Training decision trees

Terence Parr
MSDS program
University of San Francisco

UNIVERSITY OF SAN FRANCISCO

Training overview

- Training partitions feature space into rectangular hypervolumes chasing reduced y impurity in subregions
- Hypervolumes are specified by sequence 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 <u>greedily</u> 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 subregions created by that split

Fitting decision trees

subsets

MSE or gini

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

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
      $yl = y[X_{col} \le split]$
      $yr = y[X_{col} > split]$
      if $|yl| = 0$ or $|yr| = 0$ 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]
```

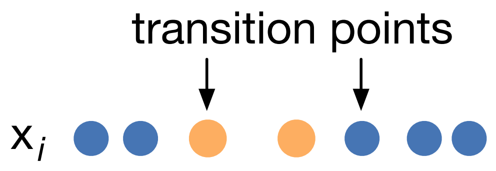
Should pick midpoint between split value and next smallest x

Decision tree prediction

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

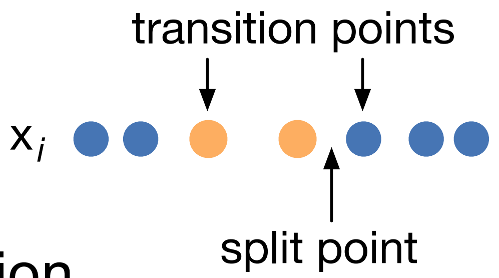
The usual bestsplit() is inefficient

- It has a nested loop; tries all combinations of p variables and worst-case n unique values in each variable at root: O(n*p)
- Cost of computing loss on all values in subregion each iteration is also expensive
- For classification, can mitigate by sorting by ith 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)



Improving generality and efficiency

- Select a subset of values as candidates, k; then we reduce O(n*p) to O(k*p) 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



UNIVERSITY OF SAN FRANCISCO

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 $|yl| = 0$ or $|yr| = 0$ 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.

Prediction

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

```
**Algorithm:** $predict(node, x)$
    **if** $node$ $is$ $leaf$ **then**
        **if** $classifier$ **then return** $mode(node.y)$
        **return** $mean(node.y)$
    **end**
    **if** $x[node.col] \leq node.split$ **then return** $\text{predict}(node.lchild, x)$
    **return** $\text{predict}(node.rchild, x)$
```