DATA 301:
Gradient Boosted Trees
(XGBoost, lightGBM)

Topics

Introduction
Bagging verses Boosting
Example
Benefits
Drawbacks
Packages
Summary

Introduction

Random forest are a collection of decision trees that are created using a technique called ‘bagging’
Which means create a bunch of independent decision trees and average (or majority) vote their results

Boosted decision trees are a collection of decision trees that are created using a technique called ‘boosting’
Which means create the trees one at a time, each new tree designed to improve upon previous trees estimates

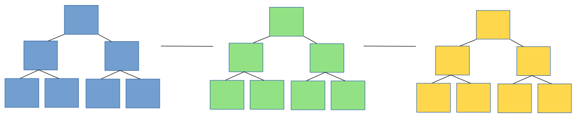
Bagging verses Boosting

Bagging

Bagging verses Boosting

Bagging

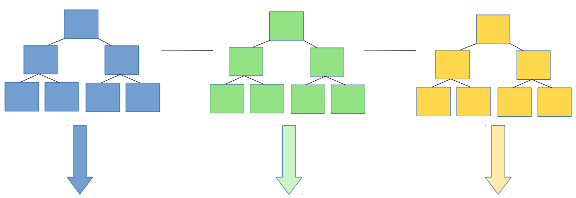
Multiple independent trees



Bagging verses Boosting

Bagging

Multiple independent trees



C1 C2 C1

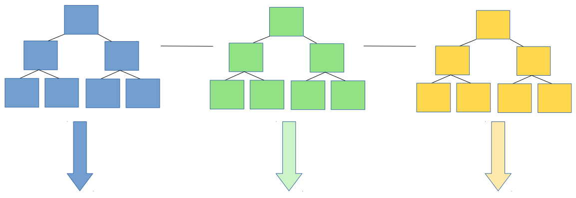
For Classification
Use majority vote

C1 C2 C1 = C1

Bagging verses Boosting

Bagging

Multiple independent trees



p1 p2 p3

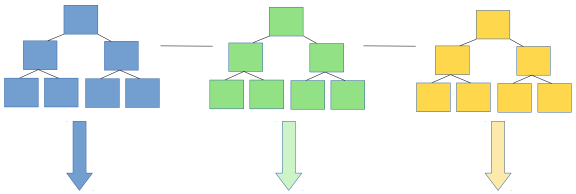
For Regression just Average results

(P1 + p2 + p3)/3 =val

Bagging verses Boosting

Bagging

Multiple independent trees



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Bagging verses Boosting

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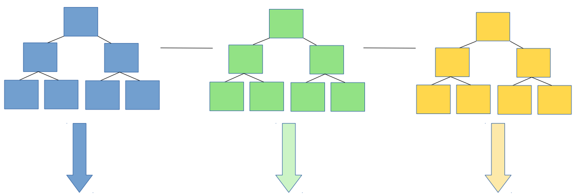
Multiple independent trees



p1 p2 p3

For Regression just Average results

(P1 + p2 + p3)/3 =val

Build trees in parrallel so very fast

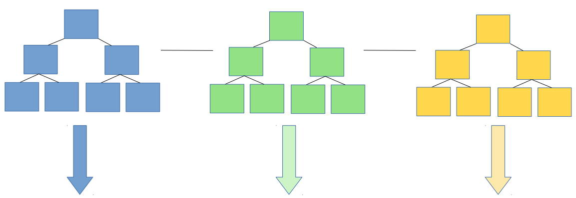
Boosting

- Start with average target value

Bagging verses Boosting

Bagging

Multiple independent trees



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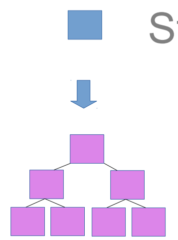
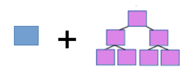


Start with average target value

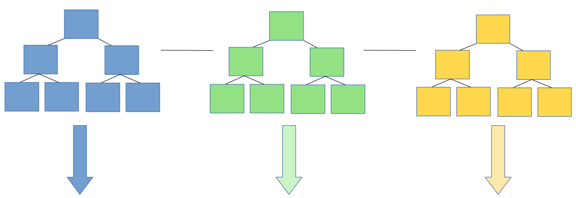
Create tree based on errors from previous ensemble and combine outputs



Bagging verses Boosting

Bagging

Multiple independent trees



p1 p2 p3

For Regression just Average results

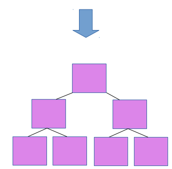
(P1 + p2 + p3)/3 =val

Lets stick with regression

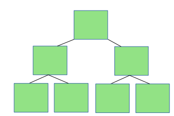
Build trees in parrallel
so very fast

Boosting

Start with average target value



Create tree based on errors from previous ensemble and combine outputs



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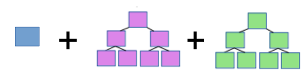
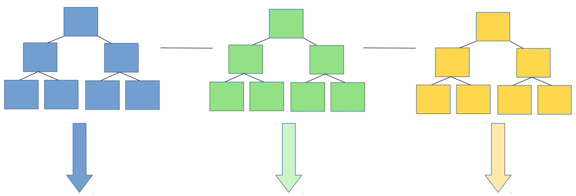


Bagging verses Boosting

Bagging

Multiple independent trees



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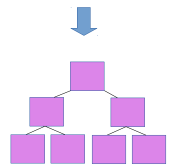

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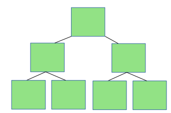

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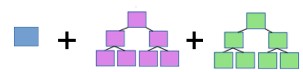
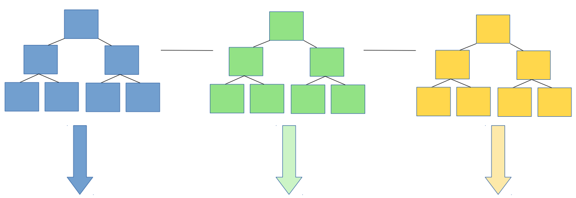


Continue until build number trees requested
Or additional trees fail to improve prediction

Bagging verses Boosting

Bagging

Multiple independent trees



p1 p2 p3

For Regression just Average results

(P1 + p2 + p3)/3 =val

Lets stick with regression

Build trees in parrallel
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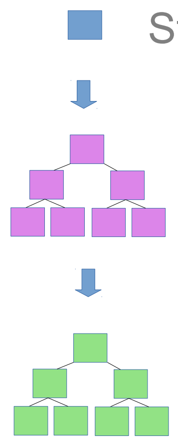
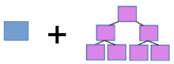
Boosting



Start with average target value

Create tree based on errors from previous ensemble and combine outputs



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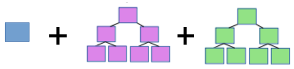

Continue until build number trees requested
Or additional trees fail to improve prediction

Build trees sequentially so slow
But more accurate than Random Forest

Example

Height	Color	Gender	Weight
1.6	Blue	Male	88
1.6	Green	Female	76
1.5	Blue	Female	56
1.8	Red	Male	73
1.5	Green	Male	77
1.4	Blue	Female	57

Average weight

71.2

Calculate average weight

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

Height	Color	Gender	Weight	Residuals
1.6	Blue	Male	88	16.8
1.6	Green	Female	76	
1.5	Blue	Female	56	
1.8	Red	Male	73	
1.5	Green	Male	77	
1.4	Blue	Female	57	

Average weight

71.2

Calculate difference between average weight and Weight
Add as new column Residuals
(1st row 88-71.2=16.8)

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

Height	Color	Gender	Weight	Residuals
1.6	Blue	Male	88	16.8
1.6	Green	Female	76	4.8
1.5	Blue	Female	56	-15.2
1.8	Red	Male	73	1.8
1.5	Green	Male	77	5.8
1.4	Blue	Female	57	-14.2

Average weight

71.2

Calculate difference between average weight and Weight
Add as new column Residuals
(1st row 88-71.2=16.8)
Do for All rows

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

Average weight

71.2

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1.6	Blue	Male	88	16.8
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1.4	Blue	Female	57	-14.2

Now build a tree to predict the Residuals using Height, Color and Gender to predict the residuals. Trees have several tuning Parameters,

max_depth= how many levels per tree

max_leaf_nodes: number terminal leaf nodes

Set max_leaf_nodes = 4 for this problem

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

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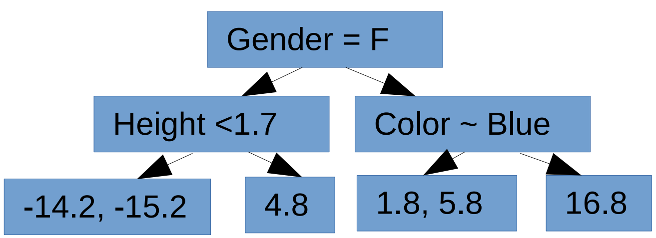

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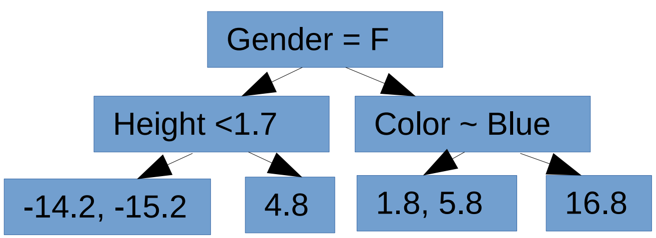

But can have a max of 4 leaf nodes

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

Average weight

71.2

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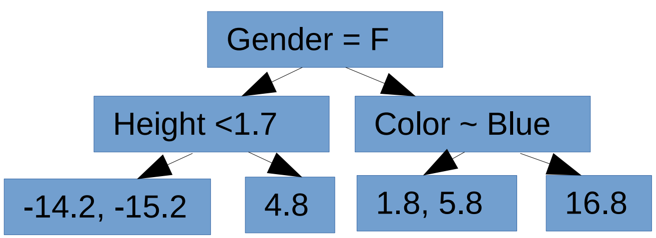

So average the leaf nodes with more than 2 values
(-14.2+-15.2)/2=-14.7
(1.8 + 5.8)/2=3.8

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

Average weight

71.2

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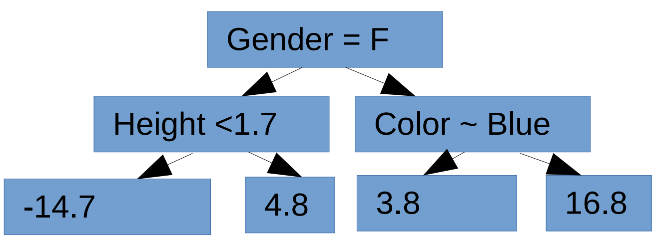

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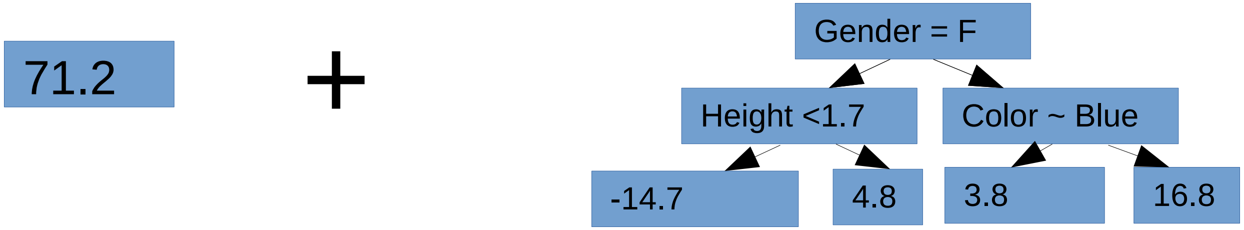
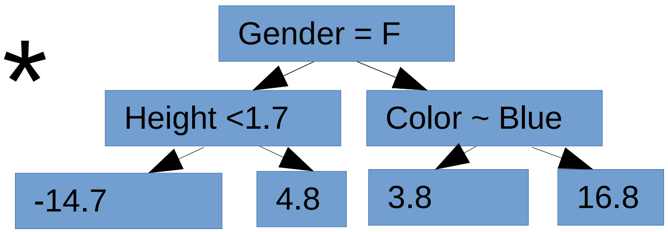


Combine new tree with
Original leaf and use to
calculate new residuals

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

71.2 + (lr)*

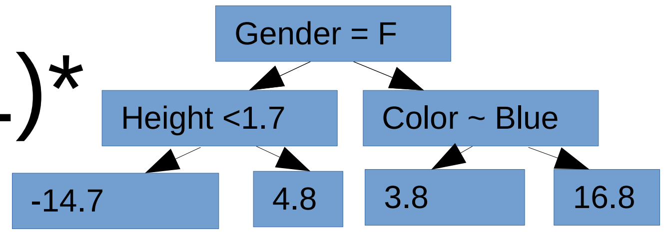


Use only part of the new trees
prediction to prevent overfitting by
Multiplying it’s output by learning rate <1

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

71.2 + (0.1)*

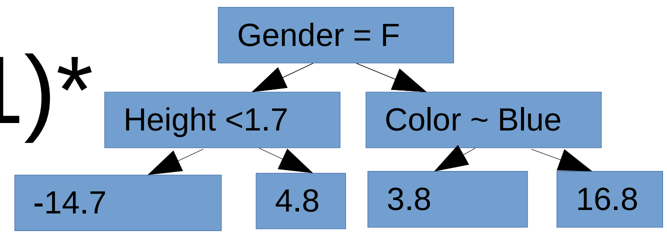


Use only part of the new trees
prediction to prevent overfitting by
Multiplying it’s output by learning rate (lr)
Lr=0.1

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

71.2 + (0.1)*



Calculate predicted weight (for row 0)
71.2 +0.1*16.8=72.9

Height	Color	Gender	Weight
1.6	Blue	Male	88
1.6	Green	Female	76
1.5	Blue	Female	56
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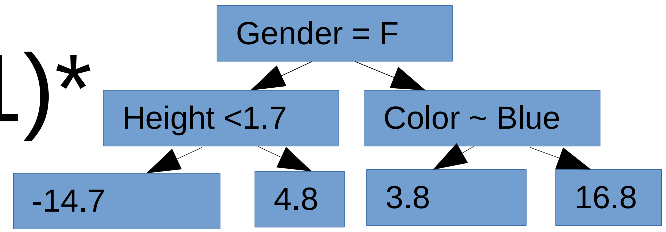

Calculate predicted weight (for row 0)
71.2 +0.1*16.8=72.9

Which is a little better than 71.2

Height	Color	Gender	Weight
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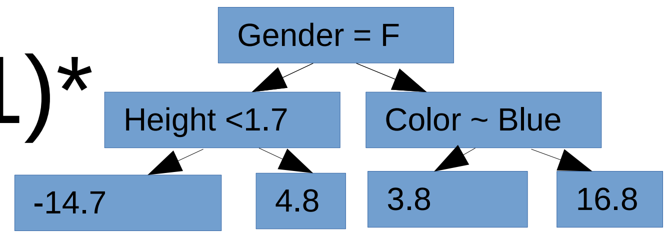

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Height	Color	Gender	Weight	Residuals
1.6	Blue	Male	88	15.1
1.6	Green	Female	76	
1.5	Blue	Female	56	
1.8	Red	Male	73	
1.5	Green	Male	77	
1.4	Blue	Female	57	

Which is a little better than 71.2

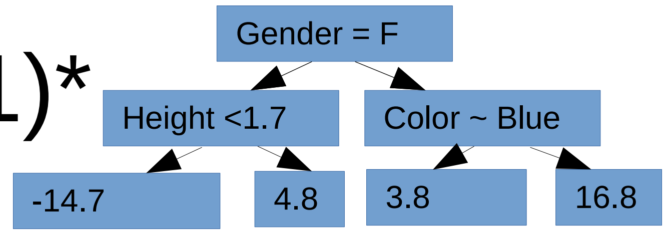
Calculate the new residuals (first row)
88-72.9=15.1

We are getting closer to the true weight

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

71.2 + (0.1)*



Calculate predicted weight (for row 0)
71.2 +0.1*16.8=72.9

Which is a little better than 71.2

Calculate the new residuals (first row)
88-72.9=15.1

Do for all rows

Height	Color	Gender	Weight	Residuals
1.6	Blue	Male	88	15.1
1.6	Green	Female	76	4.3
1.5	Blue	Female	56	-13.7
1.8	Red	Male	73	1.4
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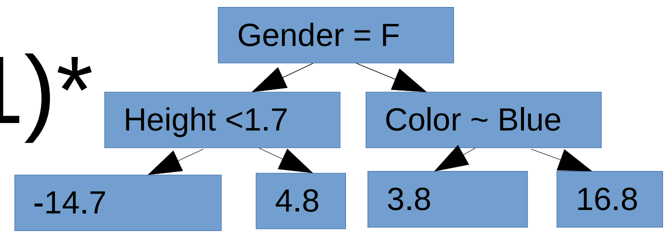
Example

71.2 + (0.1)*



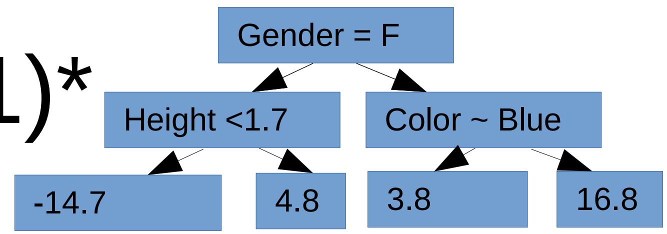
Original residuals

Residuals
16.8
4.8
-15.2
1.8
5.8
-14.2

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

71.2 + (0.1)*



Original residuals

Residuals
16.8
4.8
-15.2
1.8
5.8
-14.2

New residuals

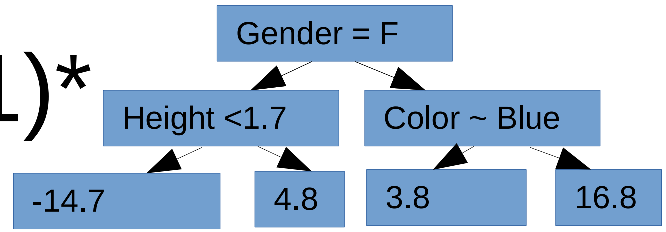
Residuals
15.1
4.3
-13.7
1.4
5.4
-12.7

Note that we are reducing the Residual size

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

71.2 + (0.1)*



Original residuals

Residuals
16.8
4.8
-15.2
1.8
5.8
-14.2

New residuals

Residuals
15.1
4.3
-13.7
1.4
5.4
-12.7

Note that we are reducing the Residual size

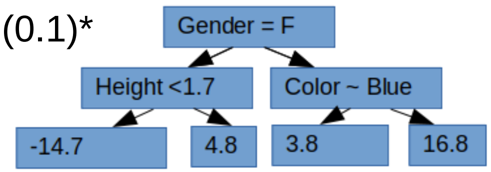
Repeat the process of calculating Residuals and building trees until Either max trees are reached or Residuals stop getting better.

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

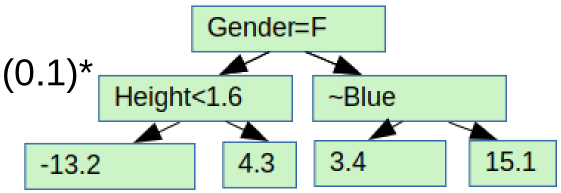
Example

When we have enough trees, we can predict weight

weight= 71.2 + (0.1)*



+ (0.1)*



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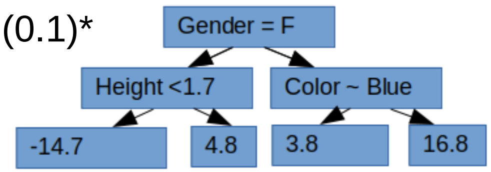

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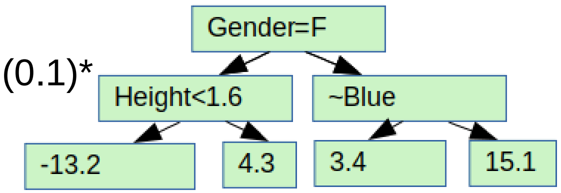


Height	Color	Gender	Weight
1.6	Blue	Male	88

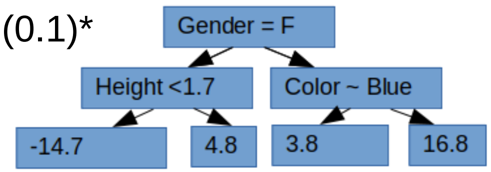
Weight= 71.2 + 0.1*16.8 + 0.1*(15.1)
= 74.39

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Example

When we have enough trees, we can predict weight

weight= 71.2 + (0.1)*



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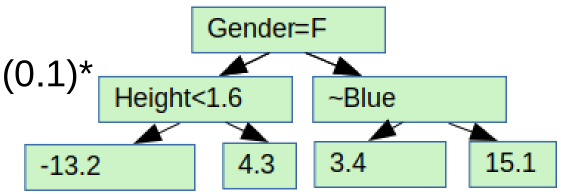

Height	Color	Gender	Weight
1.6	Blue	Male	88

Weight= 71.2 + 0.1*16.8 + 0.1*(15.1)
= 74.39

The more trees you have the more accurate it gets (at the risk of overfitting)

Example from https://www.youtube.com/watch?v=3CC4N4z3GJc

Benefits

- Reducing residual approach lets trees push wrong answers in the right direction.
- Each tree tries to improve the overall model by reducing residuals. They work together.
- More accurate than random forest, where each tree makes an independent estimate.

Drawbacks

- Trees calculated serially. Much slower than Random Forest
- More hyperparameters to tune (learning rate, max_tree_depth, max_number_leaves etc.)

Packages

- XGBoost
- lightGBM

Summary

- Gradient Boosted trees are the preferred tree ensemble given it's increase in accuracy (or F1, or R^2 or whatever performance metric of choice)
- Work with regression and classification
- Not built into scikitlearn
- Harder to tune (more hyperparameters)
- Longer to train