Training decision trees

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Training overview

- Training <u>partitions feature space</u> into rectangular hypervolumes chasing reduced y impurity in subregions
- Hypervolumes are specified by <u>sequence</u> of splits that test a single feature and 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

How to create a decision node

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

Fitting decision trees

subsets

```
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)
```

MSE or gini

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



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
                                                                 Should pick midpoint between
       if l < best[loss] then best = (col, split, l)
                                                                 split value and next smallest x
     end
  end
  return best/col/, best/split/
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```

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 $x_i = x_i$ counts to left/right
- Reduce computation by focusing on transitions points in x, effectively focusing on unique(x)

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



transition points

split point

Decision tree prediction via x subset

```
Algorithm: bestsplit(X, y, loss)
  best = (col = -1, split = -1, loss = loss(y))
  for col = 1..p do
                                                                                    Can even pick just 1 split
     candidates = \text{randomly pick } k \ll n \text{ values from } X_{col} \blacktriangleleft
                                                                                    randomly or in min..max
                                                                                    range (see "Extremely
     foreach split \in candidates do
                                                                                    random trees"); any small k
       yl = y[X \le split]
                                                                                    value works.
       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/
```



Prediction

- Start at the root node and descend through the decision nodes to the appropriate leaf
- At each decision node, test indicated specific variable's value against the split value stored in the decision node

```
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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```