. To illustrate the main ideas let's consider a simple example, and connect it to the classification scenario considered before.

Let $f : [0,1] \to [0,1]$ be a Lipschitz function, with Lipschitz constant L (*i.e.,* $|f(a) - f(b)| \leq L|a - b|,\ \forall a, b \in [0,1]$). Define the set

$$A = \{x = (x_1, x_2) : x_2 = f(x_1)\},$$

that is, the set A is the graph of function f.

Consider a partition with k^2 squared boxes (just like the ones we used in the histograms), the points in set A intersect at most $C'k$ boxes, with $C' = (1 + \lceil L \rceil)$ (and also the number of intersected boxes is at least k). The sidelength of the boxes is $1/k$ therefore the box-counting dimension of A satisfies

$$\begin{aligned} \dim_B(A) &\leq \lim_{1/k \to 0} \frac{\log C'k}{-\log(1/k)} \\ &= \lim_{k \to \infty} \frac{\log C' + \log(k)}{\log(k)} \\ &= 1. \end{aligned}$$

The result above will hold for any "normal" set $A \subseteq [0,1]^2$ that does not occupy any area. For most sets the box-counting dimension is always going to be an integer, but for some "weird" sets (called fractal sets) it is not an integer. For example, the Koch curve (see for example http://classes.yale.edu/fractals/ IntroToFrac/InitGen/InitGenKoch.html) has box-counting dimension $\log(4)/\log(3) = 1.26186\ldots$. This means that it is not quite as small as a 1-dimensional curve, but not as big as a 2-dimensional set (hence occupies no area).

To connect these concepts to our classification scenario consider a simple example. Let $\eta(x) = P(Y = 1|X = x)$ and assume $\eta(x)$ has the form

$$\eta(x) = \frac{1}{2} + x_2 - f(x_1), \quad \forall x \equiv (x_1, x_2) \in \mathcal{X}, \tag{2}$$

where $f : [0,1] \to [0,1]$ is Lipschitz with Lipschitz constant L. The Bayes classifier is then given by

$$f^*(x) = \mathbf{1}_{\{\eta(x) \geq 1/2\}} \equiv \mathbf{1}_{\{x_2 \geq f(x_1)\}}.$$

This is depicted in Figure 7. Note that this is a special, restricted class of problems. That is, we are considering the subset of all classification problems such that the joint distribution P_{XY} satisfies $P(Y = 1|X = x) = 1/2 + x_2 - f(x_1)$ for some function f that is Lipschitz. The Bayes decision boundary is therefore given by

$$A = \{x = (x_1, x_2) : x_2 = f(x_1)\}.$$

Has we observed before this set has box-counting dimension 1.

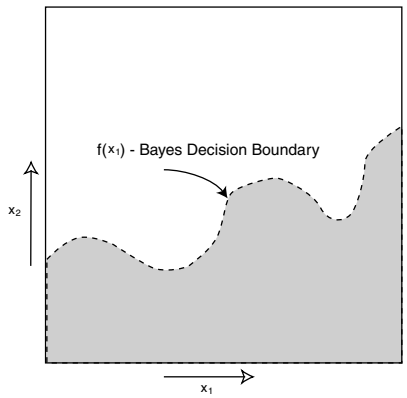


Figure 7: Bayes decision boundary for the setup described in Appendix A.