Training decision trees

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Training overview

- Training partitions feature space into rectangular hypervolumes of similar X records chosen so the associated y are similar/pure
- Hypervolumes are specified by sequence of *splits* that test a single feature and feature value at a time
- Each split becomes a decision node in decision tree
- Records in an “atomic” hypervolume form a single leaf
- Hypervolume described by conditionals on path from root to leaf
- A specific feature can be tested multiple times in single tree

How to create a decision node

- Given (X, y) for entire training set or a subregion
- Each split chosen greedily to minimize impurity in subregion y's
  - Regressor: variance or MSE
  - Classifier: gini impurity or entropy
- To choose split, exhaustively try each (x_j variable, x_j value) pair and pick the pair with min weighted average impurity for the two subregions created by that split

Fitting decision trees

subsets

MSE or gini function

Optimization: also check if y are all same or very close

```
Algorithm: $dtreefit(X,\ y,\ loss,\ min\_samples\_leaf)$
    if $|X| \leq min\_samples\_leaf$ then return Leaf($y$)
    $col, split = bestsplit(X, y, loss)$
    if $col$ = -1 then return Leaf($y$)    $(No\ better\ split?)$
    $lchild = dtreefit(X[X_{col} \leq split], y[X_{col} \leq split], loss, min\_samples\_leaf)$
    $rchild = dtreefit(X[X_{col} > split], y[X_{col} > split], loss, min\_samples\_leaf)$
    return $DecisionNode(col, split, lchild, rchild)$
```

Overall fit: pass in full (X, y) to dtreefit() and get back the decision tree

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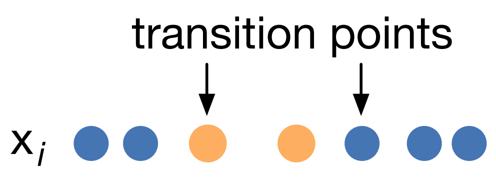
Best split var/value

```
**Algorithm:** $bestsplit(X,\ y,\ loss)$
  $best = (col = -1, split = -1, loss = loss(y))$
  **for** $col$ = $1..p$ **do**
    **foreach** $split \in X_{col}$ **do**
      $yl = y[X_{col} \leq split]$
      $yr = y[X_{col} > split]$
      **if** $|yl| < min\_samples\_leaf$ $or$ $|yr| < min\_samples\_leaf$ **then continue**
      $l = \frac{|yl| \times loss(yl) + |yr| \times loss(yr)}{|y|}$          $(weighted\ average\ of\ subregion\ losses)$
      **if** $l = 0$ **then return** $col,\ split$
      **if** $l < best[loss]$ **then** $best = (col, split, l)$
    **end**
  **end**
  **return** $best[col],\ best[split]$
```

Should pick midpoint between split value and next smallest x

The usual bestsplit() is inefficient

- It has a nested loop; tries all combinations of p variables and worst-case n unique values in each variable at root: $O(np)$
- Cost of computing loss on all values in subregion each iteration is also expensive
- For classification, can mitigate by sorting by *i*th var then we know at a specific x value, everything to left is less and right is greater; keep track of class counts to left/right
- Reduce computation by focusing on transitions points in x, effectively focusing on unique(x)



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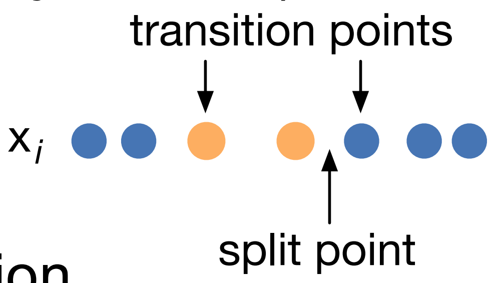
Improving generality and efficiency

- Select a subset of values as candidates, k; then we reduce O(np) to O(kp) for $k << n$ (n is often huge) (our project k=11)
- We should really pick split point between two x values: $(x^{(i)}+x^{(i-1)})/2$ (if sorted)
- More likely split point is between, not on, x values, so midpoint is good guess as to underlying distribution
- And, of course, we can reduce tree height with min_samples_leaf to restrict complexity



Decision tree prediction via x subset

```
Algorithm: bestsplit(X, y, loss)
  $best = (col = -1, split = -1, loss = loss(y))$
  for $col$ = 1..$p$ do
    $candidates$ = randomly pick $k \ll n$ values from $X_{col}$
    foreach $split \in candidates$ do
      $yl = y[X \leq split]$
      $yr = y[X > split]$
      if $|yl| < min\_samples\_leaf$ or $|yr| < min\_samples\_leaf$ then continue
      $l = \frac{|yl| \times loss(yl) + |yr| \times loss(yr)}{|y|}$        (weighted average of subregion losses)
      if $l = 0$ then return $col$, $split$
      if $l < best[loss]$ then $best = (col, split, l)$
    end
  end
  return $best[col]$, $best[split]$
```

Can even pick just 1 split randomly or in min..max range (see "Extremely random trees"); any small k value works.

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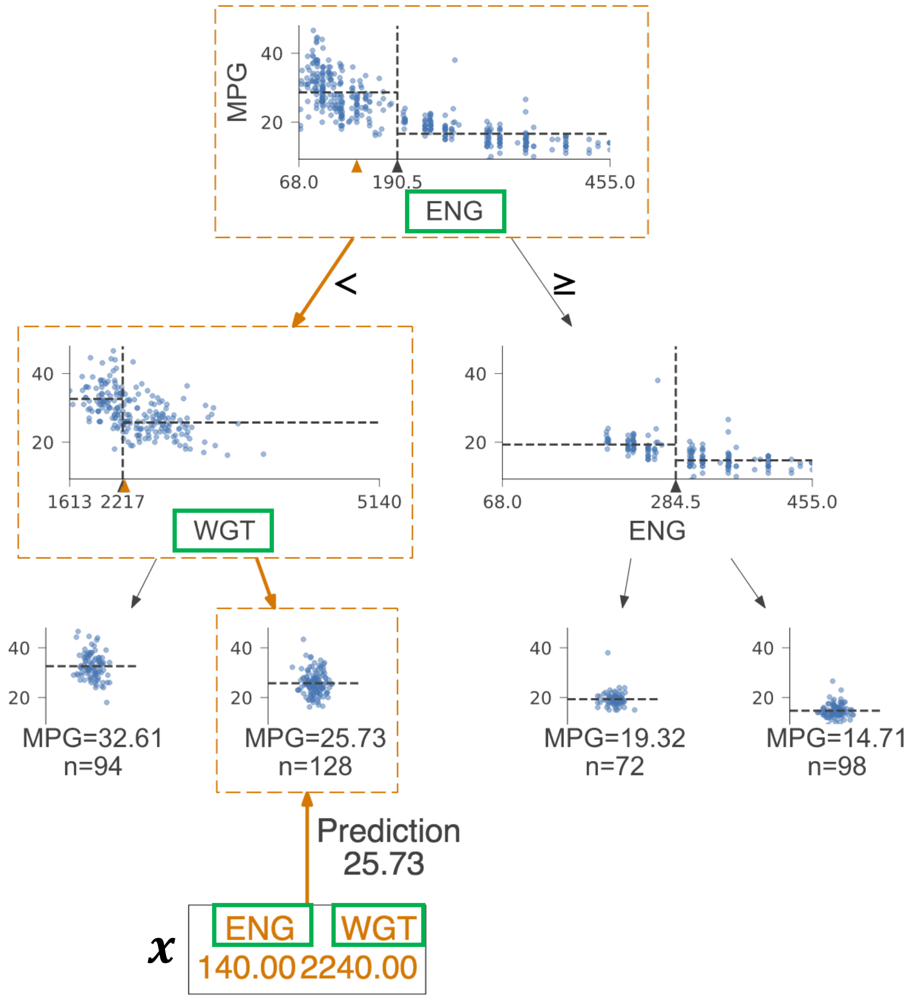
Prediction

- Start at the root node with test $\boldsymbol{x}$ and descend through decision nodes to the appropriate leaf; predict leaf mean or mode
- At each decision node, test indicated variable's x_j value against the split value stored in the decision node



Prediction algorithm

y for samples in leaf

```
1 Algorithm: predict(node,x)
2     if node is leaf then
3         if classifier then return $mode(node.y)$
4         return $mean(node.y)$
5     end
6     if $x[node.col] \leq node.split$ then return predict($node.lchild, x$)
7     return predict($node.rchild, x$)
```

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