Random Forests™

Ensembles of bootstrapped, independent trees

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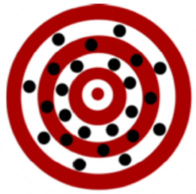
Bias / Variance (again)

Expected prediction error at x_0

$$\mathrm{E}[(Y - \hat{f}_k(x_0))^2 | X = x_0]$$

- For a single test vector x_0, **bias** "*is the squared difference between the true mean $f(x_0)$ and the expected value of the estimate*" [ESL book p37] (at least under MSE error)
  (How far off is the expected prediction from true answer?)
- **Variance** is the variance of the estimates for x_0 from models trained using tweaked training data (most common terminology)
- But high variance also implies model parameters (tree structure) vary a lot if we tweak the training data

Unbiased but high variance



Leo Breiman (1996) introduced bagging
then Random Forests (2001)
https://www.stat.berkeley.edu/~breiman/randomforest2001.pdf

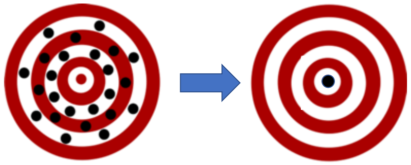
RF motivation

- Decision trees can often get training errors close to zero because we can grow very large trees to partition the feature space into tiny regions with 1 or just a few observations / samples; trees are very accurate on the training set and have **low bias**
- The downside is that decision trees overfit like mad: decision trees have **high variance** and don't generalize well

Analogy: Decision tree SF house prices

- Real estate agent builds house price model in their head by visiting lots of houses in SF
- Increase generality by averaging, say, all houses in each neighborhood: averaging smooths out variation in answers (shortening tree or increase node size)
- The cost: less precise house predictions
- Hmm…can we think of another way to average w/o introducing bias?

How can we increase generality?



- **Goal**: keep the high accuracy, but increase the generality
- So, let’s alter our decision tree model in a way that makes predictions **noisier but with same prediction expected value** (don’t intro any bias)
- To compensate for the noise and claw back some accuracy, make an ensemble of such trees; ensemble predicts average or majority vote of trees
- Averaging predictions reduces variance without introducing bias so ensemble is **accurate on average**
- The expected value of full strength model is same as expectation of altered model's prediction

Target image credit: http://ficscience.blogspot.com/2011/02/technicalities-of-technical-terms.html

The key trick is amnesia

- Random forests are all about adding a bit of amnesia to the training process
- We will restrict the trees by training each on a randomly selected subset of the training data: **bagged trees**
- Further, we will have training purposely forget about some features as we create decision nodes: **random forests**

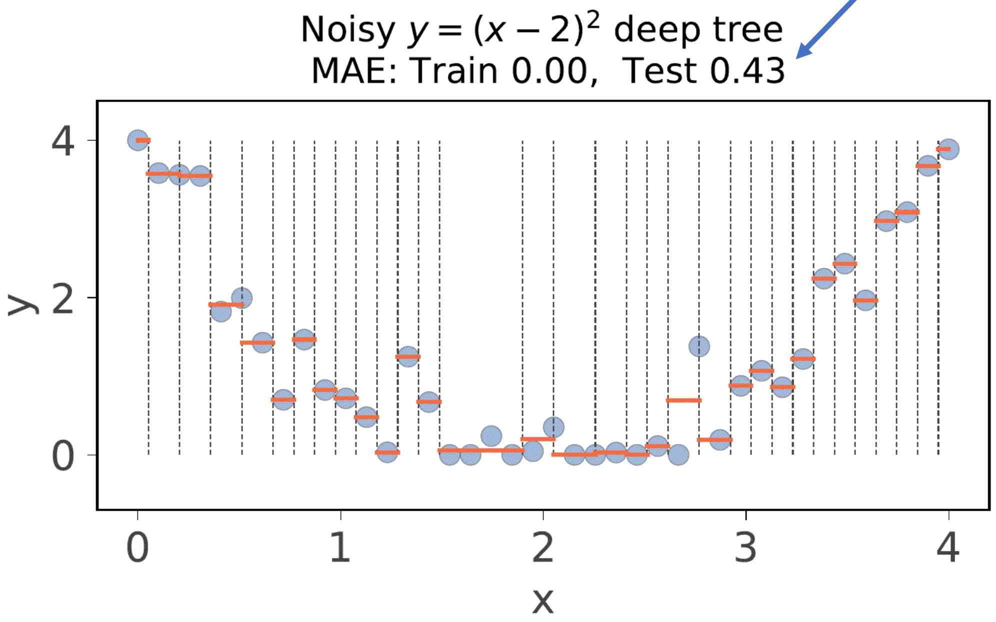
Analogy: Crowdsourcing SF house prices

- Recruit multiple real estate agents to build house price models in their heads by visiting lots of houses; then each agent can estimate prices of unvisited houses
- Agents choose and examine house subsets **independently**
- There will be some overlap in visited houses sets but the subsets will be *independent and identically distributed* (*i.i.d.*)
- An agent trained on an i.i.d. subset is not biased (they have same expectation) but is less accurate—a prediction for one house might be too low but a prediction for another house might be too high
- The variance of the ensemble average will be much tighter than the variance of an individual tree's prediction
- Averaging all agents' predictions reduces variance and is unbiased

Ex: Overfit decision trees regressors

- Animation shows 1D feature space partitioning of i.i.d. sample sets
- Slightly different training data sets can yield very different decision trees
- Clearly the trees have gotten way too specific to the data set
- Notice how the training error is 0 but (20% hold out) test error is terrible!

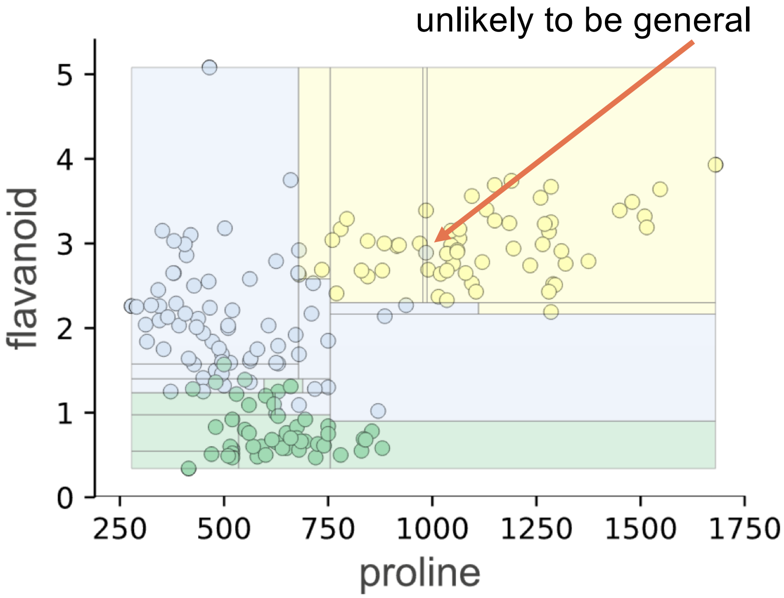
Uh oh!



See https://github.com/parrt/msds621/blob/master/notebooks/trees/random-forests.ipynb

Ex: Overfit decision tree classifiers

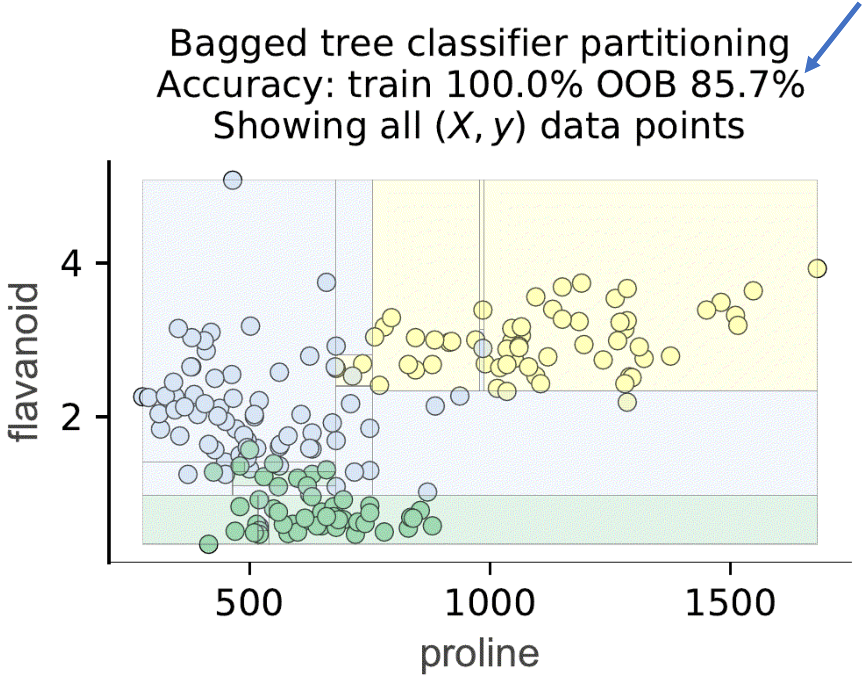
- Here is a previous example where partitioning trapped a lonely blue in a sea of yellow
- In practice, we're given just one data set so let's do some sampling to get some i.i.d. "copies"
- Then see how different data sets give different partitioning (from different trees)



Partitioning from bootstrapped data[†]

- *Bootstrap* (X, y) to simulate multiple i.i.d. data sets[†]
- Each set gets ~63% of unique (X, y) data (sample n records with replacement)
- Animation shows 2D feature space partitions from various bootstraps
- Partitioning clearly varies a lot between bootstraps
- *OOB* == "out of bag" (more later)

amnesia

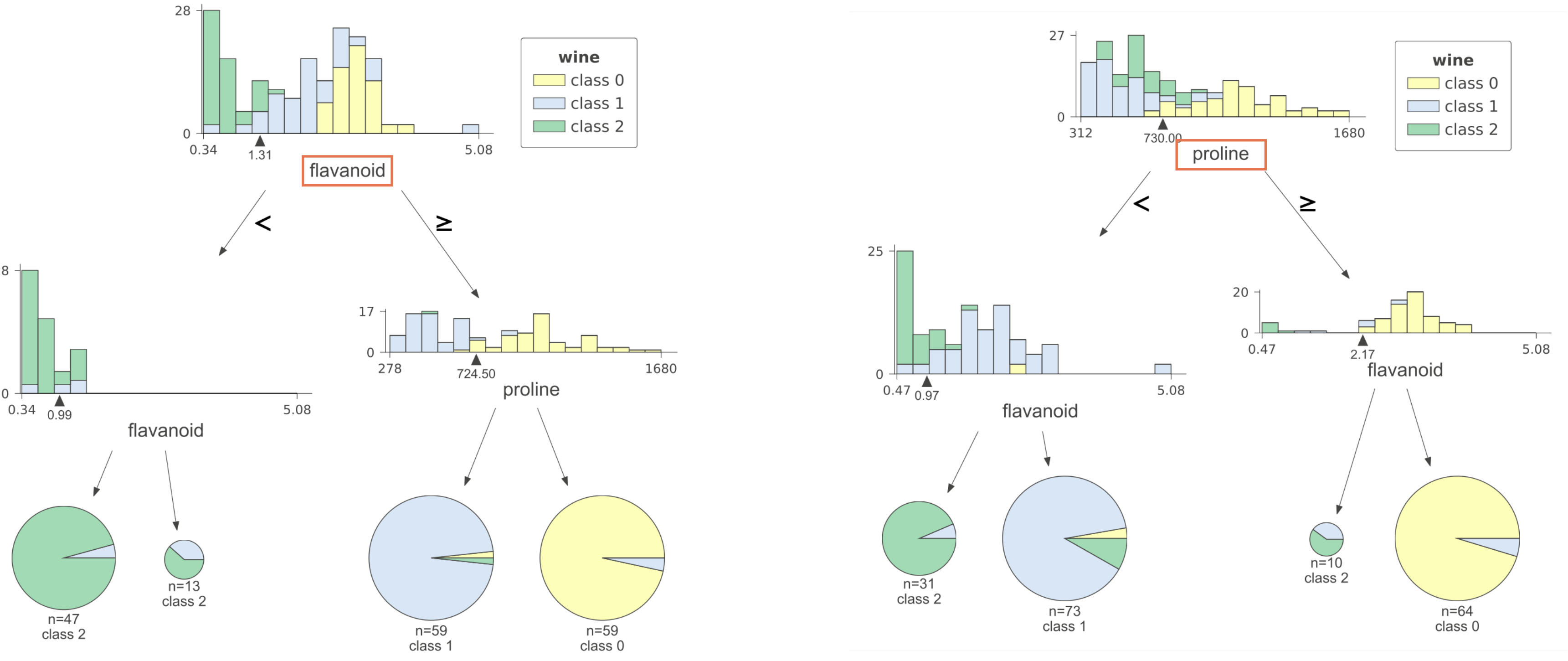


Uh oh!
Varies

[†] Bootstraps are technically *conditionally independent*, conditioned on nature of original X, which could be weird by chance or by the way it was collected/obtained.

Bootstrapping gives slightly different trees

`DecisionTreeClassifier(max_depth=2)`



Same tree construction algorithm running on slightly different bootstraps

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Aside: Code for bootstrapping

NumPy

```
# Bootstrap: sample with replacement
n = len(y)
idx = np.random.randint(0,n,size=n)
X_train = X[idx]
y_train = y[idx]
```

```
# get OOB (out-of-bag) samples
mask = np.ones(n, dtype=bool)
mask[idx] = False
X_test = X[mask]
y_test = y[mask]
```

Pandas

```
# If data in dataframe
df = df.sample(len(df), replace=True)
```

See https://github.com/parrt/msds621/blob/master/notebooks/trees/random-forests.ipynb

Bagged trees

Training trees on bootstrapped samples and aggregating predictions

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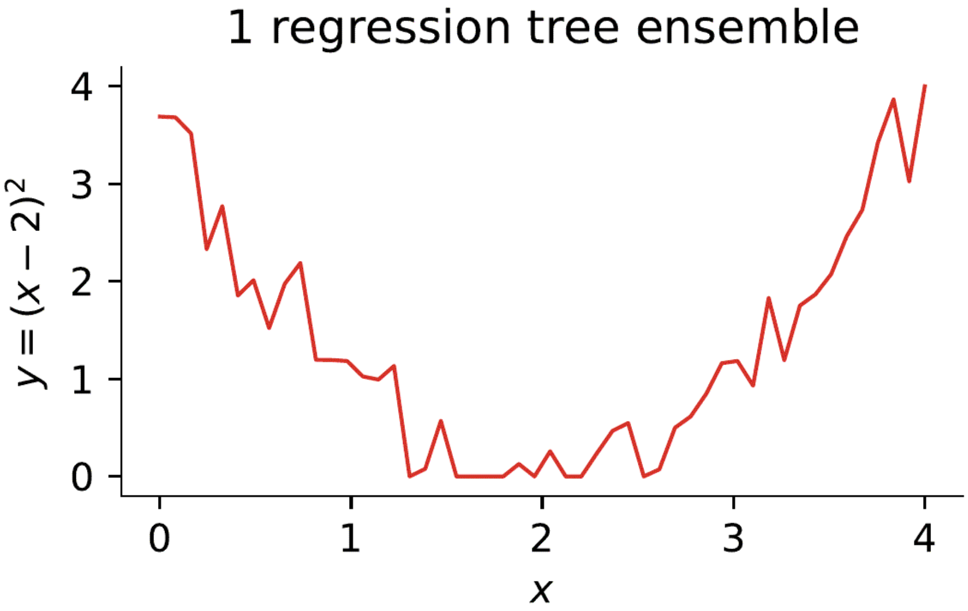
Ensemble of high-variance regression trees

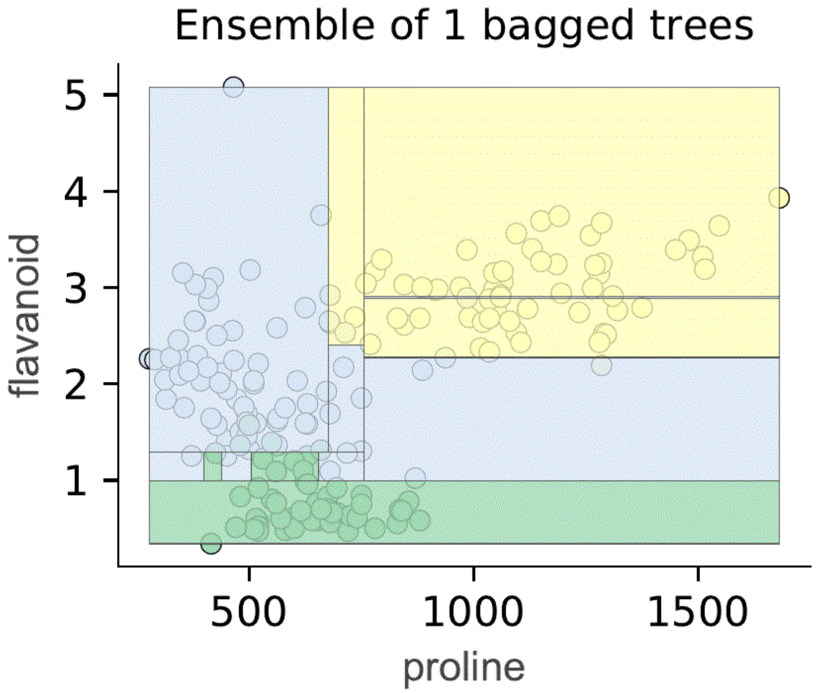
- Animation shows how averaging the prediction of an ensemble of overfit trees actually produces a reasonable combined prediction
- As we add trees, the average prediction (red line) smooths out to reveal the underlying quadratic distribution from which we draw noisy samples
- Note: variance of individual tree predictions stays high regardless of number of trees, but the variance of the ensemble average tightens (the magic of C.L.T.)



Repeatedly drawing new noisy training sets

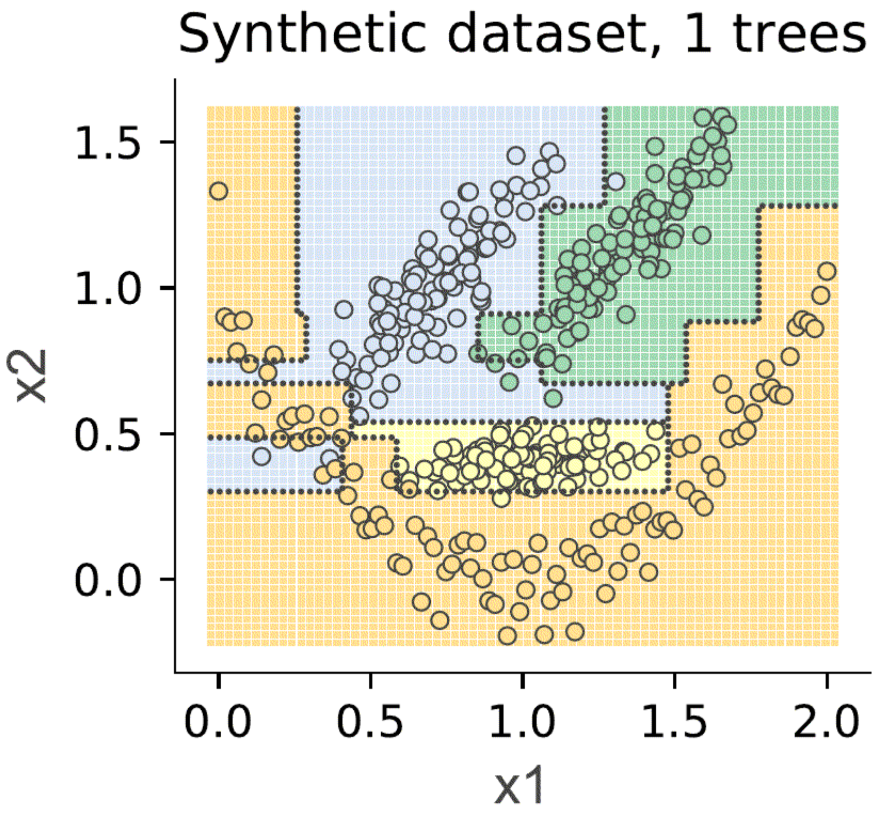
Ensemble of high-var. classification trees

- Animation shows overlapping prediction regions from multiple classifier trees
- Training data for each tree is bootstrapped from the original (X, y) data
- As we add trees, the averaged prediction regions become more stable and the decision boundaries more complex
- "Bag" is *bootstrap aggregation*



Ensemble classifier on synthetic data set

- Animation shows prediction regions from multiple bagged classifier trees
- Colored tiles indicate the probabilities of the various classes; e.g., yellow-orange color indicates uncertainty between those two classes
- What's prob. of class k at tile?
  - proportion of trees that predict k



Animation uses probability space visualization I added to dtreeviz

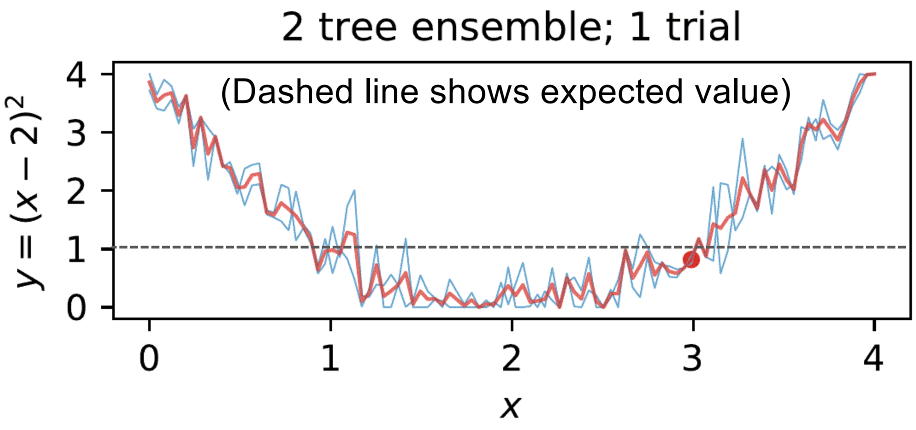
Ensemble's effect on bias and variance

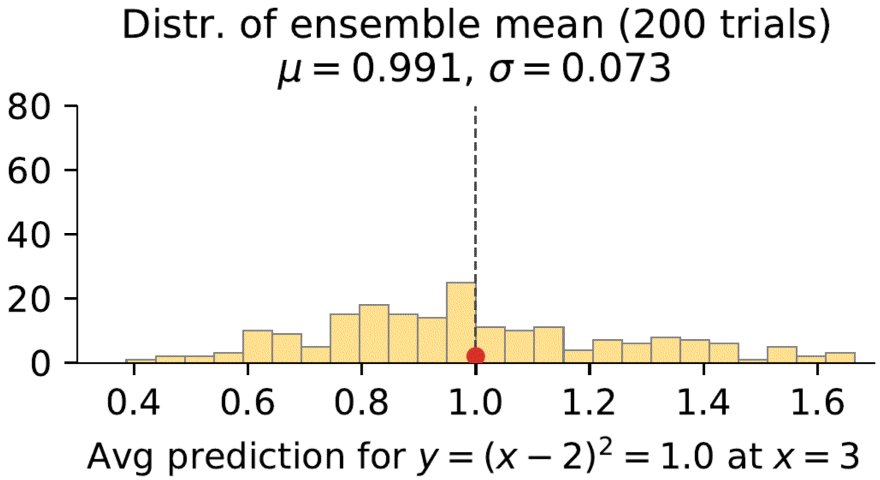
- Train T trees on T i.i.d. X data sets
- Central limit theorem says that if variance of an i.i.d. random variable is σ^2, the variance of the average of T such vars is σ^2/T
- So, as we add trees, the variance of the ensemble prediction will shrink, which means better generality
- After, say, 100 trees though we're not going to get a more general model, but will get better estimates of the true prediction for a single test record (squeezing out some more noise)
- The average of the tree predictions is the same as the expected prediction from any tree trained on one of the X sets (since i.d.)
- If individual trees had different expectations, adding trees would increase bias

See page 588 ESLII book

Ex: variance of ensemble prediction

- Animation shows tree and ensemble predictions on left for T trees; variance of predictions in blue tree predictions doesn't change with the number of trees but red line get tighter / less noisy with more trees
- At $x = 3$, expected value of ensemble is 1.0; create 200 separate ensembles of size T and compute variance of ensemble predictions at $x = 3$; distribution of ensemble average shown on the right





Problem: trees are not independent thinkers

- With real estate agent analogy, we implicitly assumed agents were independent thinkers, and not clones
- But, decision trees are like robot clones and, given the same bit of data, yield the exact same bit of tree
- Imagine worst case: bootstrapping yields T identical sets so ensemble gives exactly the same prediction as any single tree
- In practice, if there is one strongly predictive var out of p, then all trees would be similar; initial root splits, and many others, would likely be same

Random Forests

Ensembles of de-correlated bagged trees

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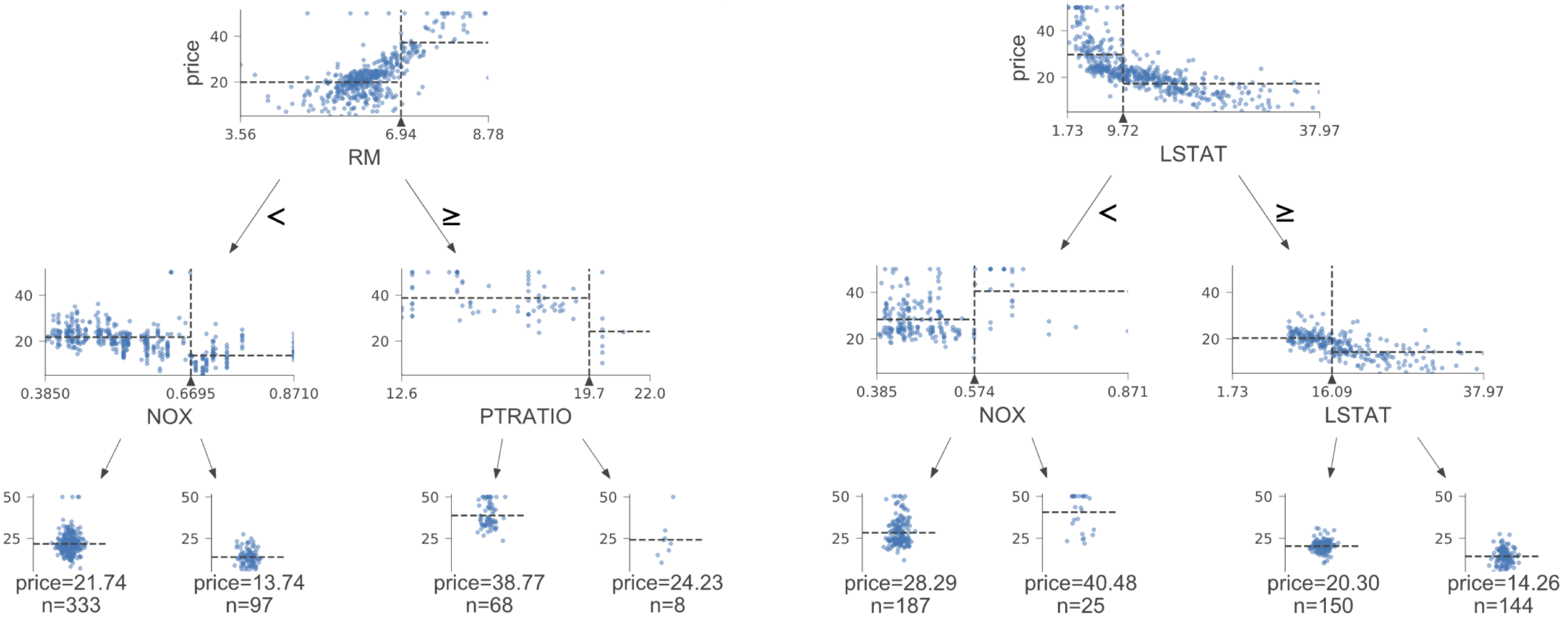
Making trees independent thinkers

- Bagging overcomes most of the overfitting, but we can improve generality a little by further restricting the tree training process itself in an effort to make trees think more independently
- Restrict the available features when searching for a decision node split; choose from m randomly selected features (**amnesia** again!)
- Choose max features per split, $m \leq p$, such as m = sqrt(p)
- Make sure chance of selecting predictive variables (m/p) is high enough to find predictive variables (See ESLII p596)
- Let validation error be your guide to choosing m
- A *random forest* is then just an ensemble of decision trees trained on bootstraps and whose feature selection strategy has a bit of amnesia

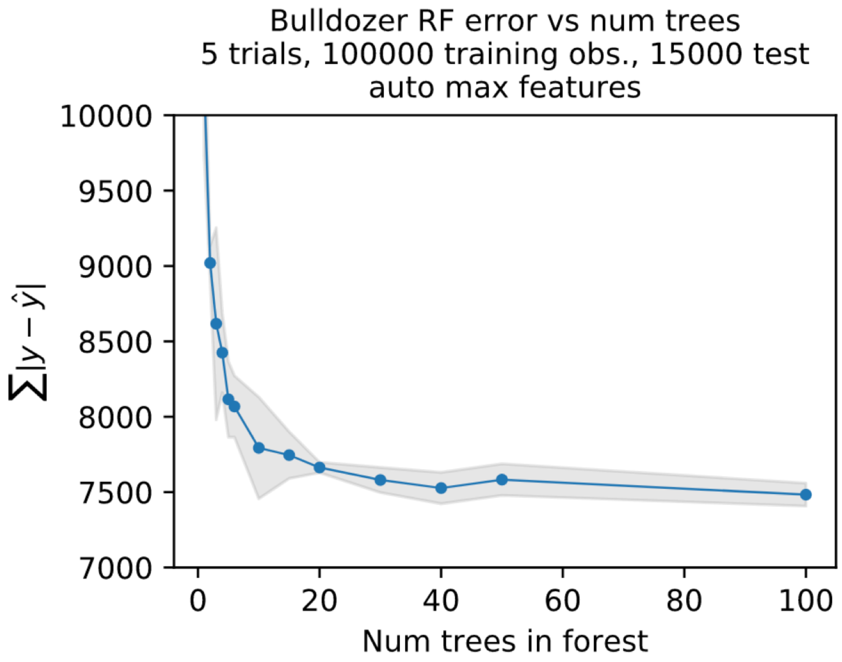
Ex: Effect of limiting feature set but using full data set

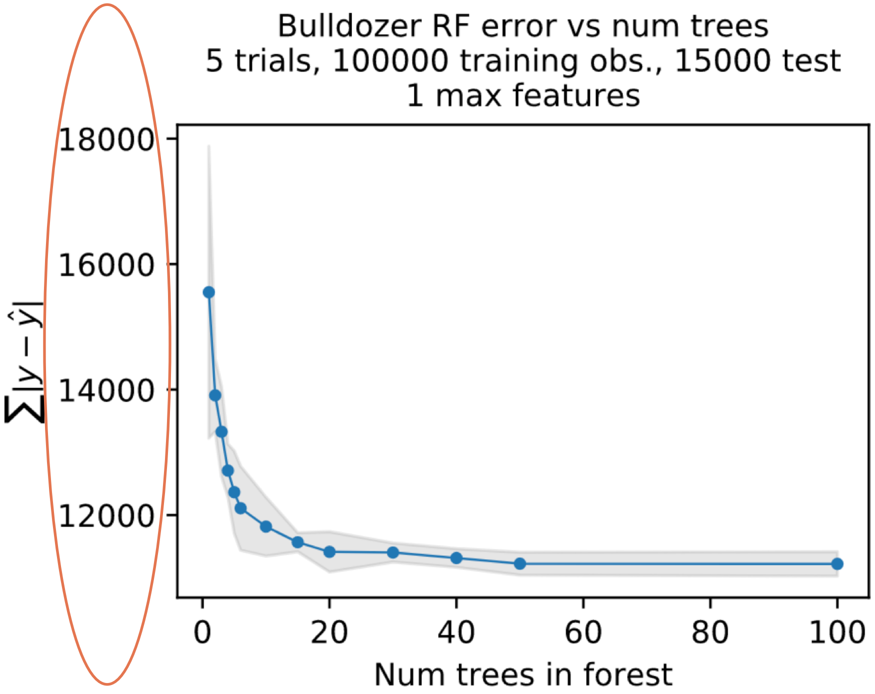
2 trees trained on **entire** Boston set with m=5 (of 13)



Choose from 5 randomly selected features during EACH split

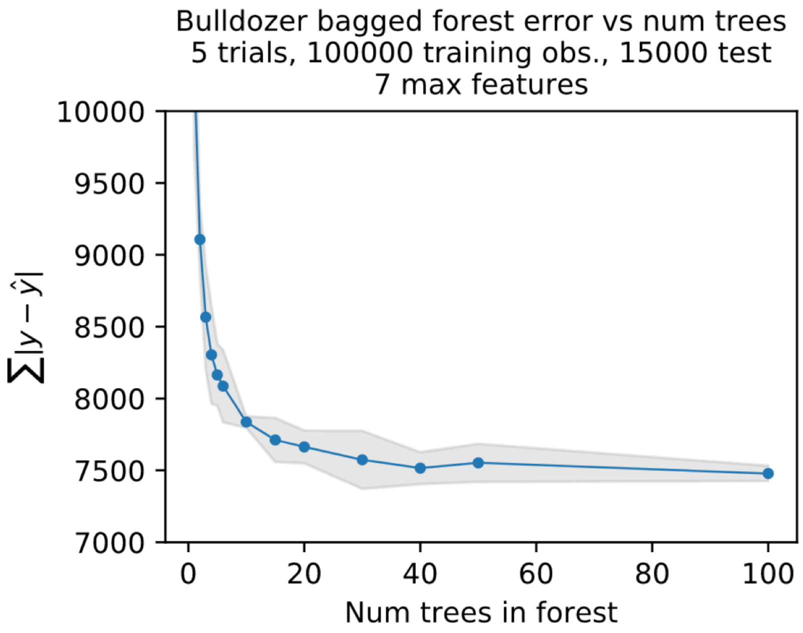
If max_features too low, bad accuracy





Effect of forest size on accuracy

- Why does accuracy improve greatly (initially) as we add trees?
  - Each tree sees only 2/3 of data so adding bootstrapped trees increases use of training data
  - Variance is tightening quickly as we average even just a few trees
- Why does accuracy asymptotically approach a minimum instead of continual improvement?
  - With enough trees, ensemble sees 100% of the training data; it's approaching the accuracy of single decision tree in ideal world
  - We've squeezed out all bias and variance that we can with this model



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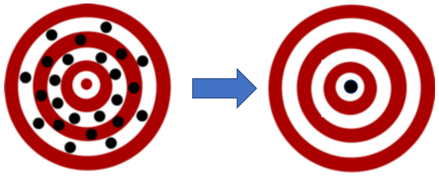
Properties (see *Breiman 2001*)



- p4 "*Random forests do not overfit as more trees are added*" **Why**?
  - New trees get averaged in so each additional tree has less individual effect
  - New trees <u>balance each other out</u>, one might be too high, another too low
- p7 "*It's relatively robust to y outliers and X noise*" **Why**?
  - y outliers get shunted to their own leaf since doing so reducing loss function, particularly if squared-error is used
  - Noise X variables aren't predictive so not chosen as split vars
- p10 Bagging helps more, the more unstable the model. **Why**?
  - Averaging is a smoothing operator, squeezing predictions to true value
  - If model is low variance already, there is no point in bagging

Properties continued

- RFs are scale and range insensitive in features and target y **Why**?
  - Comparing feature values in decision nodes, not doing math on them
  - Computing mean or mode of y to predict
- ESLII p596 "*Classifiers are less sensitive to variance [than regressors]*" **Why**?
  - (not sure haha) I believe it has something to do with mode vs mean (mode is same until a threshold whereas mean is influenced by any value added, unless it is also the mean)

Bootstrapping vs subsampling

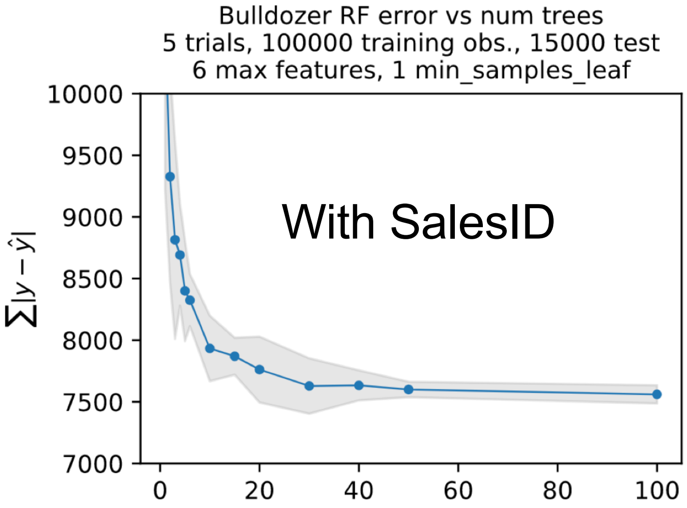
- Bootstrapping is sampling with replacement vs subsampling w/o replacement
- 😯 Friedman and Hall (2000): subsampling also works, showing that training trees with $n/2$ subsamples is similar in bias/variance to bagging http://statweb.stanford.edu/~jhf/ftp/bag.pdf
- Smaller training set is a big win in terms of speed
- Using even smaller fractions of n improve generality (reduce variance) because trees are less correlated (they work on different data chunks); note that each tree would become less accurate as n subsample size decreases

RF Tuning strategy

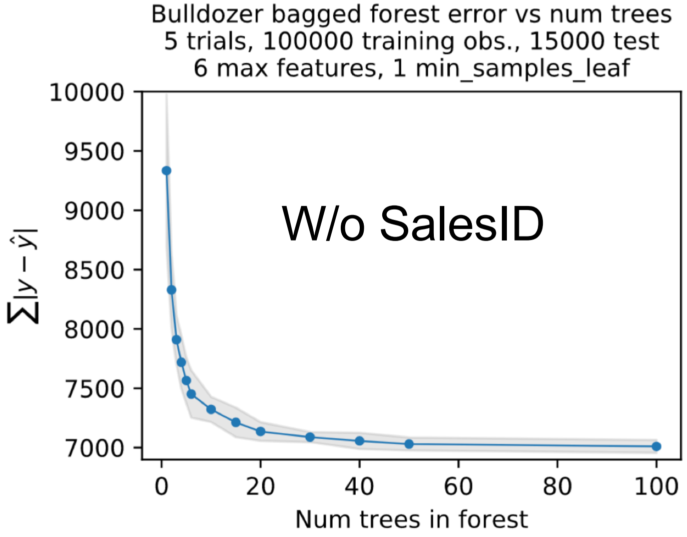
- Good news: very little tuning needed
- Goal: minimize validation error
- Start with maybe 20 trees and work upwards til validation error stops getting better; or just pick 100
- Sklearn uses max_features= sqrt(p) by default; try dropping this to log(p), or similar; ESLII suggests $p/3$ for regression and sqrt(p) for classification
- Try adjusting min samples per leaf: 1, 3, 5, 10, 25, 100
- Can also try grid search, but I never bother;
  Start with num trees, then tune the others

Feature engineering beats model tuning

- SalesID: unique record ID, and is never seen again in future predictions
- Is that useful for prediction? No
- Does the model think it's useful? Yes
- Model is overfit not on noise but on falsely-predictive feature
  - Could be that sales ID correlates with inflation or change in type of models sold in auction creates "trend" in sale prices
- A case where using LESS data improves the model a lot ($500 diff)
- Dropping useless features also often gives a small bump



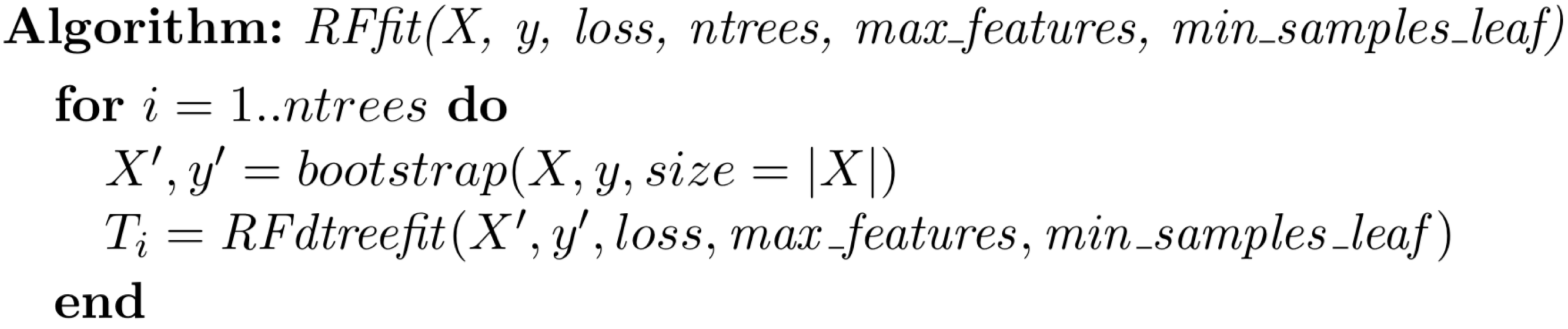
Bulldozer RF error vs num trees
5 trials, 100000 training obs., 15000 test
6 max features, 1 min_samples_leaf



Bulldozer bagged forest error vs num trees
5 trials, 100000 training obs., 15000 test
6 max features, 1 min_samples_leaf

The RF algorithms

Fitting RFs



```
Algorithm: $RFfit(X,\ y,\ loss,\ ntrees,\ max\_features,\ min\_samples\_leaf)$
  for $i = 1..ntrees$ do
    $X', y' = bootstrap(X, y, size = |X|)$
    $T_i = RFdtreefit(X', y', loss, max\_features, min\_samples\_leaf)$
  end
```

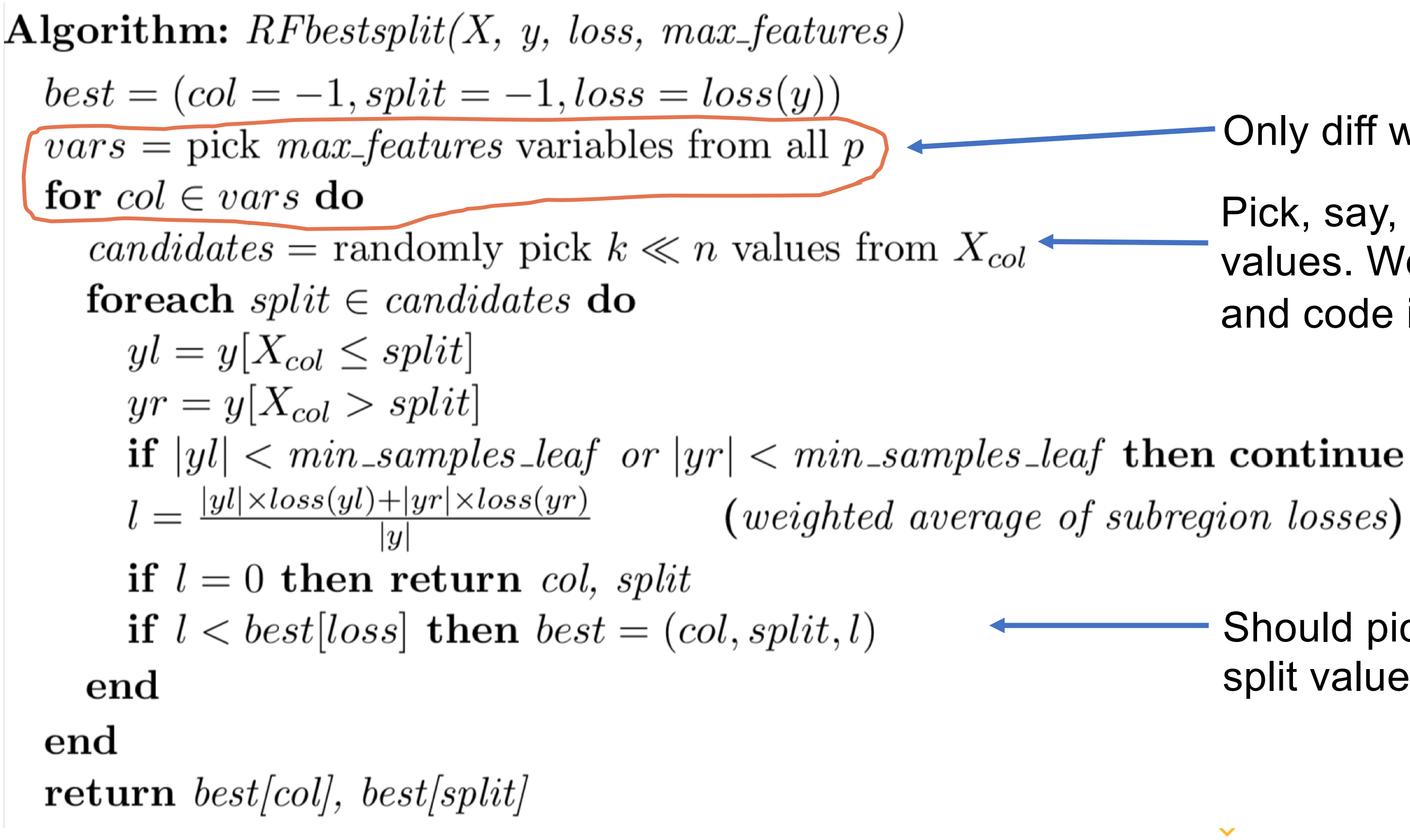
For regression, pass in loss = MSE or stddev
For classifier, pass in loss = gini

Fitting a single tree in RF

Same as decision tree except we pass max_features to RFbestsplit()

```
**Algorithm:** $RFdtreefit(X,\ y,\ loss,\ max\_features,\ min\_samples\_leaf)$
    **if** $|X| \le min\_samples\_leaf$ **then** return Leaf($y$)
    $col, split = RFbestsplit(X, y, loss,\ max\_features)$
    **if** $col$ = $-1$ **then** return Leaf($y$)
    $lchild = RFdtreefit(X[X_{col} \le split], y[X_{col} \le split], ...)$
    $rchild = RFdtreefit(X[X_{col} > split], y[X_{col} > split], ...)$
    **return** $DecisionNode(col, split, lchild, rchild)$
```

Finding best split in decision node in RF



```
Algorithm: $RFbestsplit(X,\ y,\ loss,\ max\_features)$
  $best = (col = -1, split = -1, loss = loss(y))$
  $vars$ = pick $max\_features$ variables from all $p$
  for $col \in vars$ do
    $candidates$ = randomly pick $k \ll n$ values from $X_{col}$
    foreach $split \in candidates$ 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 $best[col],\ best[split]$
```

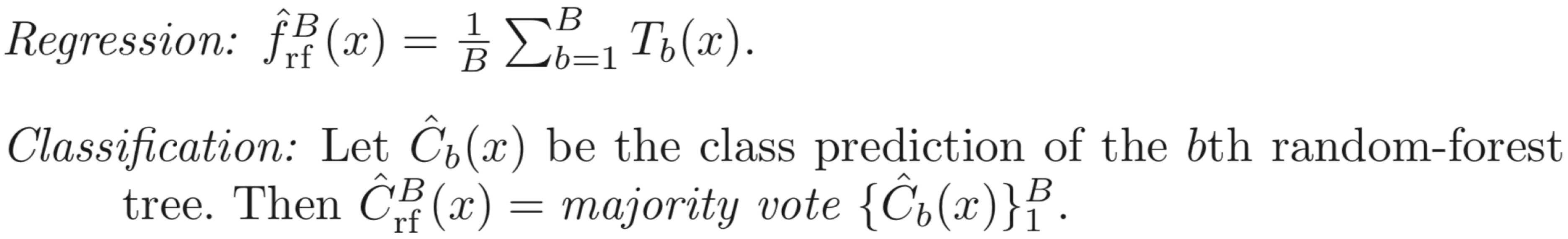
Only diff with decision tree

Pick, say, 11 not all possible X values. We get better generality and code is much faster!

Should pick midpoint between split value and next smallest X

Simplest RF prediction (ESLII p588)

- But doesn’t use all information to make best prediction
- Should use weighted averages / votes



Regression: $\hat{f}^B_{\text{rf}}(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x).$

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}^B_{\text{rf}}(x) = \textit{majority vote } \{\hat{C}_b(x)\}_1^B.$

RF prediction

Weighted average of y values among the leaves reached by running x down each tree

```
**Algorithm:** $RFpredict_{regr}(\{T_1..T_{ntrees}\},\ x)$
  **Let** $leaves = \{leaf(T_t, x)\ \forall\, t = 1..ntrees\}$
  $nobs = \sum_{t=1}^{ntrees} |leaves_t|$
  $ysum = \sum_{t=1}^{ntrees} \sum_{y \in leaves_t} y$
  **return** $\frac{1}{nobs} ysum$
```

```
**Algorithm:** $RFpredict_{class}(\{T_1..T_{ntrees}\},\ x)$
  $counts[k] = 0\ \forall$ classes $k$
  **foreach** $t = 1..ntrees$ **do**
    $leaf = leaf(T_t, x)$          ($leaf$ $reached$ $by$ $x$)
    **foreach** $y \in leaf$ **do**
      $counts[y]$ += 1          ($track$ $count$ $of$ $leaf$ $modes$)
    **end**
  **end**
  **return** argmax($counts$)
```

Count all y votes among the leaves reached by running x down each tree

Extremely randomized trees (Geurts *et al* 2006)

- The variable/value pair is highly sensitive to the training set, and responsible for much of the error rate
- "*The optimal cut-point was shown to depend very strongly on the particular learning sample used…this cut-point variance appeared to be responsible for a significant part of the error rates of tree-based methods.*" https://link.springer.com/article/10.1007/s10994-006-6226-1
- Geurts wondered if more randomness could reduce variance further
- Pick random split value in min(X[:,j]) .. max(X[:,j]), ignoring individual X_j values!
- Like RF, select $m \leq p$ variables and choose var/value with lowest loss
- Fits using entire X training set, not bootstrap and not subsample (trying to increase accuracy of prediction/decrease noise)
- Our use of just 11 (not n) X candidate values in the project is similar (an effort to reduce variance and increase speed)

RF advantages

- Ensemble of decision trees trained on different bootstraps that sometimes forgetting about features during training
- Prediction is ensemble average or majority vote (weighted)
- Easy to understand, efficient, excellent accuracy, interpretable
- Very little tuning is required
- Gracefully handles label-encoded categorical variables, no need to normalize numerical variables
- Robust to noise in X, y and nonpredictive variables
- Built-in out of bag validation sets
- Negative: cannot extrapolate beyond support data