Random forests

STAT 471

November 9, 2021

Where we are

✓ **Unit 1:** Intro to modern data mining

✓ **Unit 2:** Tuning predictive models

✓ **Unit 3:** Regression-based methods

Unit 4: Tree-based methods

Unit 5: Deep learning

Lecture 1: Growing decision trees

Lecture 2: Tree pruning and bagging

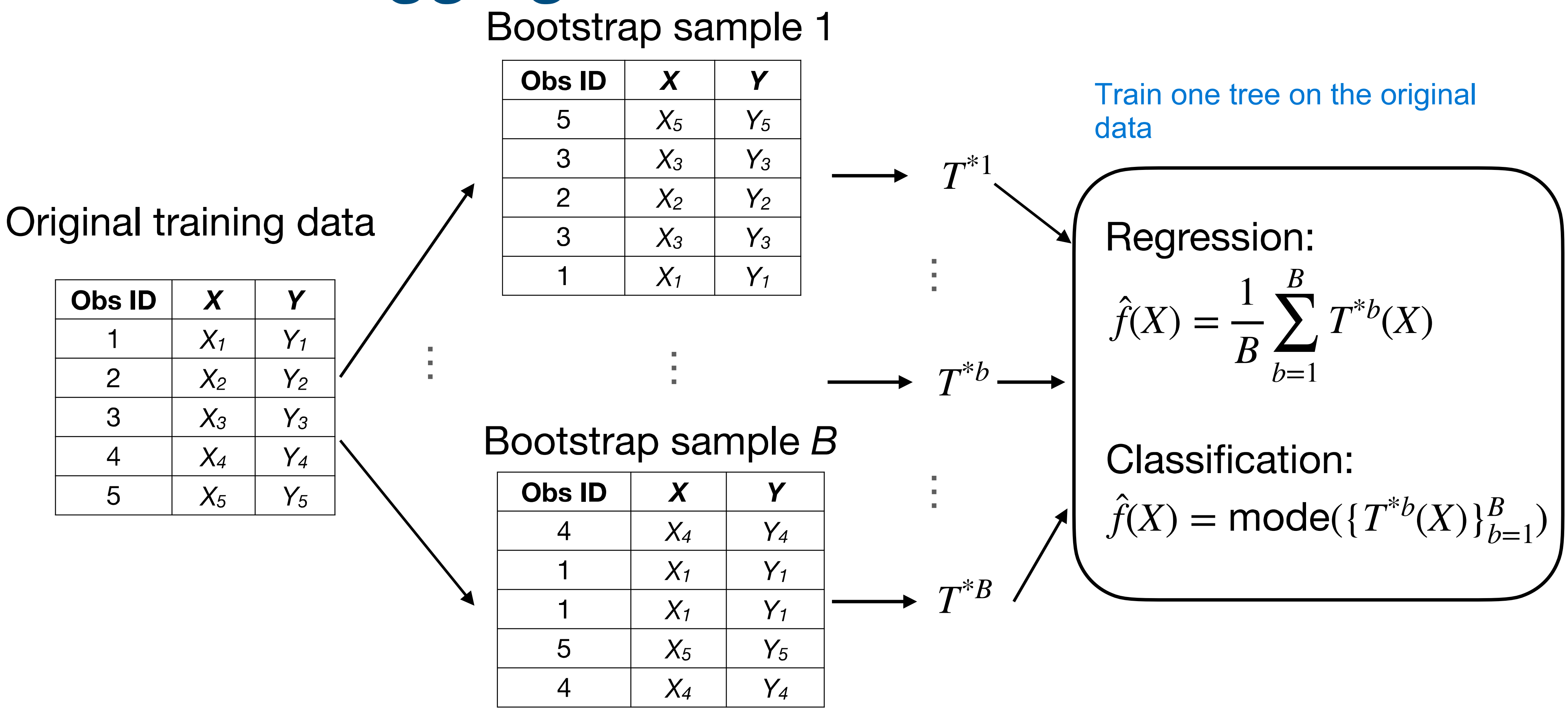
Lecture 3: Random forests

Lecture 4: Boosting

Lecture 5: Unit review and quiz in class

Homework 4 due the following Wednesday.

Recall: Bagging



Original training data

Obs ID	*X*	*Y*
1	X_1	Y_1
2	X_2	Y_2
3	X_3	Y_3
4	X_4	Y_4
5	X_5	Y_5

Bootstrap sample 1

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2	X_2	Y_2
3	X_3	Y_3
1	X_1	Y_1

Bootstrap sample *B*

Obs ID	*X*	*Y*
4	X_4	Y_4
1	X_1	Y_1
1	X_1	Y_1
5	X_5	Y_5
4	X_4	Y_4

Train one tree on the original data

Regression:

$$\hat{f}(X) = \frac{1}{B}\sum_{b=1}^{B} T^{*b}(X)$$

Classification:

$$\hat{f}(X) = \text{mode}(\{T^{*b}(X)\}_{b=1}^{B})$$

Variance reduction of bagging

The bagging prediction is defined by $\hat{f}(X) = \frac{1}{B}\sum_{b=1}^{B} T^{*b}(X)$.

Suppose Corr$[T^{*b_1}(X), T^{*b_2}(X)] = \rho \in [0,1]$. Then, we can derive that

$$\text{Var}[\hat{f}(X)] = \frac{1}{B^2}\sum_{b_1=1}^{B}\sum_{b_2=1}^{B} \text{Cov}[T^{*b_1}(X), T^{*b_2}(X)] \approx \left(\frac{1}{B} + \frac{B-1}{B}\rho\right) \text{Var}[T(X)] \approx \rho \cdot \text{Var}[T(X)],$$

where $T(X)$ is a single decision tree. Take-aways:

Variance of the bagging estimate is row time the variance of a single tree

- The variance is reduced by a factor of $\rho =$ Corr$[T^{*b_1}(X), T^{*b_2}(X)]$, so the less correlated the bootstrapped trees prediction are, the better.

- As long as B is large enough, the variance reduction is about the same.

The bootstrap tree predictions are better

Random forest is just like bagging but with extra step that reduces correlation among trees and further reduces variance

Random forests: More variance reduction

Random forests are the same as bagging, but with one key modification:

At each split point of each tree:

- Randomly sample a subset of $m \leq p$ features
- Split on the best feature *among this subset*

Intuition: Sampling features at each split decorrelates the trees, reducing variance and therefore boosting prediction performance.

Hopefully each individual tree is still roughly unbiased even though it has access to a smaller number of features at each split.

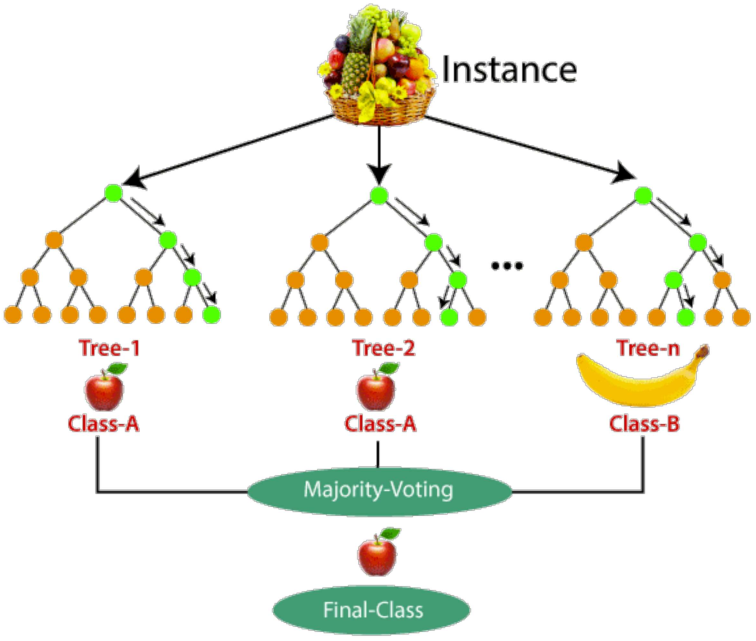


Image source: https://www.section.io/engineering-education/introduction-to-random-forest-in-machine-learning/

Note that setting $m = p$ recovers bagging.

At every step would be including all features

Have to decide which region should split and which

Random forests

For each bootstrap sample, you randomly sample M candidate variables and grow a decision tree, and then you predict same way as bagging

Parameters:

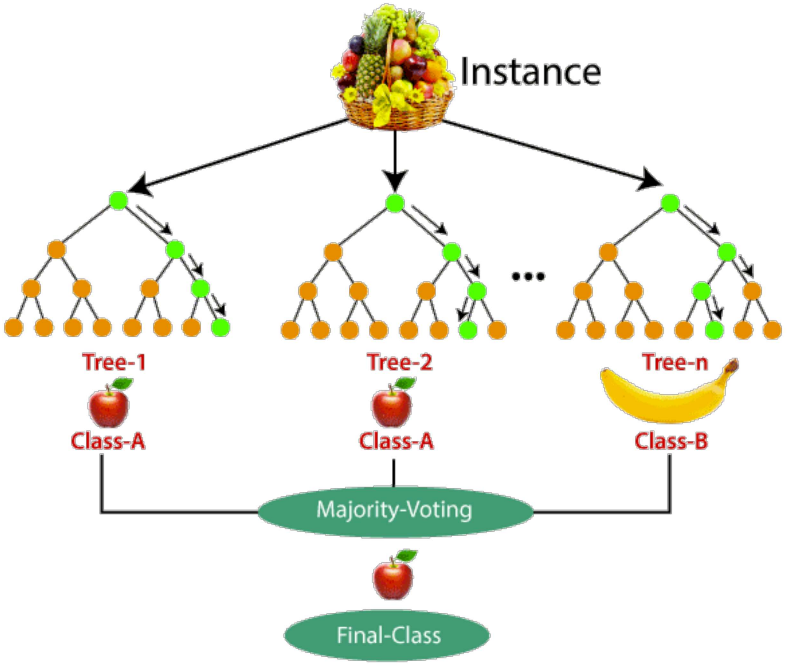
- B: number of bootstrap samples
- m: number of variables to sample at each split
- criterion to stop splitting, like max number of nodes and/or min samples per node

Training:

- Extract B bootstrap samples from your training data
- For each bootstrap sample $b = 1,\ldots,B$,
  - Grow a decision tree based on the bootstrap sample, randomly sampling m candidate variable to split on at each step, until stopping criterion is met

Prediction:

- aggregate the decision trees using the mean (for regression) or mode (for classification)



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A bias-variance trade-off in choosing m

If m is larger, the random forest will have lower bias (it can better fit the underlying trend) but higher variance (more correlated trees).

The higher m is, the more similar the set of features the tree is considering

If m is smaller, the random forest will have higher bias (it might not be able to fit the underlying trend as well) but lower variance (less correlated trees).

If m is smaller, not allowing to use all features and trees will be less correlated

Default choices: $m = p/3$ for regression and $m = \sqrt{p}$ for classification.

For best predictive performance, m should be tuned.

Random forest, in comparison to deep learning is more plug and play

Final tree is average of predictions of all trees. There is no "super" tree, but B trees that make up the "forest"

Tuning random forests via out-of-bag error

We usually tune prediction methods via cross-validation. For random forests, there is a clever and computationally faster alternative: out-of-bag error.

The idea behind cross-validation is that we want to using parts of our training data as validation sets. By bootstrapping, random forests already do this!

For each bootstrap sample, define the “bag” to be the set of unique training observations in the sample. Then, predictions based on that tree can be made on the out-of-bag (OOB) samples.

When we use bootstrapping, doing something very similar to CV

Bootstrap sample *b*

Obs ID	***X***	***Y***
5	X_5	Y_5
3	X_3	Y_3
2	X_2	Y_2
3	X_3	Y_3
1	X_1	Y_1

$\longrightarrow T^{*b}$

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$\longrightarrow T^{*b}$

4	X_4	Y_4

out-of-bag *b*

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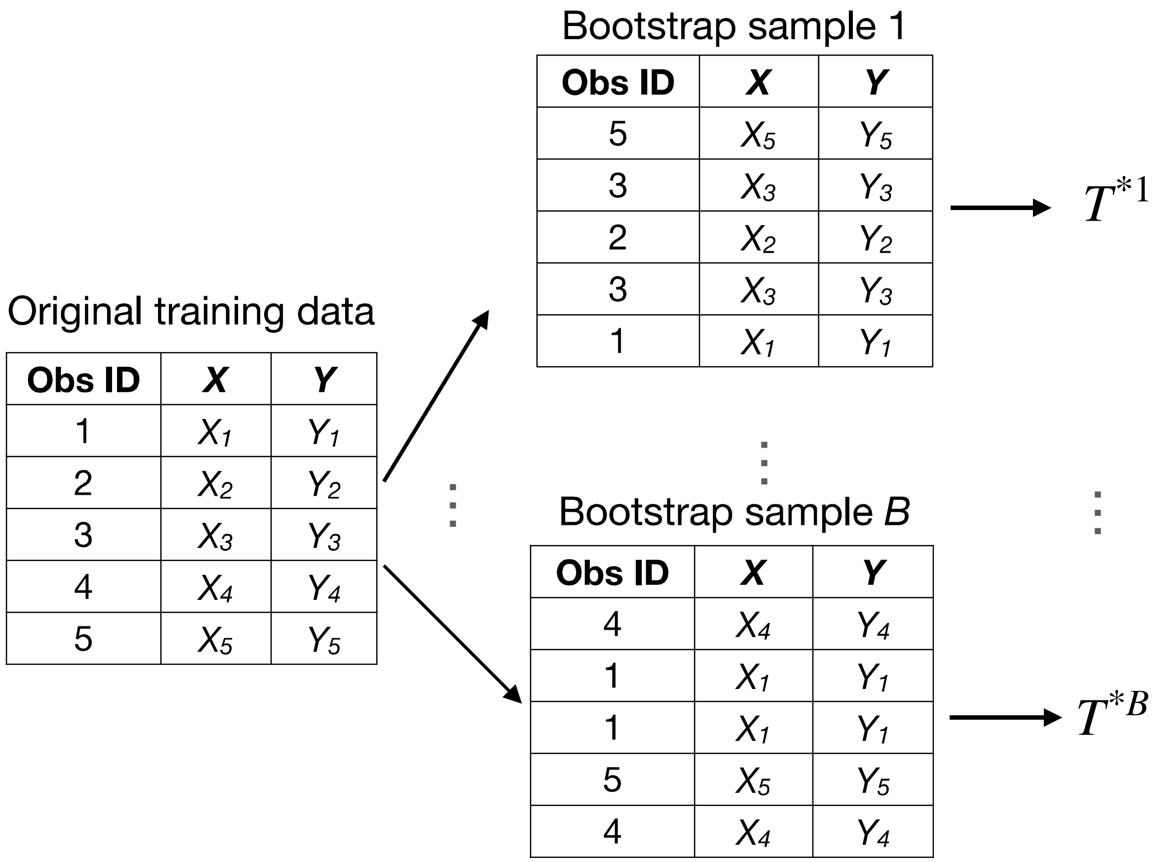
out-of-bag *b*

$$\longrightarrow T^{*b} \longrightarrow T^{*b}(X_4)$$

Out of bag error



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Bootstrap sample 1

Obs ID	X	Y
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$\longrightarrow T^{*1}$

⋮

Bootstrap sample *B*

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4	X_4	Y_4
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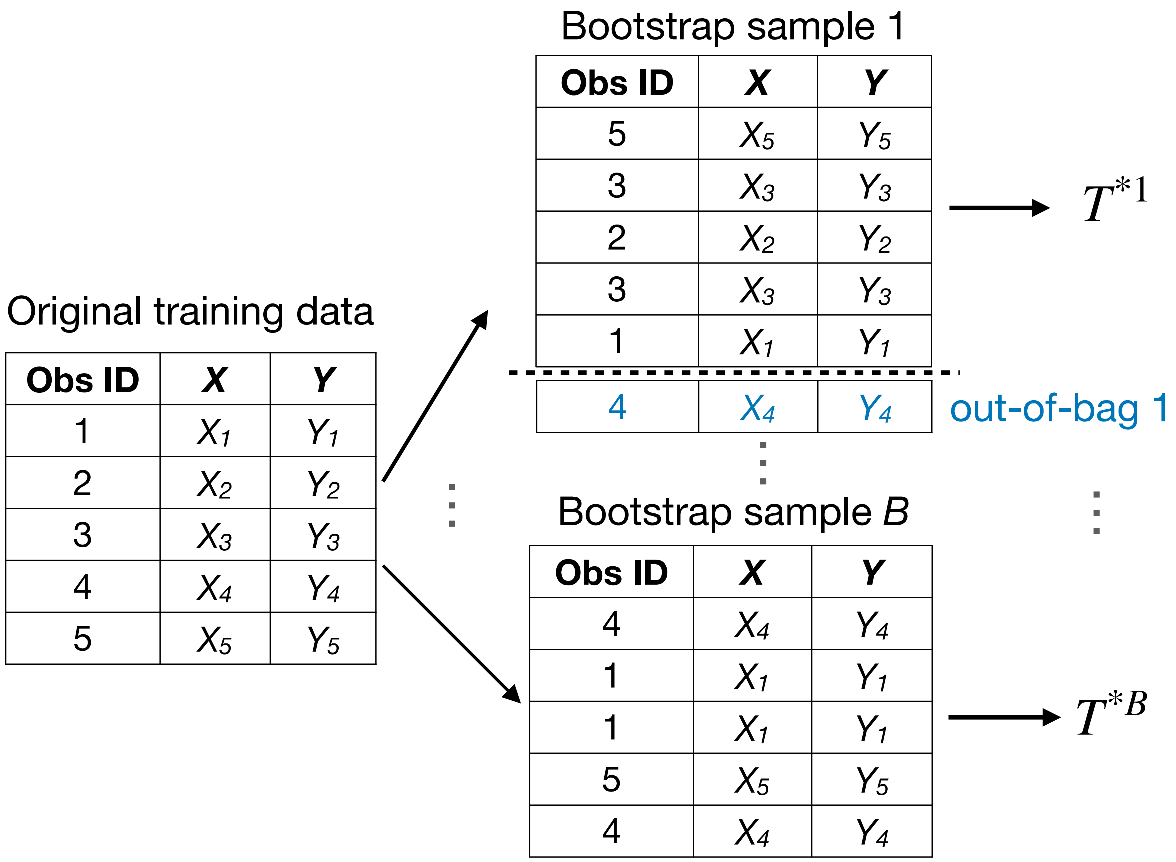
1	X_1	Y_1
5	X_5	Y_5
4	X_4	Y_4

$\longrightarrow T^{*B}$

Have a bunch of bootstrap samples

Each sample has its own out of bag sample

Out of bag error



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$\longrightarrow T^{*1}$

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out-of-bag 1

Bootstrap sample *B*

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1	X_1	Y_1
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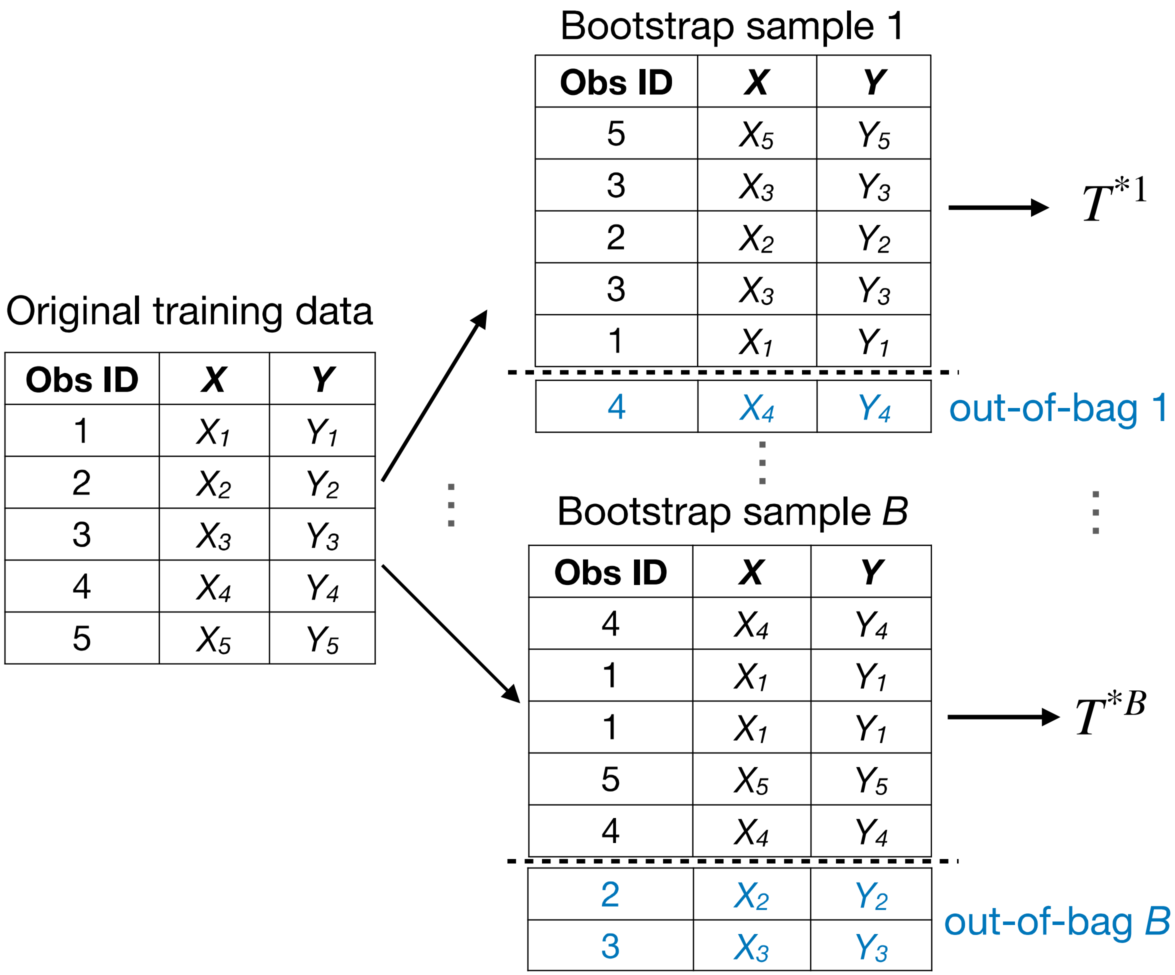
$\longrightarrow T^{*B}$

Out of bag error



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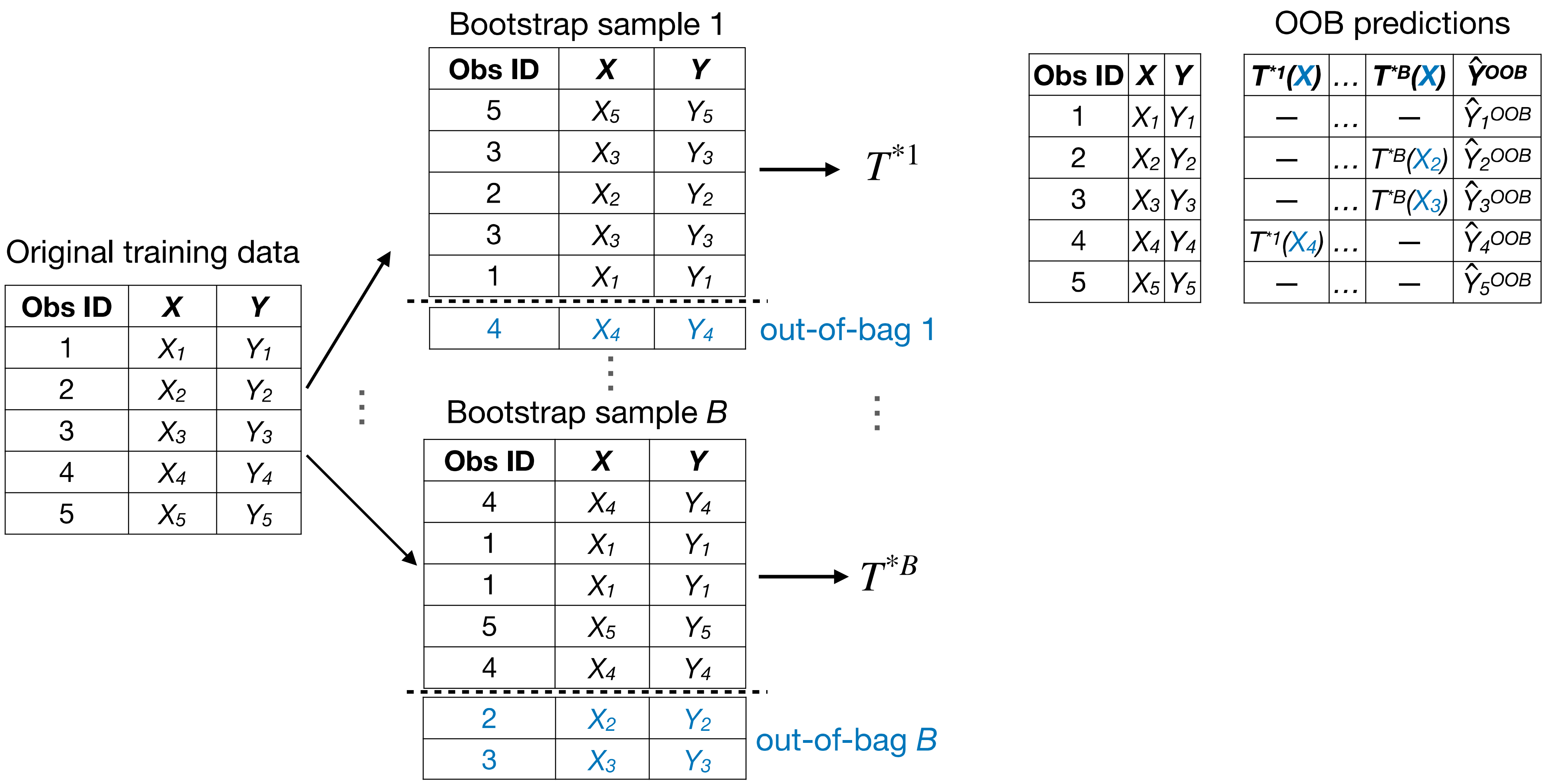
$\longrightarrow T^{*B}$

2	X_2	Y_2
3	X_3	Y_3

out-of-bag *B*

Out of bag error



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out-of-bag 1

$\longrightarrow T^{*1}$

Bootstrap sample B

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4	X_4	Y_4
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3	X_3	Y_3

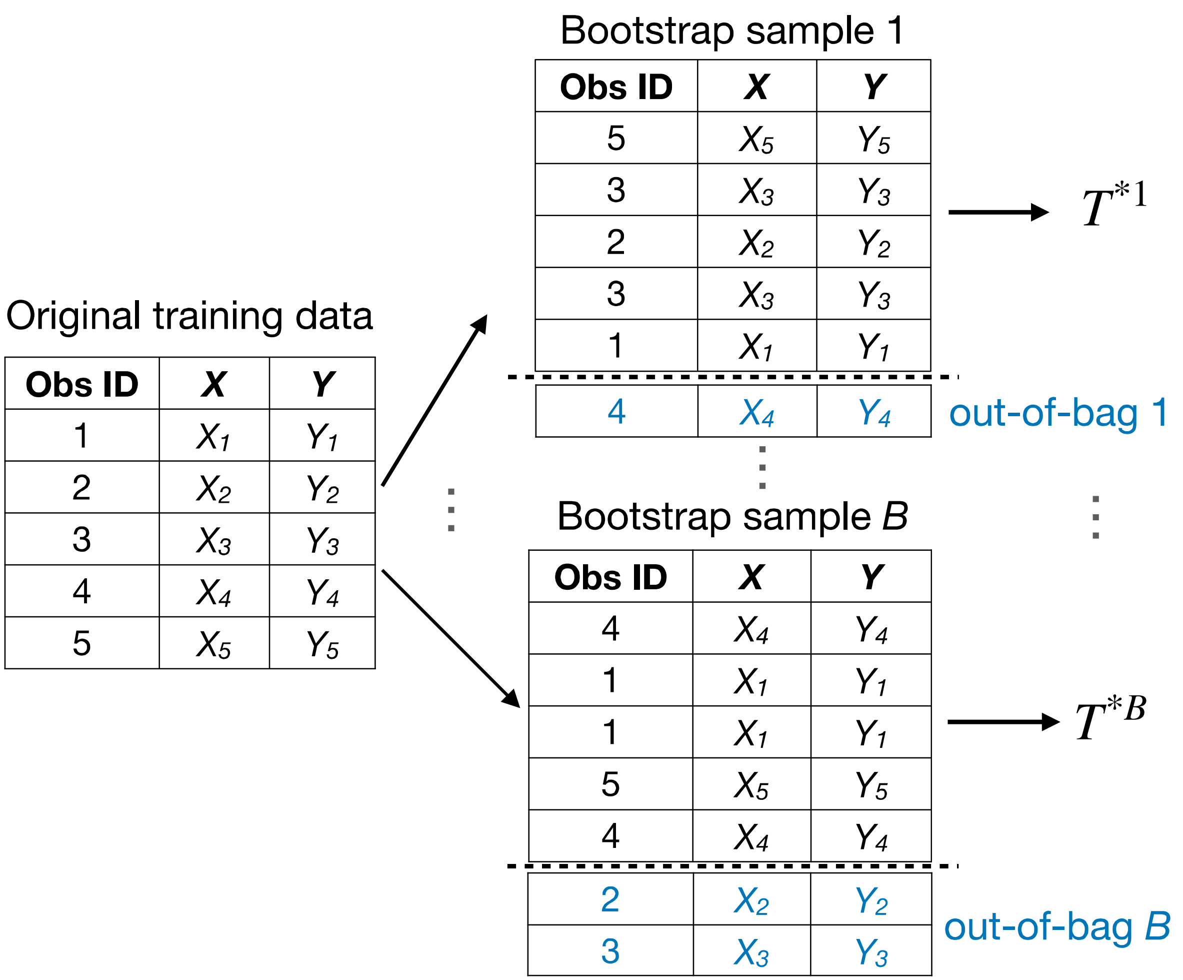
out-of-bag B

$\longrightarrow T^{*B}$

OOB predictions

Obs ID	X	Y	$T^{*1}(X)$	…	$T^{*B}(X)$	$\hat{Y}^{OOB}$
1	X_1	Y_1	—	…	—	$\hat{Y}_1^{OOB}$
2	X_2	Y_2	—	…	$T^{*B}(X_2)$	$\hat{Y}_2^{OOB}$
3	X_3	Y_3	—	…	$T^{*B}(X_3)$	$\hat{Y}_3^{OOB}$
4	X_4	Y_4	$T^{*1}(X_4)$	…	—	$\hat{Y}_4^{OOB}$
5	X_5	Y_5	—	…	—	$\hat{Y}_5^{OOB}$

Out of bag error



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—	…	—	$\hat{Y}_1^{OOB}$
—	…	$T^{*B}(X_2)$	$\hat{Y}_2^{OOB}$
—	…	$T^{*B}(X_3)$	$\hat{Y}_3^{OOB}$
$T^{*1}(X_4)$	…	—	$\hat{Y}_4^{OOB}$
—	…	—	$\hat{Y}_5^{OOB}$

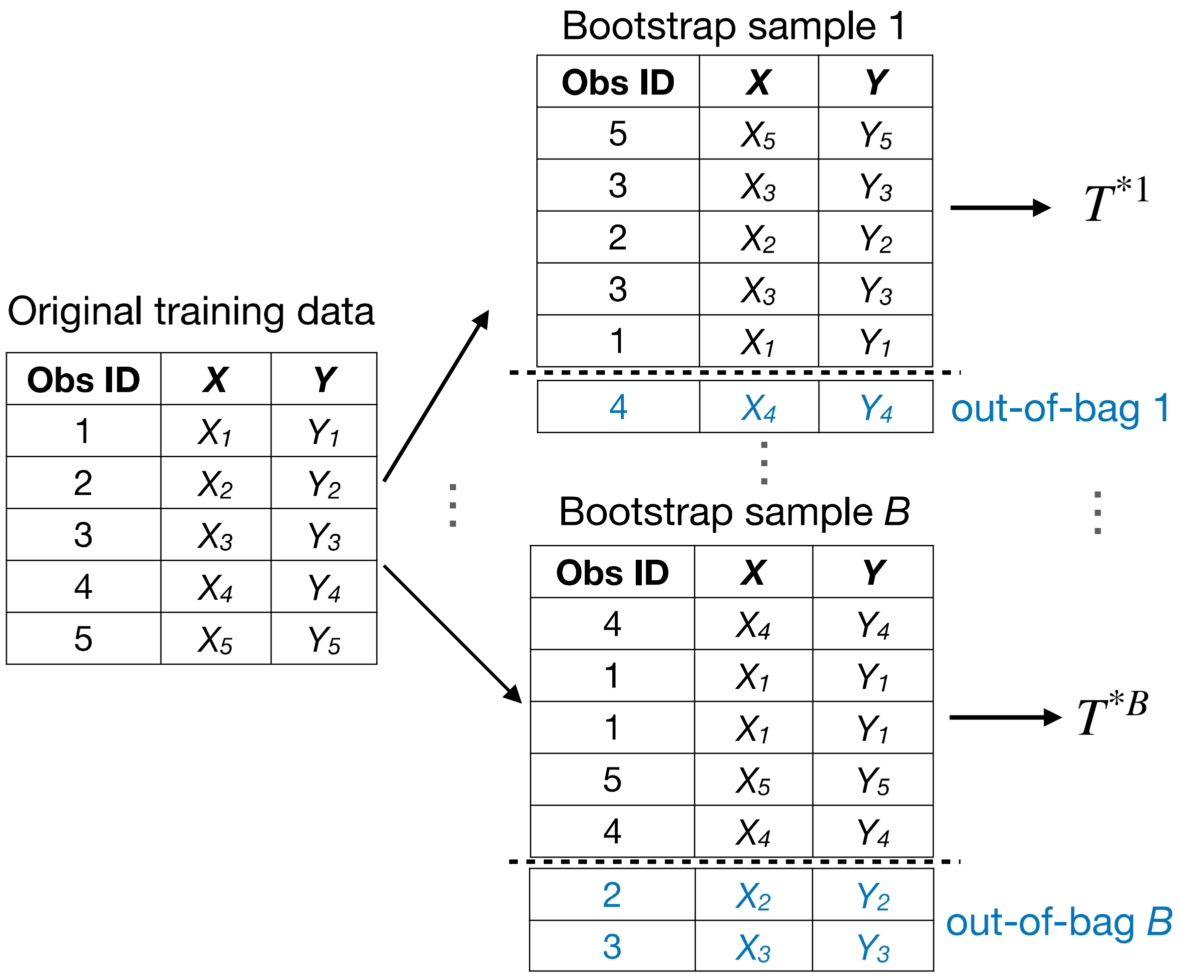
Regression:

$$\hat{Y}_i^{\text{OOB}} = \text{mean}\{T^{*b}(X_i)\}_{i \in \text{OOB}_b}$$

$$\text{OOB err} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i^{\text{OOB}})^2$$

Out of bag error

Average across rows to get OOB predictions



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out-of-bag 1

$\longrightarrow T^{*1}$

Bootstrap sample *B*

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out-of-bag *B*

$\longrightarrow T^{*B}$

OOB predictions

Obs ID	*X*	*Y*	$T^{*1}(X)$	…	$T^{*B}(X)$	$\hat{Y}^{OOB}$
1	X_1	Y_1	–	…	–	$\hat{Y}_1^{OOB}$
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3	X_3	Y_3	–	…	$T^{*B}(X_3)$	$\hat{Y}_3^{OOB}$
4	X_4	Y_4	$T^{*1}(X_4)$	…	–	$\hat{Y}_4^{OOB}$
5	X_5	Y_5	–	…	–	$\hat{Y}_5^{OOB}$

Regression:

$$\hat{Y}_i^{\text{OOB}} = \text{mean}\{T^{*b}(X_i)\}_{i \in \text{OOB}_b}$$

$$\text{OOB err} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i^{\text{OOB}})^2$$

Classification:

$$\hat{Y}_i^{\text{OOB}} = \text{mode}\{T^{*b}(X_i)\}_{i \in \text{OOB}_b}$$

$$\text{OOB err} = \frac{1}{n}\sum_{i=1}^{n} I(Y_i \neq \hat{Y}_i^{\text{OOB}})$$

Parameters to tune (or not)

Random forests generally work pretty well even if not tuned (i.e. if default parameter choices are used).

However, parameters can be tuned using OOB error to improve performance:

- m: most important tuning parameter
- criteria to stop splitting: can be tuned but growing trees about as deep as possible generally works pretty well
- B: least necessary to tune; just choose a large value like 100-1000.

Recommendation is to tune on M

Interpretability and variable importance measures

Compared to trees, main drawback of random forests is reduced interpretability.

However, variable importance measures can help improve the interpretability.

Two types of variable importance measures are used for random forests:

- purity based importance: how much improvement in node purity results from splitting on a feature

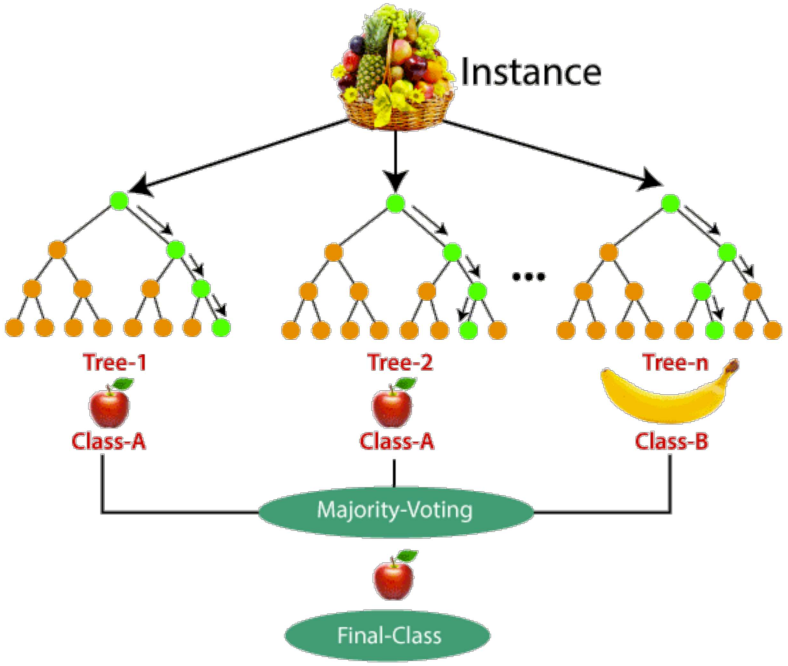
- OOB prediction based importance: how much deterioration in prediction accuracy results from scrambling a feature out of bag

Purity-based variable importance

Consider the construction of one tree. For each split, note the feature that was split on and resulting reduction in RSS or Gini index (i.e. improvement in purity).

Define the importance of each feature in this single tree by summing up the improvement in purity for all splits based on this feature.

For random forests, we can average this quantity over all of the trees to get a purity-based variable importance metric.



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OOB prediction based variable importance

Recall the OOB error introduced a few slides ago.

For each feature j and each tree, consider making predictions on the OOB data after first scrambling feature j. We can therefore get a scrambled OOB error.

For each feature j, we can define an OOB-prediction-based variable importance by the difference in OOB error when this feature is scrambled and when it is not.

X =

X_0	X_1	…	X_j	…	X_{p-1}
12	0		a		1.5
-3	1		b		-0.7
5	0		c		0.2
16	0		d		-3.5
-7	1		e		0.9

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$\xrightarrow{\text{scramble}}$

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Regular OOB predictions

$T^{*1}(X)$	…	$T^{*B}(X)$	$\hat{Y}^{OOB}$
—	…	—	$\hat{Y}_1^{OOB}$
—	…	$T^{*B}(X_2)$	$\hat{Y}_2^{OOB}$
—	…	$T^{*B}(X_3)$	$\hat{Y}_3^{OOB}$
$T^{*1}(X_4)$	…	—	$\hat{Y}_4^{OOB}$
—	…	—	$\hat{Y}_5^{OOB}$

→ Regular OOB error

Scrambled OOB predictions

$T^{*1}(X)$	…	$T^{*B}(X)$	$\hat{Y}^{OOB}$
—	…	—	$\hat{Y}_1^{OOB}$
—	…	$T^{*B}(X_2)$	$\hat{Y}_2^{OOB}$
—	…	$T^{*B}(X_3)$	$\hat{Y}_3^{OOB}$
$T^{*1}(X_4)$	…	—	$\hat{Y}_4^{OOB}$
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—	…	—	$\hat{Y}_5^{OOB}$

→ Regular OOB error

Scrambled OOB predictions

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$T^{*1}(X_4)$	…	—	$\hat{Y}_4^{OOB}$
—	…	—	$\hat{Y}_5^{OOB}$

→ Scrambled OOB error

Var. Imp. = scrambled OOB err - regular OOB err

Summary

- Random forests are a fancier version of bagging based on random sub-sampling of m features at each split point.

- They improve on bagging by de-correlating the bootstrapped decision trees and therefore reducing the variance of the method.

- OOB error is a nice alternative to cross-validation error for random forests, and can be used to tune parameters such as m.

- Random forests usually give much better prediction performance than individual decision trees, but at the cost of interpretability.

- Nevertheless, there are a couple ways to measure variable importance in random forests, giving us some interpretability.

Random forests are a state-of-the-art tool for predictive modeling.