

Data Mining Criteria for Tree-Based Regression and Classification

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ABSTRACT

This paper is concerned with the construction of regression and classification trees that are more adapted to data mining applications than conventional trees. To this end, we propose new splitting criteria for growing trees. Conventional splitting criteria attempt to perform well on both sides of a split by attempting a compromise in the quality of fit between the left and the right side. By contrast, we adopt a data mining point of view by proposing criteria that search for interesting subsets of the data, as opposed to modeling all of the data equally well. The new criteria do not split based on a compromise between the left and the right bucket; they effectively pick the more interesting bucket and ignore the other.

As expected, the result is often a simpler characterization of interesting subsets of the data. Less expected is that the new criteria often yield whole trees that provide more interpretable data descriptions. Surprisingly, it is a “flaw” that works to their advantage: The new criteria have an increased tendency to accept splits near the boundaries of the predictor ranges. This so-called “end-cut problem” leads to the repeated peeling of small layers of data and results in very unbalanced but highly expressive and interpretable trees.

Keywords

CART, splitting criteria, Boston Housing data, Pima Indians Diabetes data

1. INTRODUCTION

We assume familiarity with the basics of classification and regression trees. A standard reference is Breiman et al. [3], hereafter referred to as CART; a concise introduction can be

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found in Venables and Ripley [10], and a more theoretical one in Ripley [8].

Readers should know that tree construction consists of a greedy growing phase driven by a binary splitting criterion, followed by a pruning phase based on cost-complexity measures and/or estimates of generalization error. The growing phase yields the discoveries, the pruning phase the statistical protection against random structure. With the pruning phase in mind, the growing phase is free to overgrow the tree.

We are here concerned only with the growing phase, and hence with the splitting criteria that drive it. A typical criterion measures the quality of a proposed split in terms of a size-weighted sum of losses or impurities of the left and the right side of the split: $\text{crit}(\text{split}_{L,R}) = w_L \text{loss}_L + w_R \text{loss}_R$. Such weighted sums constitute a compromise between the two sides. By contrast, the new splitting criteria proposed here combine the impurities of the left and right buckets of a split in such a way that low impurity of just one bucket results in a low value of the splitting criterion. These criteria need to be developed for regression and classification trees separately. Section 3 deals with regression, and Section 4 with classification.

This work originated in the course of a marketing study at AT&T in which the first author was involved. Due to the proprietary nature of the original marketing data, we demonstrate our proposals instead on public datasets from the UC Irvine Machine Learning Repository [6]. Because interpretability is the focus of this paper, we present these datasets in greater detail than usual. For the same reason we also include a larger number of tree displays than usual.

2. SIMPLICITY AND INTERPRETABILITY OF TREES

We state the intent and some of the main points of the present work:

- Data mining, in contrast to traditional statistics, is not concerned with modeling all of the data. Data mining involves the search for interesting *parts* of the data. Therefore:
- The goal is *not* to achieve superior performance in terms of global performance measures such as residual sums of squares, misclassification rates, and their out-of-sample versions. (The R^2 values and misclassification rates reported in the examples are only given for general interest.)

- The aspects of trees with which we experimented — simplicity and interpretability — are not easily quantifiable. We leave it as an open problem to find quantifications of these intuitive notions. Note that simplicity is not identical with size of a tree. This is a corollary of the example discussed next:
- The splitting criteria proposed here often generate highly unbalanced trees. Against a perception that more balanced trees are more interpretable, we argue that balance and interpretability are largely independent. In fact, there exists a type of maximally unbalanced tree that is highly interpretable, namely, those with cascading splits on the same variable, as illustrated in Figure 1. The simplicity of these trees stems from the fact that all nodes can be described by one or two clauses, regardless of tree depth. In Figure 1, it is apparent from the mean values in the nodes that the response shows a monotone increasing dependence on the predictor x . In the examples below we will show that tree fragments similar to the one shown in Figure 1 occur quite convincingly in real data.
- The original intent that started the present work was to develop a datamining version of trees that produces in effect simple rules for interesting subsets. In so far, the intent was not much different from that of the rule-induction literature (see for example [4]). We found, however, that our proposals produced not only locally interesting nuggets but globally more interpretable trees than conventional tree-growing methods. Therefore, the present proposals compete with trees more than with rules.

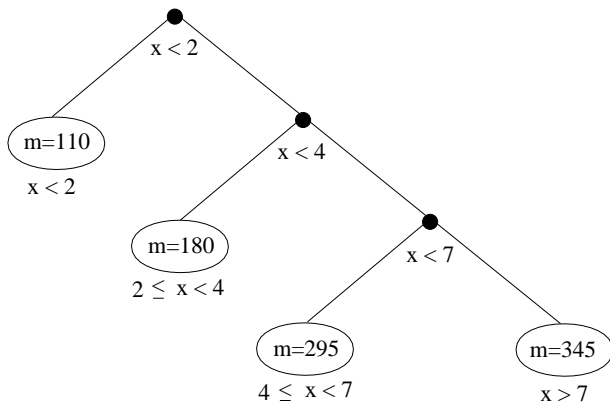


Figure 1: An artificial example of a simple and interpretable yet unbalanced tree

3. REGRESSION TREES

In regression, the impurity measure for buckets is the variance of the response values, and the splitting criterion is a compromise between left and right side bucket in terms of a weighted average of the variances:

$$crit_{LR} = \frac{1}{N_L + N_R} (N_L \hat{\sigma}_L^2 + N_R \hat{\sigma}_R^2) , \quad (1)$$

where we used the following notations for size, mean and variance of buckets:

$$\begin{aligned} N_L &= \#\{n | x_n \leq c\} , & N_R &= \#\{n | x_n > c\} , \\ \hat{\mu}_L &= \frac{1}{N_L} \sum_{n \in L} y_n , & \hat{\mu}_R &= \frac{1}{N_R} \sum_{n \in R} y_n , \\ \hat{\sigma}_L^2 &= \frac{1}{N_L} \sum_{n \in L} (y_n - \hat{\mu}_L)^2 , & \hat{\sigma}_R^2 &= \frac{1}{N_R} \sum_{n \in R} (y_n - \hat{\mu}_R)^2 , \end{aligned}$$

x being the splitting variable and c the splitting value.

The new splitting criteria will do away with the compromise and respond to the presence of just one interesting bucket. “Interesting” could mean high purity in terms of small variance of the response, or it could mean a high or a low mean value of the response. Thus we wish to identify pure buckets ($\hat{\sigma}^2$ small) or extreme buckets ($\hat{\mu}$ extreme) as quickly as possible. This leads us to the following two criteria:

- Criterion R1: *One-sided purity*

In order to find a single pure bucket, we replace the weighted average of left and right variances by their minimum:

$$crit_{LR} = \min(\hat{\sigma}_L^2, \hat{\sigma}_R^2)$$

By minimizing this criterion over all possible splits, we find a split whose left *or* right side is the single bucket with smallest variance (purity). Note that for subsequent splits, both the high-purity bucket *and* the ignored bucket are candidates for further splitting. Thus, ignored buckets get a chance to have further high-purity buckets split off later on. Typically, a high-purity bucket is less likely to be split again.

- Criterion R2: *One-sided extremes*

In order to find one single bucket with a high mean, use the mean as the criterion value and pick the larger of the two:

$$crit_{LR} = \max(\hat{\mu}_L, \hat{\mu}_R)$$

Implicitly one of the bucket with the lower mean is ignored. By maximizing this criterion over all possible splits, we find a split whose left or right side is the single bucket with the highest mean. — An obvious dual for finding buckets with low means is:

$$crit_{LR} = \min(\hat{\mu}_L, \hat{\mu}_R)$$

These criteria are a more radical departure from conventional approaches because they dispense with the notion of purity altogether. The notion of purity seems to have been large unquestioned in the tree literature. Mean values have not been thought of as splitting criteria although they are often of more immediate interest than variances. From the present point of view, minimizing a variance-based criterion is a circuitous route to take when searching for extreme means.

At this point, a natural criticism of the new criteria may arise: their potentially excessive greediness. The suspicion is that they capture spurious groups on the periphery of the variable ranges, thus exacerbating the so-called “end cut problem” (CART, p. 313). not in the conclusion. First, the end cut problem exists but it can be controlled with a minimum bucket size requirement or a penalty for small bucket size. Second, there is an argument that the criteria for one-sided extremes may have a chance of succeeding in

	Regression Trees	Classification Trees
One-sided purity	$\min(\hat{\sigma}_L^2, \hat{\sigma}_R^2)$	$\min(p_L^0 p_L^1, p_R^0 p_R^1)$
One-sided extreme	$\max(\hat{\mu}_L, \hat{\mu}_R)$	$\max(p_L^1, p_R^1)$

Table 1: Synopsis of the new regression and classification criteria.

many situations: in real data the dependence of the mean response on the predictor variables is often monotone; hence extreme response values are often found on the periphery of variable ranges, just the kind of situations to which the criteria for one-sided extremes would respond. Finally, recall that the present goal is not to achieve superior fit but enhanced interpretability.

4. TWO-CLASS CLASSIFICATION TREES

We consider only the two-class situation and leave more than two classes as an open problem. The class labels are denoted 0 and 1. Given a split into left and right buckets, let $p_L^0 + p_L^1 = 1$, $p_R^0 + p_R^1 = 1$ be the probabilities of 0 and 1 on the left and on the right, respectively. Here are some of the conventional measures of loss or impurity, expressed for the left bucket:

- Misclassification rate: $\min(p_L^0, p_L^1)$. Implicitly one assigns the bucket to a class by majority vote and estimates the misclassification rate by the proportion of the other class.
- Entropy: $-p_L^0 \log p_L^0 - p_L^1 \log p_L^1$. This can also be interpreted as the expected value of the minimized negative log-likelihood of the Bernoulli model for $Y \in \{0, 1\}$, $n \in L$.
- The Gini index: $p_L^0 p_L^1$. It can be interpreted as the Mean Squared Error (*MSE*) when fitting the mean, p_L^1 , to the Bernoulli variable $Y \in \{0, 1\}$, $n \in L$: $MSE_L = E_L(Y - p_L^1)^2 = p_L^0 p_L^1$.

These impurity criteria for buckets are conventionally blended into compromise criteria for splits by forming weighted sums of the left and right buckets. Denoting with $p_L + p_R = 1$ the marginal probabilities of the left and the right bucket given the mother bucket, the compromise takes this form:

misclassification rate :

$$p_L \min(p_L^0, p_L^1) + p_R \min(p_R^0, p_R^1)$$

entropy :

$$p_L (-p_L^0 \log p_L^0 - p_L^1 \log p_L^1) + p_R (-p_R^0 \log p_R^0 - p_R^1 \log p_R^1)$$

Gini index :

$$p_L p_L^0 p_L^1 + p_R p_R^0 p_R^1$$

These impurity functions are the smaller the stronger the majority of either label is. Misclassification rate is problematic because it may lead to many indistinguishable splits, some of which may be intuitively more desirable than others. The problem is illustrated, for example, in (CART, p.96). One therefore uses entropy or the Gini index instead, both of which avoid the problem. CART uses the Gini index, while C4.5 Quinlan [7] and *S-Plus* (Statsci [9], or Venables and Ripley [10]) use entropy. For two classes there does not seem to exist a clear difference in performance between entropy and the Gini index. In the multi-class case, however, Breiman [2] has brought to light significant differences.

We now approach two-class classification the same way as regression by attempting to identify pure or extreme buckets as quickly as possible. While the criteria for regression trees are based on variances or means, the criteria for classification trees are only based on the probabilities of class 0 and 1. For one-sided purity, the goal can be restated as finding splits with just one bucket that has a clear majority label. Another approach is to select a class of interest, 1, say, and look for buckets that are very purely class 1. For example, in a medical context, one might want to quickly find buckets that show high rates of mortality, or high rates of treatment effect. As in Section 3, we introduce two criteria for splitting, corresponding to the two approaches:

- Criterion C1: *One-sided purity*

In order to find a single pure bucket, regardless of its class, we replace the weighted average with the minimum:

$$crit_{LR} = \min(p_L^0, p_L^1, p_R^0, p_R^1),$$

which is equivalent to

$$crit_{LR} = \min(p_L^0 p_L^1, p_R^0 p_R^1)$$

because $\min(p_L^0, p_L^1)$ and $p_L^0 p_L^1$ are monotone transformations of each other. The criteria are also equivalent to

$$crit_{LR} = \max(p_L^0, p_L^1, p_R^0, p_R^1)$$

because if one of p_L^0, p_L^1 is maximum, the other is minimum. This latter criterion expresses the idea of pure buckets more directly.

- Criterion C2: *One-sided extremes*

Having chosen class 1, say, as the class of interest, the criterion that searches for a pure class 1 bucket among L and R is

$$crit_{LR} = \min(p_L^0, p_R^0),$$

which is equivalent to the more intuitive form

$$crit_{LR} = \max(p_L^1, p_R^1).$$

Table 3 shows a synopsis of the new criteria for regression and two-class classification.

5. AN EXAMPLE OF REGRESSION TREES: THE BOSTON HOUSING DATA

Following CART, we demonstrate the application of the new splitting criteria on the Boston Housing data. These well-known data were originally created by Harrison and Rubinfeld [5], and they were popularized by Belsley, Kuh and Welsch [1]. Data files are available from the UC Irvine Machine Learning Repository [6].

Harrison and Rubinfeld's main interest in the data was to investigate how air pollution concentration (NOX) affects

the value of single family homes in the suburbs of Boston. Although NOX turned out to be a minor factor if any, the data have been frequently used to demonstrate new regression methods. These data are such well-treaded ground that if anything new is found in them, it should be remarkable. The data contain the median housing values as a response, and 13 predictor variables for 506 census tracts in the Boston area; see Table 2 for details.

We constructed several trees based on both CART and the new criteria. To facilitate comparisons, all trees were generated with equal size, namely, 16 terminal nodes. A minimum bucket size of 23 was chosen, which is about 5% of the overall sample size (506). The resulting trees are displayed in Figures 3 through 6. For each node, the mean response (m) and the size (sz) is given. Here is a summary of the main features of these trees:

1. *CART*, Figure 3
Somewhat balanced tree of depth 6. The major variables are RM (3x, = 3 times) and above all LSTAT (6x). Minor variables appearing once each are NOX, CRIM, B, PTRATIO, DIS, INDUS, with splits mostly in the expected directions. Two of the top splits act on the size of the homes (RM), and below it, especially for areas with smaller homes, an monotone decreasing dependence on the fraction of lower status population (LSTAT) is apparent. Except for the peeling on RM at the top and the subsequent peeling on LSTAT, the tree is not simple.
2. *One-sided purity*, Figure 4
Unbalanced tree of depth 9. The minor variable PTRATIO (1x) is allowed the first split with a small bucket of size 9%; apparently a cluster of school districts has significantly worse pupil-to-teacher ratios than the majority. Crime-infested neighborhoods are peeled off next in a small bucket of size 5% (CRIM, 1x) with extremely low mean. NOX makes surprisingly 3 appearances, which would have made Harrison and Rubinfeld happy. In the third split from the top, NOX breaks off 12% of highly polluted areas with a low bucket mean of 16, as compared to 25 for the rest. LSTAT (3x) creates next a powerful split into buckets of size 41% and 34%, with means of 30 and 19, respectively. RM (2x) plays a role only in “high-status” neighborhoods.
3. *One-sided extremes: high mean*, Figure 5
An extremely unbalanced tree. There are no single powerful splits, only peeling splits with small buckets on one side. The repeated appearance of just two variables, RM (2x, levels 1 and 3) and LSTAT (8x), however, tells a powerful story: For highest housing prices (bucket mean 45), the size of homes ($RM > 7.59$) is the only variable that matters. For $RM < 7.08$, a persistent monotone decreasing dependence on LSTAT takes over, down to a median housing value of about 17. This simple interplay between RM and LSTAT lends striking interpretability to the tree and tells a simple but convincing story. At the bottom, crime (CRIM, 2x) and pollution (NOX, 1x) show some remaining smaller effects in the expected directions.
4. *One-sided extremes: low mean*, Figure 6
Again an extremely unbalanced tree. It tells a similar story as the previous one, but greater precision is

achieved for low housing values, because this is where the criterion looks first. The first peeling split sets aside a 5% bucket of crime-infested neighborhoods with lowest housing values around 10. The second lowest mean bucket ($B < 100$) consists of 5% census tracts with high African-American population ($63\% \pm 32\%$; due to an arcane transformation). Thereafter, monotone decreasing dependence on LSTAT takes over in the form of six peeling splits, followed by monotone increasing dependence on RM in the form of five peeling splits. These two successive monotone dependencies are essentially the same as in the previous tree, which found them in reverse order due to peeling from high to low housing values.

After perusing the last two trees and their crisp stories, it is worthwhile to return to the CART tree of Figure 3 and apply the lessons learnt. We see in retrospect that the CART tree tries to tell the same story of monotone dependence on LSTAT and RM, but because of its favoring of balanced splits, it is incapable of clearly layering the data: The split on LSTAT at the second level divides into buckets of size 51% and 34%, of which only the left bucket further divides on LSTAT. By comparison, the high means criterion creates at level 3 a split on LSTAT with buckets of sizes 9% and 77%, clearly indicating that the left bucket is only the first of a half dozen “tree rings” in ascending order of LSTAT and descending order of housing price.

In summary, it appears that, in spite of the highest R^2 value, the CART tree is considerably harder to interpret compared to the extreme means trees. Even the one-sided purity criterion has certain advantages for “data mining” in that it is better able to find interesting small buckets. Ironically the greater end-cut problem of the new criteria works in their favor. Conversely, CART’s end-cut problem is not sufficiently strong to allow it to clearly detect monotone dependencies and express them in terms of highly unbalanced layering trees.

After a tree-based analysis that resulted in an interpretable tree, it is plausible to re-express the tree in terms of linear models by describing monotone dependencies with linear or additive terms and localizing them with suitable dummy variables. For example, the tree generated with the low means criterion might suggest a linear model of the following form:

$$\begin{aligned}
 MEDVAL = & \beta_{CRIM} * 1_{[CRIM > 15.79]} \\
 & + \beta_B * 1_{[B \leq 100.08]} * 1_{[CRIM \leq 15.79]} \\
 & + \beta_{LSTAT} * LSTAT * 1_{[LSTAT > 10.14]} \\
 & \quad * 1_{[B > 100.08]} * 1_{[CRIM \leq 15.79]} \\
 & + \beta_{RM} * RM * 1_{[LSTAT \leq 10.14]} * 1_{[B > 100.08]} \\
 & \quad * 1_{[CRIM \leq 15.79]} \\
 & + ERROR
 \end{aligned}$$

This type of exercise shows the power of adaptive model building that is implicit in interpretable trees.

6. AN EXAMPLE OF CLASSIFICATION TREES: PIMA INDIANS DIABETES

We demonstrate the application of the new criteria for classification trees with the Pima Indians Diabetes data (Pima data, for short). These data were originally owned

Variable	description
CRIM	crime rate
ZN	proportion of residential land zoned for lots over 25,000 sq. ft
INDUS	proportion of non-retail business acres
CHAS	Charles River dummy variable (=1 if tract bounds river; 0 otherwise)
NOX	nitric oxides concentration, pphm
RM	average number of rooms per dwelling
AGE	proportion of owner-occupied units built prior to 1940
DIS	weighted distances to five Boston employment centers
RAD	index of accessibility to radial highways
TAX	full-value property tax rate per \$10,000
PTRATIO	pupil teacher ratio
B	$1000 * (Bk - 0.63)^2$ where Bk is the proportion of blacks
LSTAT	percent lower status population
response	median value of owner occupied homes in \$1000's

Table 2: Predictor Variables for the Boston Housing Data.

by the “National Institute of Diabetes and Digestive and Kidney Diseases,” but they are now available from the UC Irvine Machine Learning Repository [6].

The class labels of the Pima data are 1 for diabetes and 0 otherwise. There are 8 predictor variables for 768 patients, all females, at least 21 years of age, and of Pima Indian heritage near Phoenix, AZ. Among the 768 patients, 268 tested positive for diabetes (class 1). For details see Table 3 and the documentation at the UC Irvine Repository.

We constructed four trees based on entropy and the new criteria. A minimum bucket size of 35 was imposed, amounting to about 5% of the overall sample size (768). The resulting trees are shown in Figures 7 through 10. For each node, the proportion (p) of each class and the size (sz) are given. Here is a summary of the trees:

1. *Entropy*, Figure 7

Typical balanced tree of depth 6. The strongest variable is PLASMA (5x), which creates a very successful split at the top. BODY (3x) is the next important variable, but much less so, followed by PEDIGREE (3x) and AGE (2x). The class ratios in the terminal buckets range from 1.00:0.00 on the left to 0.16:0.84 on the right. All splits are in the expected direction. Overall, the tree is plausible but does not have a simple interpretation.

2. *One-sided purity*, Figure 8

Extremely unbalanced tree of depth 12. In spite of the depth of the tree, its overall structure is simple: As the tree moves to the right, layers high in class 0 (no diabetes) are being shaved off, and, conversely, as the tree steps left, layers high in class 1 (diabetes) are shaved off (with the exception of the BP split near the bottom). The top of the tree is dominated by BODY and PLASMA, while AGE and PEDIGREE play a role in the lower parts of the tree, where the large rest bucket gets harder and harder to classify.

3. *One-sided extremes: high class 0*, Figure 9

Extremely unbalanced tree with simple structure: Because the criterion searches for layers high in class 0

(no diabetes), the tree keeps stepping to the right. In order to describe conditions under which class 0 is prevalent, it appears that only BODY and PLASMA matter. The tree shows a sequence of interleaved splits on these two variables, indicating a combined monotone dependence on them. See below for an investigation of this behavior. For interpretability, this tree is the most successful one.

4. *One-sided extremes: high class 1*, Figure 10

Another extremely unbalanced tree with simple structure: The criterion searches for layers high in class 1 (diabetes), which causes the tree to step to the left. The top split on PLASMA identifies a 0.86 diabetic bucket of size 9.9%. BODY refines it to 90%. This is the major story because the remaining cascade to the left works off a bucket with a fraction 0.71 non-diabetics, obviously with only mild success.

From the trees and the summary, it becomes clear that PLASMA is the most powerful predictor, followed by BODY. In particular the third tree is almost completely dominated by these two variables. Their interleaved appearance down this tree suggests a combined monotone dependence which should be studied more carefully. Figure 2 shows how the third tree in Figure 9 tries to approximate the class probability surface with a step function on axes-aligned rectangular tiles.

Variable	description
PRGN	number of times pregnant
PLASMA	plasma glucose concentration at two hours in an oral glucose tolerance test
BP	diastolic blood pressure (mm Hg)
THICK	Triceps skin fold thickness (mm)
INSULIN	two hour serum insulin (μ U/ml)
BODY	body mass index (weight in $kg/(height\ in\ m)^2$)
PEDIGREE	diabetes pedigree function
AGE	age (years)
RESPONSE	class variable (=1 if diabetes; 0 otherwise)

Table 3: Predictor Variables for the Pima Indians Diabetes Data.

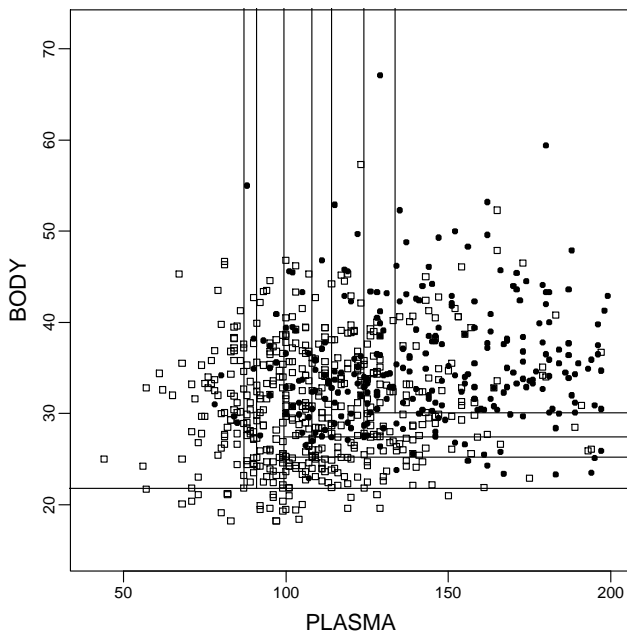


Figure 2: The Pima Diabetes Data, BODY against PLASMA. The plain is tiled according to the buckets of the tree in Figure 9. Open squares: no diabetes (class 0), filled circles: diabetes (class 1).

7. SUMMARY

The following are a few conclusions from our experiments:

- Hyper-greedy data mining criteria can produce highly interpretable trees.
- Highly unbalanced trees can reveal monotone dependence.
- The end-cut “problem” can turn into a virtue.
- If trees are grown for interpretation, global measures for quality of fit are not very informative.

The following are a few topics that merit further research:

- Develop quality measures for interpretability and simplicity of trees.

- Extend the new 2-class criteria to more than two classes.
- Develop more sophisticated methods to control bucket size.

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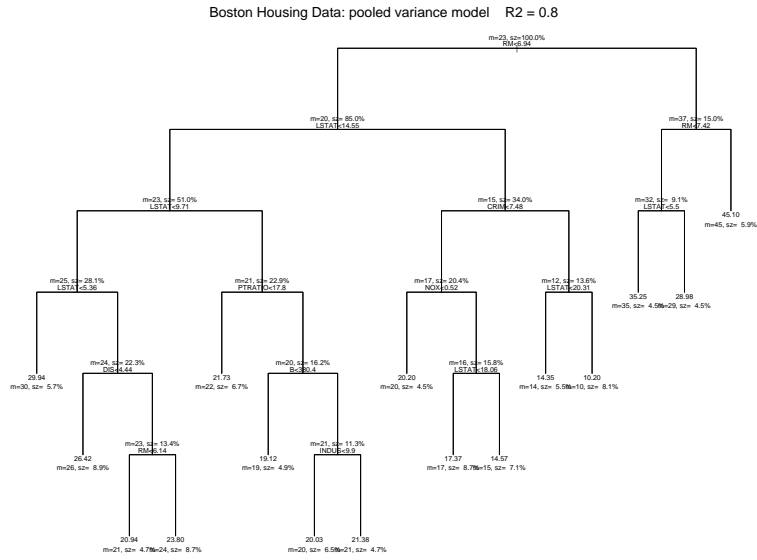


Figure 3: The Boston Housing Data, Regression Tree 1, CART Criterion.

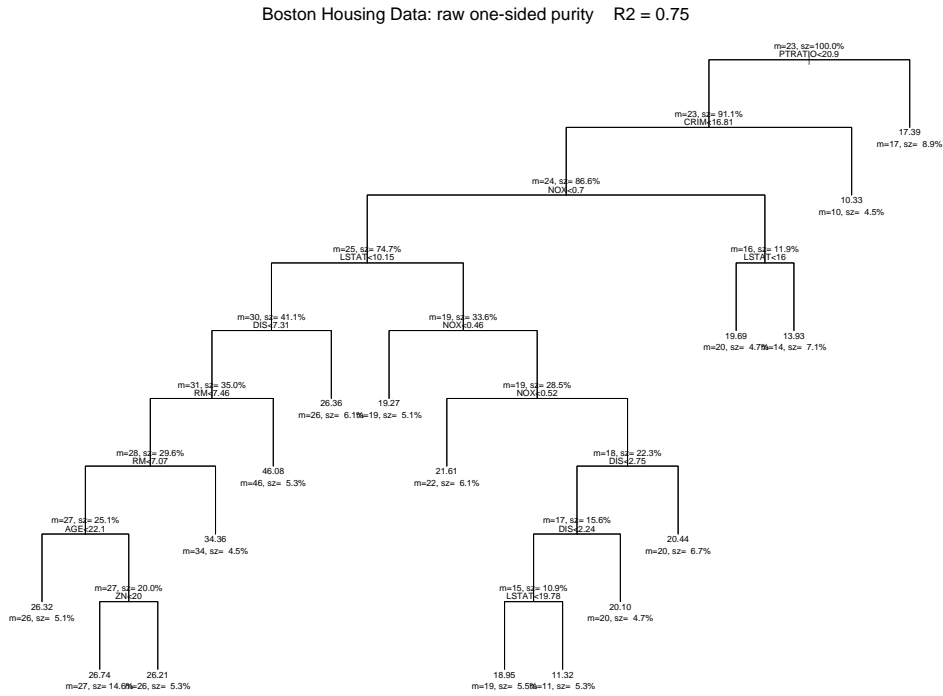
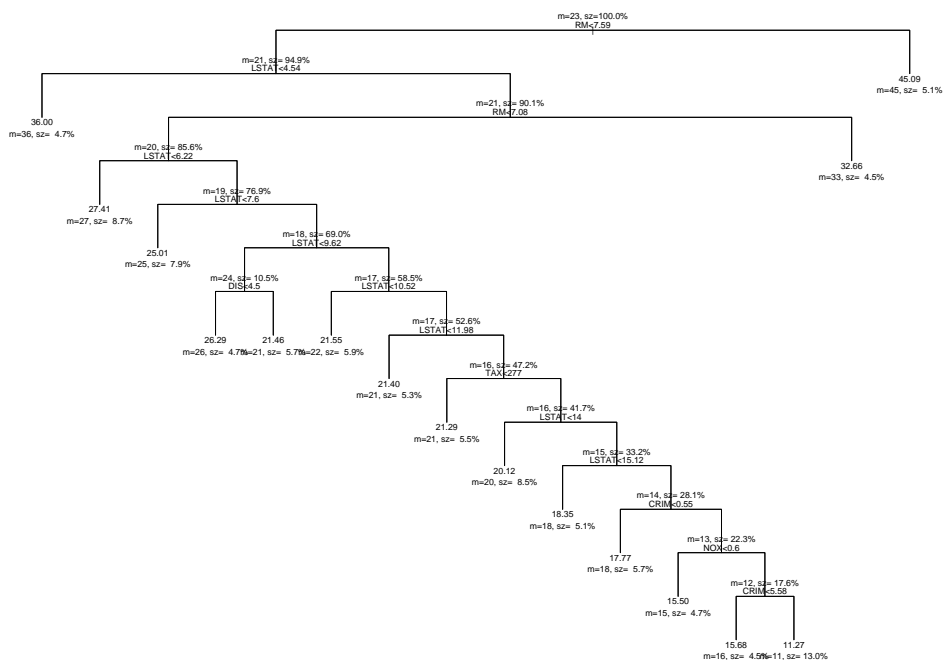


Figure 4: The Boston Housing Data, Regression Tree 2, One-Sided Purity Criterion.

Boston Housing Data: one-sided extremes (high means) $R^2 = 0.78$



Pima Data: entropy misclass. error = 0.21 (162/768)

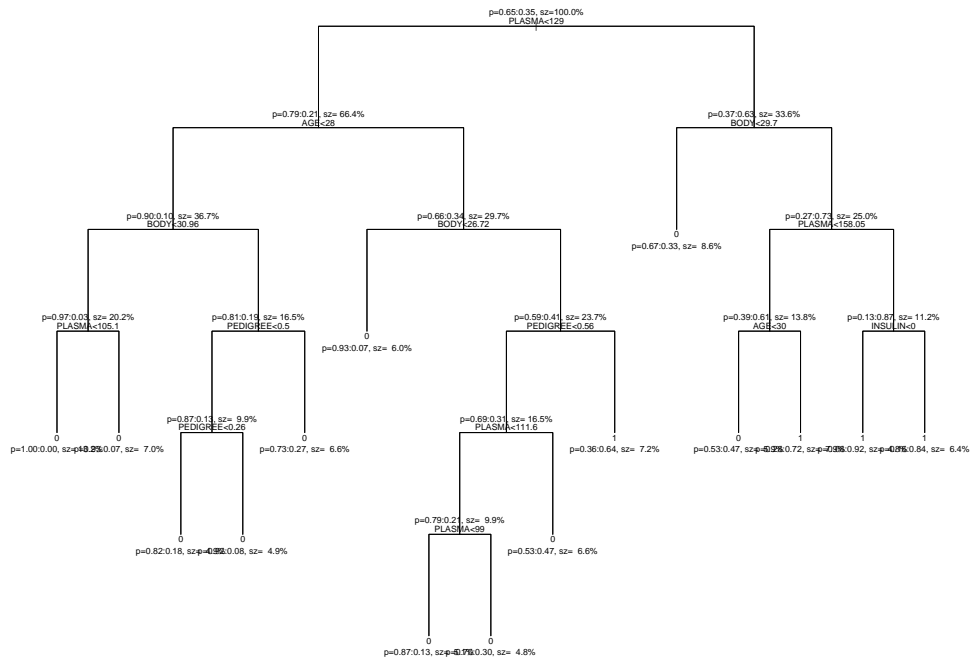


Figure 7: The Pima Indian Diabetes Data, Tree 1, Entropy.

Pima Data: one-sided purity misclass. error = 0.21 (163/768)

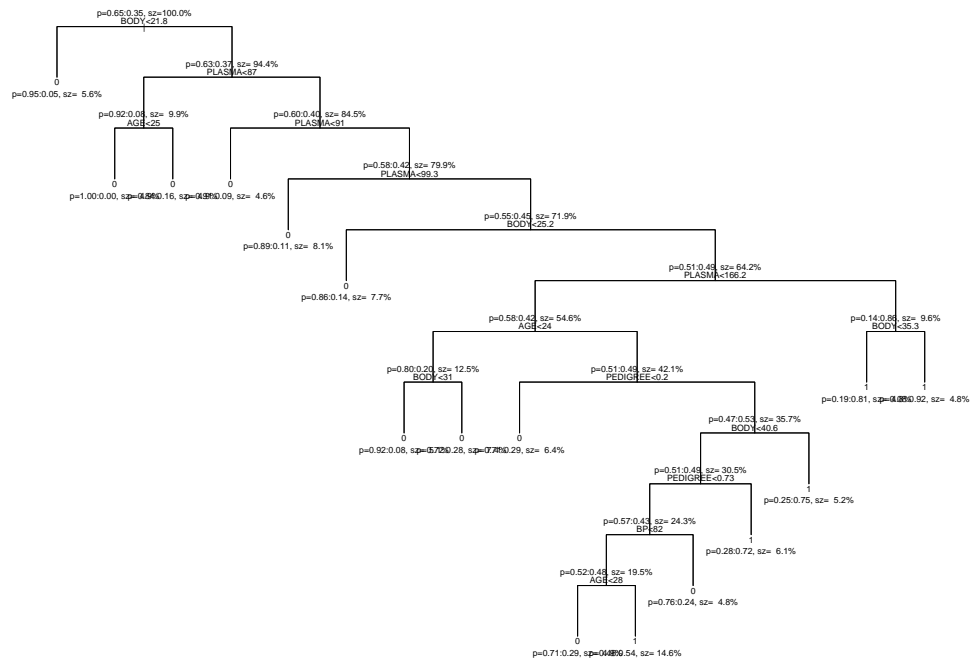


Figure 8: The Pima Indian Diabetes Data, Tree 2, One-Sided Purity.

