Data Mining
Classification Trees (2)

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Basic Tree Construction Algorithm (control flow)

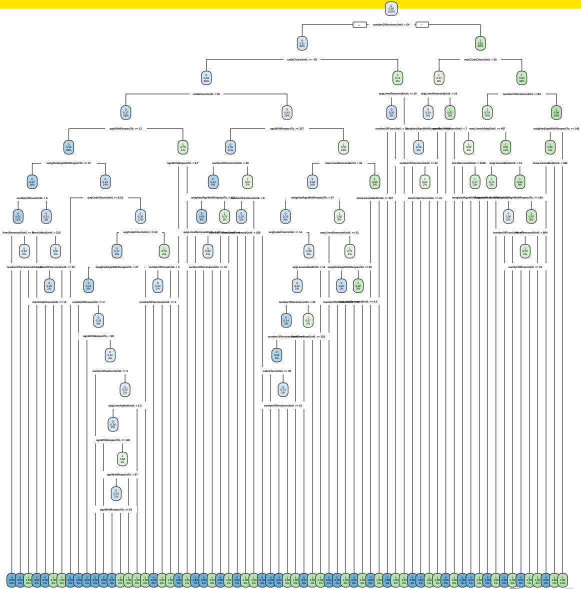
Construct tree

nodelist $\leftarrow$ {{training data}}
Repeat
current node $\leftarrow$ select node from nodelist
nodelist $\leftarrow$ nodelist $-$ current node
if impurity(current node) > 0
then
S $\leftarrow$ set of candidate splits in current node
s* $\leftarrow \arg\max_{s \in S}$ impurity reduction(s,current node)
child nodes $\leftarrow$ apply(s*,current node)
nodelist $\leftarrow$ nodelist $\cup$ child nodes
fi
Until nodelist $= \varnothing$

Overfitting and Pruning

- The tree growing algorithm continues splitting until all leaf nodes contain examples of a single class.
- This results in a tree with zero resubstitution error.
- Is this a good tree for predicting the class of new examples?
- Not unless the problem is truly "deterministic"!
- Problem of *overfitting*.

An Overfitted Tree on Bug Prediction Data



Proposed Solutions

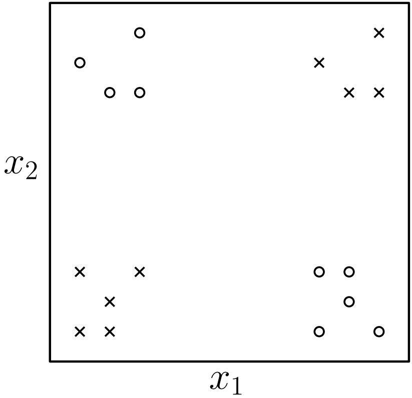
How can we prevent overfitting?

- Stopping rules, e.g. don't expand a node if:
  - the impurity reduction of the best split is below some threshold, or
  - the number of training examples falling into that node is too small.
- Pruning: grow a very large tree and merge back nodes.

Stopping Rules

Disadvantage: sometimes you first have to make a weak split to be able to follow up with a good split.

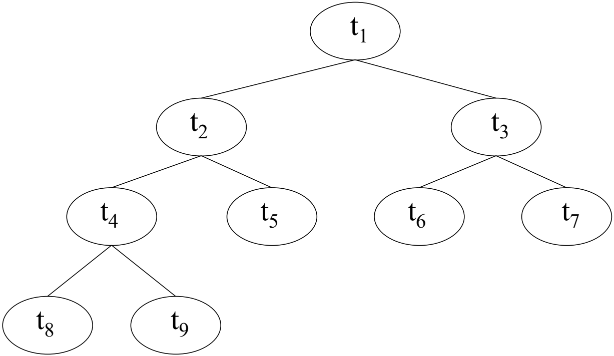
Since we only look one step ahead we may miss the good follow-up split.



Pruning

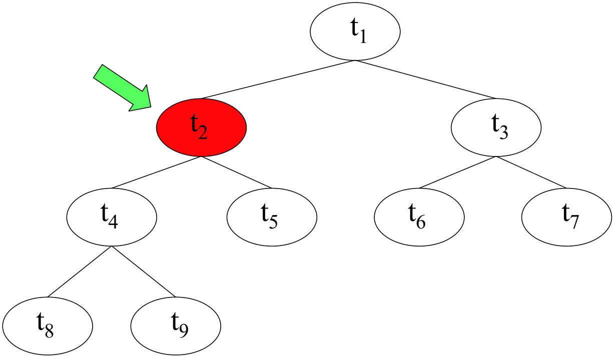
- To avoid the problem of stopping rules, we first grow a very large tree T_{max} on the training sample, and then *prune* this large tree.
- Objective: select the pruned subtree that has lowest *true* error rate.
- Problem: how to find this pruned subtree?
- Cost-complexity pruning (Breiman et al.; CART), also called *weakest link* pruning.

Terminology: Tree T

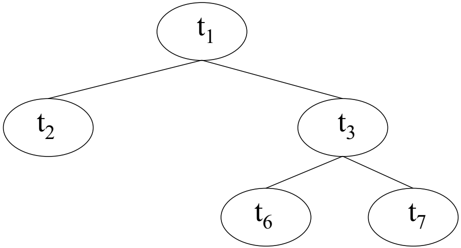


$\tilde{T}$ denotes the collection of leaf nodes of tree T.
$\tilde{T} = \{t_5, t_6, t_7, t_8, t_9\}, |\tilde{T}| = 5$

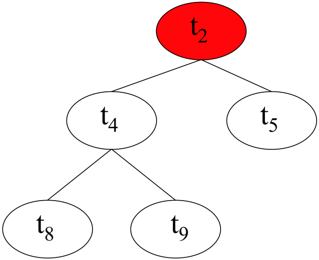
Terminology: Pruning T in node t_2



Terminology: T after pruning in t_2: $T - T_{t_2}$



Terminology: Branch T_{t_2}



$\tilde{T}_{t_2} = \{t_5, t_8, t_9\}, |\tilde{T}_{t_2}| = 3$

Cost-complexity pruning

- A pruned subtree of T is a tree obtained by pruning T in 0 or more nodes.
- The total number of pruned subtrees of a balanced binary tree with ℓ leaf nodes is

$$\lfloor 1.5028369^{\ell} \rfloor$$

- With just 40 leaf nodes we have approximately 12 million pruned subtrees.
- Exhaustive search not recommended.
- Basic idea of cost-complexity pruning: reduce the number of pruned subtrees we have to consider by selecting the ones that are the "best of their kind" (in a sense to be defined shortly...)

Total cost of a tree

Strike a balance between fit and complexity. Total cost $C_\alpha(T)$ of tree T

$$C_\alpha(T) = R(T) + \alpha|\tilde{T}|$$

Total cost consists of two components:

- resubstitution error $R(T)$, and
- a penalty for the complexity of the tree $\alpha|\tilde{T}|, (\alpha \geq 0)$.

Note: $R(T) = \dfrac{\text{number of wrong classifications made by } T}{\text{number of examples in the training sample}}$

Tree with lowest total cost

- Depending on the value of α, different pruned subtrees will have the lowest total cost.
- For $\alpha = 0$ (no complexity penalty) the tree with smallest resubstitution error wins.
- For higher values of α, a less complex tree that makes a few more errors might win.

As it turns out, we can find a nested sequence of pruned subtrees of T_{max}, such that the trees in the sequence minimize total cost for consecutive intervals of α values.

Smallest minimizing subtree

Theorem:

For any value of α, there exists a smallest minimizing subtree $T(\alpha)$ of T_{max} that satisfies the following conditions:

1. $T(\alpha)$ minimizes total cost for that value of α:
   $C_\alpha(T(\alpha)) = \min_{T \leq T_{\text{max}}} C_\alpha(T)$
2. $T(\alpha)$ is a pruned subtree of all trees that minimize total cost:
   if $C_\alpha(T) = C_\alpha(T(\alpha))$ then $T(\alpha) \leq T$.

Note: $T' \leq T$ means T' is a pruned subtree of T.

Sequence of subtrees

Construct a *decreasing sequence* of pruned subtrees of $T_{\max}$

$$T_{\max} > T_1 > T_2 > T_3 > \ldots > \{t_1\}$$

(where t_1 is the root node of the tree) such that T_k is the smallest minimizing subtree for $\alpha \in [\alpha_k, \alpha_{k+1})$.

Note: From a computational viewpoint, the important property is that T_{k+1} is guaranteed to be a pruned subtree of T_k. No backtracking is required.

Decomposition of total cost

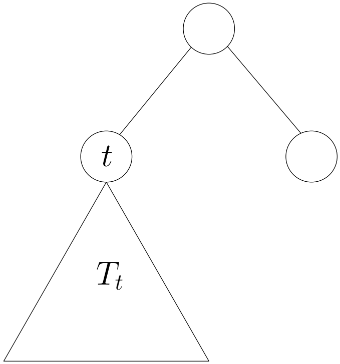
The total cost of a tree is the sum of the contributions of its leaf nodes:

$$C_\alpha(T) = R(T) + \alpha|\tilde{T}| = \sum_{t \in \tilde{T}} (R(t) + \alpha)$$

$R(t)$ is the number of errors we make in node t if we predict the majority class, divided by the total number of observations in the training sample.

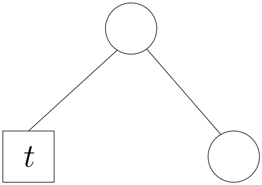
Effect on cost of pruning in node t

Before pruning in t



$C_\alpha(T_t) = \sum_{t' \in \tilde{T}_t} (R(t') + \alpha)$

After pruning in t



$C_\alpha(\{t\}) = R(t) + \alpha$

Finding the T_k and corresponding α_k

T_t: branch of T with root node t.
After pruning in t, its contribution to total cost is:

$$C_\alpha(\{t\}) = R(t) + \alpha,$$

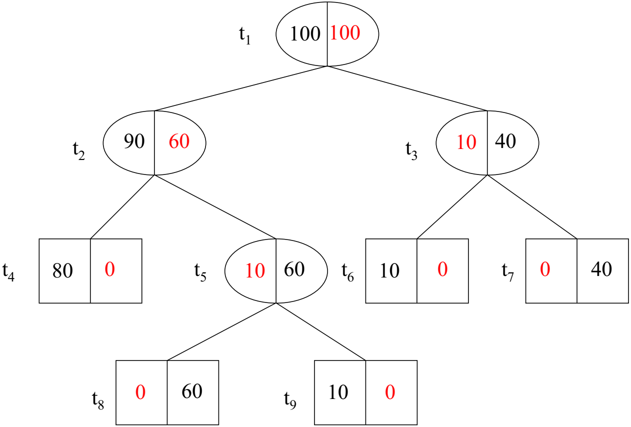
The contribution of T_t to the total cost is:

$$C_\alpha(T_t) = \sum_{t' \in \tilde{T}_t} (R(t') + \alpha) = R(T_t) + \alpha|\tilde{T}_t|$$

The tree obtained by pruning in t becomes better than T when

$$C_\alpha(\{t\}) = C_\alpha(T_t)$$

Computing contributions to total cost of T



$$C_\alpha(\{t_2\}) = R(t_2) + \alpha = \frac{3}{10} + \alpha$$
$$C_\alpha(T_{t_2}) = R(T_{t_2}) + \alpha|\tilde{T}_{t_2}| = \alpha|\tilde{T}_{t_2}| + \sum_{t' \in \tilde{T}_{t_2}} R(t') = 3\alpha + 0$$

Solving for α

The total cost of T and $T - T_t$ become equal when

$$C_\alpha(\{t\}) = C_\alpha(T_t),$$

At what value of α does this happen?

$$R(t) + \alpha = R(T_t) + \alpha|\tilde{T}_t|$$

Solving for α we get

$$\alpha = \frac{R(t) - R(T_t)}{|\tilde{T}_t| - 1}$$

Note: for this value of α total cost of T and $T - T_t$ is the same, but $T - T_t$ is preferred because we want the *smallest* minimizing subtree.

Computing $g(t)$: the "critical" α value for node t

- For each non-terminal node t we compute its "critical" *alpha* value:

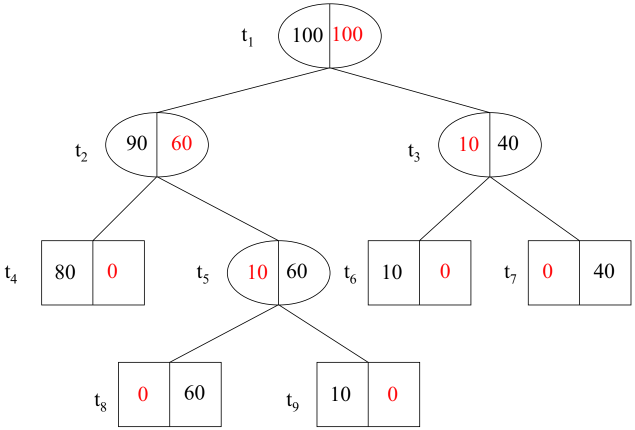
$$g(t) = \frac{R(t) - R(T_t)}{|\tilde{T}_t| - 1}$$

In words:

$$g(t) = \frac{\text{increase in error due to pruning in } t}{\text{decrease in \# leaf nodes due to pruning in } t}$$

- Subsequently, we prune in the nodes for which $g(t)$ is the smallest (the "weakest links").
- This process is repeated until we reach the root node.

Computing $g(t)$: the "critical" α value for node t



$$g(t_1) = \frac{1}{8}, g(t_2) = \frac{3}{20}, g(t_3) = \frac{1}{20}, g(t_5) = \frac{1}{20}.$$

Computing $g(t)$: the "critical" α value for node t

Calculation examples:

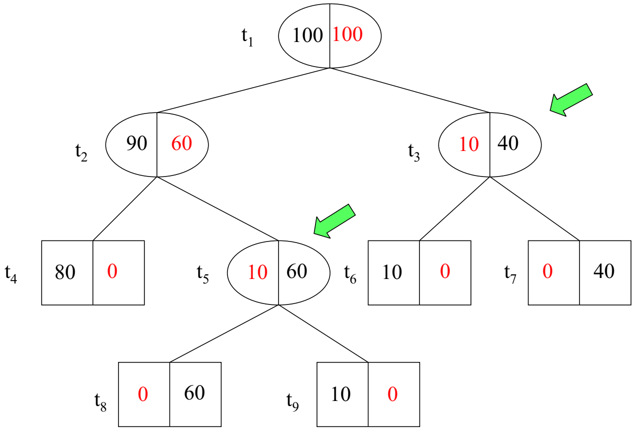
$$g(t_1) = \frac{R(t_1) - R(T_{t_1})}{|\tilde{T}_{t_1}| - 1} = \frac{1/2 - 0}{5 - 1} = \frac{1}{8}$$

$$g(t_2) = \frac{R(t_2) - R(T_{t_2})}{|\tilde{T}_{t_2}| - 1} = \frac{3/10 - 0}{3 - 1} = \frac{3}{20}$$

$$g(t_3) = \frac{R(t_3) - R(T_{t_3})}{|\tilde{T}_{t_3}| - 1} = \frac{1/20 - 0}{2 - 1} = \frac{1}{20}$$

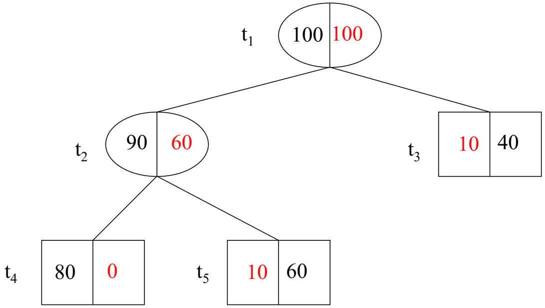
$$g(t_5) = \frac{R(t_5) - R(T_{t_5})}{|\tilde{T}_{t_5}| - 1} = \frac{1/20 - 0}{2 - 1} = \frac{1}{20}$$

Finding the weakest links



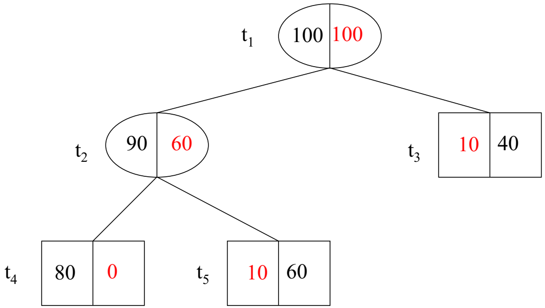
$g(t_1) = \frac{1}{8}, g(t_2) = \frac{3}{20}, g(t_3) = \frac{1}{20}, g(t_5) = \frac{1}{20}.$

Pruning in the weakest links



By pruning the weakest links we obtain the next tree in the sequence.

Repeating the same procedure



$g(t_1) = \frac{2}{10}, g(t_2) = \frac{1}{4}$.

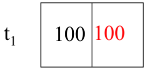
Computing $g(t)$: the "critical" α value for node t

Calculation examples:

$$g(t_1) = \frac{R(t_1) - R(T_{t_1})}{|\tilde{T}_{t_1}| - 1} = \frac{1/2 - 1/10}{3 - 1} = \frac{2}{10}$$

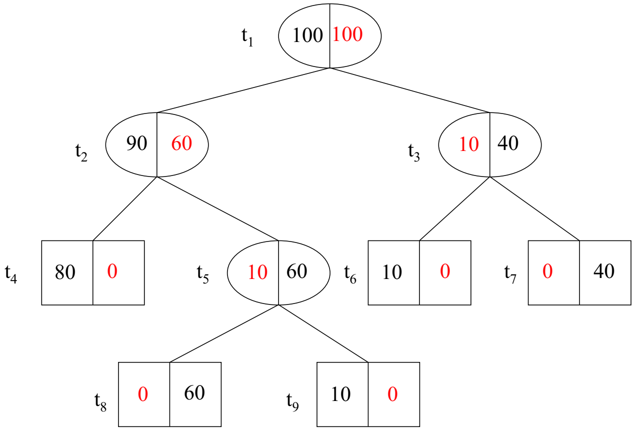
$$g(t_2) = \frac{R(t_2) - R(T_{t_2})}{|\tilde{T}_{t_2}| - 1} = \frac{3/10 - 1/20}{2 - 1} = \frac{1}{4}$$

Going back to the root



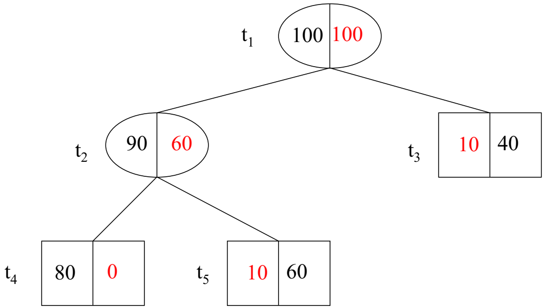
We have arrived at the root so we're done.

The best tree for $\alpha \in [0, \frac{1}{20})$



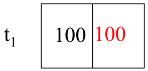
The big tree is the best for values of α below $\frac{1}{20}$.

The best tree for $\alpha \in [\frac{1}{20}, \frac{2}{10})$



When α reaches $\frac{1}{20}$ this tree becomes the best.

The best tree for $\alpha \in [\frac{2}{10}, \infty)$



When α reaches $\frac{2}{10}$ the root wins and we're done.

Computing the Pruning Sequence

$T_1 \leftarrow T(\alpha = 0)$; $\alpha_1 \leftarrow 0$; $k \leftarrow 1$
While $T_k > \{t_1\}$ do
For all non-terminal nodes $t \in T_k$
$g_k(t) \leftarrow \frac{R(t) - R(T_{k,t})}{|\tilde{T}_{k,t}| - 1}$
$\alpha_{k+1} \leftarrow \min_t g_k(t)$
Visit the nodes in post-order and prune
whenever $g_k(t) = \alpha_{k+1}$ to obtain T_{k+1}
$k \leftarrow k + 1$
od

Note: $T_{k,t}$ is the branch of T_k with root node t,
and T_k is the pruned tree in iteration k.

Algorithm to compute T_1 from $T_{\max}$

If we don't continue splitting until all nodes are pure,
then $T_1 = T(\alpha = 0)$ may not be the same as $T_{\max}$.

Compute T_1 from $T_{\max}$

$T' \leftarrow T_{\max}$
Repeat
Pick any pair of terminal nodes ℓ and r
with common parent t in T'
such that $R(t) = R(\ell) + R(r)$, and set
$T' \leftarrow T' - T_t$ (i.e. prune T' in t)
Until no more such pair exists
$T_1 \leftarrow T'$

Selection of the final tree: using a test set

Pick the tree T from the sequence with the lowest error rate $R^{ts}(T)$ on the test set.

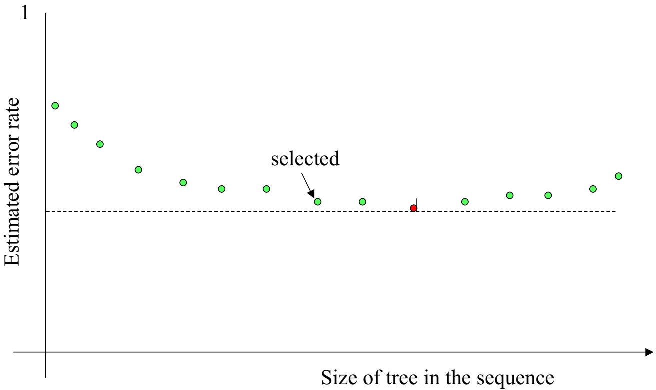
This is an *estimate* of the true error rate $R^*(T)$ of T.

The standard error of this estimate is

$$SE(R^{ts}) = \sqrt{\frac{R^{ts}(1 - R^{ts})}{n_{test}}},$$

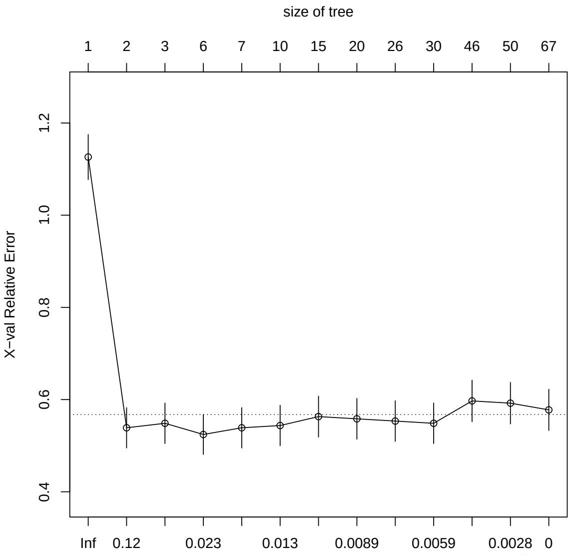
where n_{test} is the number of observations in the test set.

Selection of the final tree: the 1-SE rule

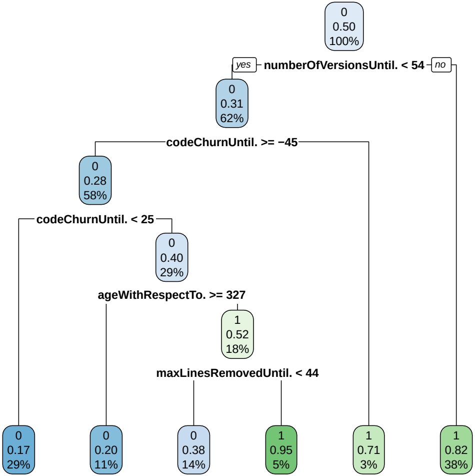


1-SE rule: select the smallest tree with R^{ts} within one standard error of the minimum.

Bug Prediction Tree Pruning Sequence



Bug Prediction Tree after Pruning



Cross-Validation

- When the data set is relatively small, it is a bit of a waste to set aside part of the data for testing.
- A way to avoid this problem is to use *cross-validation*.

Cross-Validation

1. Divide data into v folds.
2. Train on $v - 1$ folds.
3. Predict on the remaining fold.
4. Leave out each of the v folds in turn.

Cross-Validation

First iteration: train on folds 1-4, predict on fold 5

fold	X	Y	$\hat{Y}$
1			
2			
3			
4			
5			$\hat{Y}^{(5)}$

Cross-Validation

Second iteration:

fold	X	Y	$\hat{Y}$
1			
2			
3			
4			$\hat{Y}^{(4)}$
5			

Cross-Validation

Third iteration:

fold	X	Y	$\hat{Y}$
1			
2			
3			$\hat{Y}^{(3)}$
4			
5			

Cross-Validation

Fourth iteration:

fold	X	Y	$\hat{Y}$
1			
2			$\hat{Y}^{(2)}$
3			
4			
5			

Cross-Validation

Fifth iteration:

fold	X	Y	$\hat{Y}$
1			$\hat{Y}^{(1)}$
2			
3			
4			
5			

Cross-Validation

In the end we have out-of-sample predictions for all cases!

fold	X	Y	$\hat{Y}$
1			$\hat{Y}^{(1)}$
2			$\hat{Y}^{(2)}$
3			$\hat{Y}^{(3)}$
4			$\hat{Y}^{(4)}$
5			$\hat{Y}^{(5)}$

1. Perform cross-validation for different hyper-parameter settings (e.g. different values for α).
2. Compute prediction error for each parameter setting.
3. Pick setting with lowest error.
4. Train with selected setting on complete data set.

v-fold cross-validation (general)

Let C be a complexity parameter of a learning algorithm (like α in the classification tree algorithm). To select the best value of C from a range of values $c_1, \ldots, c_m$ we proceed as follows.

1. Divide the data into v groups $G_1, \ldots, G_v$.
2. For each value c_i of C
    1. For each group $j = 1, \ldots, v$
        1. Train with $C = c_i$ on all data *except* group G_j.
        2. Predict on group G_j.
    2. Compute the CV prediction error for $C = c_i$.
3. Select the value c^* of C with the smallest CV prediction error.
4. Train on the complete training sample with $C = c^*$

Selecting the best pruned subtree with cross-validation

Grow a tree on the full data set, and compute $\alpha_1, \alpha_2, \ldots, \alpha_K$ and $T_1 > T_2 > \ldots > T_K$.

Recall that T_k is the smallest minimizing subtree for $\alpha \in [\alpha_k, \alpha_{k+1})$.

Determine the grid of complexity values as follows:

$c_1 = 0$,
$c_2 = \sqrt{\alpha_2 \alpha_3}$,
$c_3 = \sqrt{\alpha_3 \alpha_4}$,
$\ldots$,
$c_{K-1} = \sqrt{\alpha_{K-1} \alpha_K}$,
$c_K = \infty$.

c_k is the "representative" value for T_k.

Selecting the best pruned subtree with cross-validation

Divide the data set into v groups $G_1, G_2, \ldots, G_v$ and for each group G_j

1. Grow a tree on all data *except* G_j, and determine the smallest minimizing subtrees $T^{(j)}(c_1), T^{(j)}(c_2), \ldots, T^{(j)}(c_K)$ for this reduced data set.
2. Compute the error of $T^{(j)}(c_k)$ $(k = 1, \ldots, K)$ on G_j.

From among $c_1, \ldots, c_K$, determine the value c^* that minimizes cross-validation error, and select the tree $T(\alpha = c^*)$ from the original pruning sequence.

Regression Trees

We can also apply tree-based models to problems with numeric targets.

Three elements are necessary to specify a tree growing algorithm:

1. A way to select a split at every non-terminal node.
2. A rule for determining when a node is terminal.
3. A rule for assigning a predicted value $\hat{y}(t)$ to every terminal node t.

Prediction Rule

In leaf nodes, we predict the average target value of all cases falling into that node.

$$\hat{y}(t) = \bar{y}(t) = \frac{1}{N(t)} \sum_{i \in t} y_i,$$

where $N(t)$ is the number of cases falling into node t.

We predict the value of c that minimizes the residual sum of squares (RSS):

$$RSS(t) = \sum_{i \in t} (y_i - c)^2.$$

Exercise: show that $c = \bar{y}(t)$ minimizes RSS.

Splitting Rule

The mean squared error (MSE) of a tree T is given by:

$$R(T) = \frac{1}{N} \sum_{t \in \tilde{T}} \sum_{i \in t} (y_i - \bar{y}(t))^2$$

where N is the size of the learning sample.

The contribution of node t to the MSE of T is

$$R(t) = \frac{1}{N} \sum_{i \in t} (y_i - \bar{y}(t))^2,$$

so we can write

$$R(T) = \sum_{t \in \tilde{T}} R(t).$$

Splitting Rule

The best split s^* of t is that split which most decreases $R(T)$.

The decrease in $R(T)$ of a (binary) split s in node t is given by:

$$\Delta R(s,t) = R(t) - R(\ell) - R(r),$$

where ℓ and r denote the left and right child created by the split respectively.

Stopping and Pruning

Continue until all nodes are pure? Not likely!

Don't split node t if $N(t) < nmin$, where $nmin$ is some small number (e.g. $nmin = 5$).

Pruning is identical to cost-complexity pruning for classification problems, using cost function

$$C_\alpha(T) = R(T) + \alpha|\tilde{T}|.$$

Note that in classification problems $R(T)$ denoted the classification error on the training sample, whereas in regression problems $R(T)$ is the mean squared error on the training sample.

Bug Prediction Data of Eclipse Classes

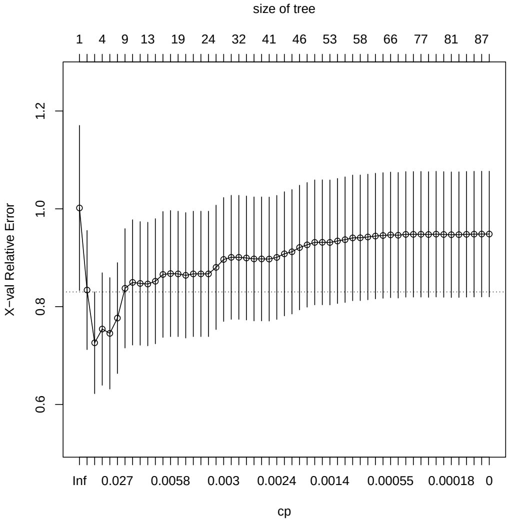
Change metrics:

`numberOfVersionsUntil`	`numberOfFixesUntil`	`numberOfRefactoringsUntil`
`numberOfAuthorsUntil`	`linesAddedUntil`	`maxLinesAddedUntil`
`avgLinesAddedUntil`	`linesRemovedUntil`	`maxLinesRemovedUntil`
`avgLinesRemovedUntil`	`codeChurnUntil`	`maxCodeChurnUntil`
`avgCodeChurnUntil`	`ageWithRespectTo`	`weightedAgeWithRespectTo`

Distribution of number of bugs ($N = 997$):

bugs	0	1	2	3	4	5	6	7	8	9
count	791	138	31	15	8	2	4	3	3	2

Bug Prediction Regression Tree Pruning Sequence



Bug Prediction Pruned Regression Tree

Top: average number of bugs
Bottom: percentage of training examples