

DATA 301:

Gradient Boosted Trees

(lightGBM, catboost)

Topics

Introduction

Bagging verses Boosting

Example

Boosting Benefits

Boosting 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

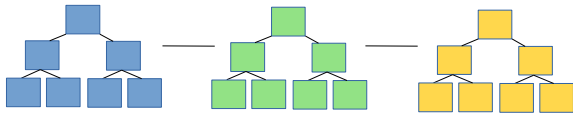
Bagging verses Boosting

Bagging

Bagging verses Boosting

Bagging

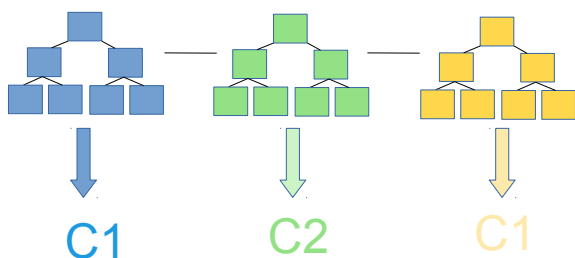
Multiple independent trees



Bagging verses Boosting

Bagging

Multiple independent trees



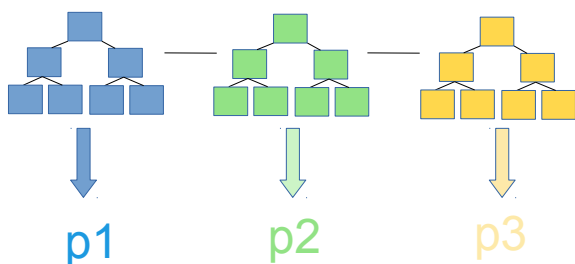
For Classification
Use majority vote

C1 C2 C1 = C1

Bagging verses Boosting

Bagging

Multiple independent trees



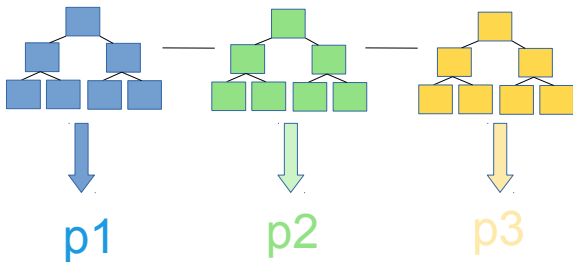
For Regression just Average results

$$(p1 + p2 + p3)/3 = \text{val}$$

Bagging versus Boosting

Bagging

Multiple independent trees



For Regression just Average results

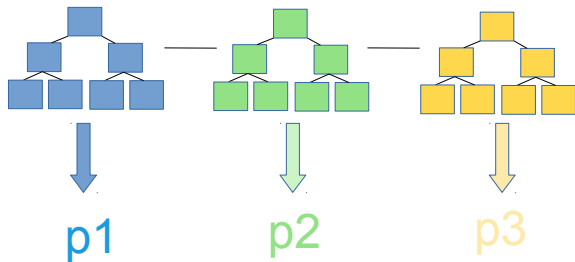
$$(p1 + p2 + p3)/3 = \text{val}$$

Build trees in parallel
so very fast

Bagging verses Boosting

Bagging

Multiple independent trees



For Regression just Average results

$$(p1 + p2 + p3)/3 = \text{val}$$

Build trees in parallel
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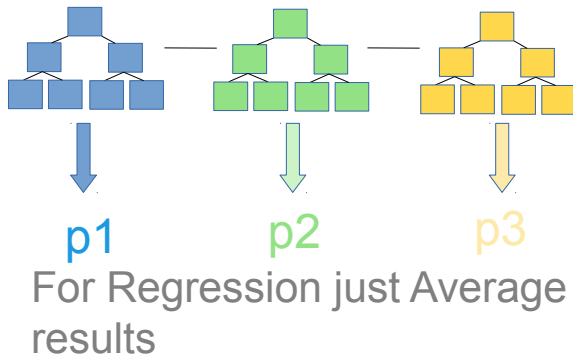
Boosting

■ Start with average target value

Bagging versus Boosting

Bagging

Multiple independent trees

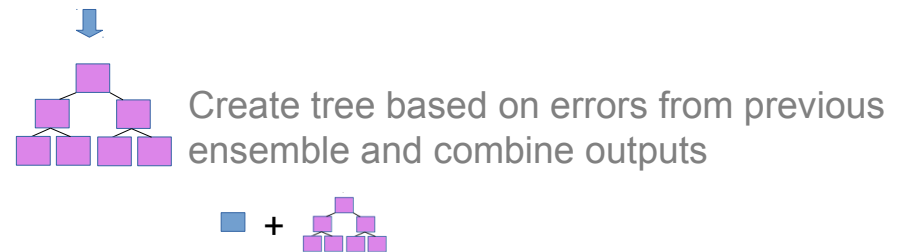


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Boosting

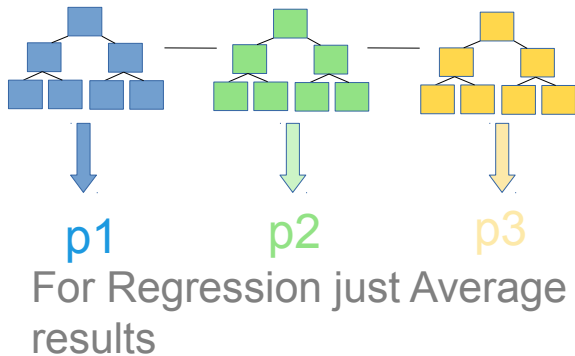
Start with average target value



Bagging versus Boosting

Bagging

Multiple independent trees

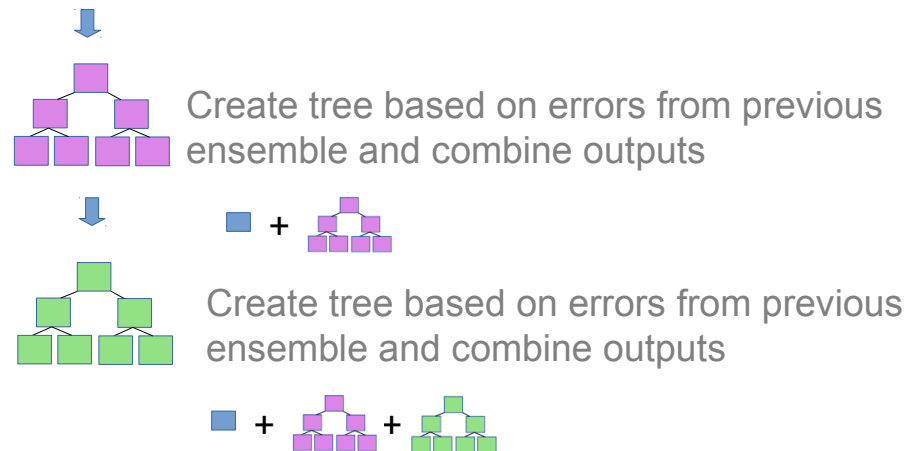


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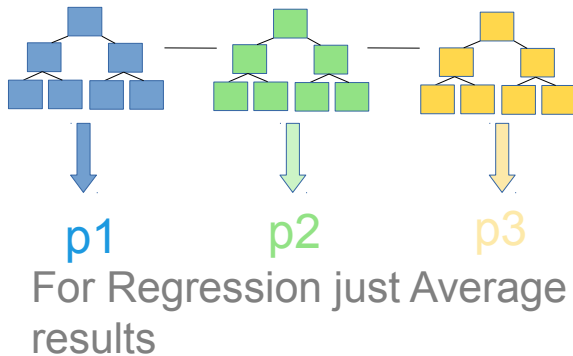
Start with average target value



Bagging versus Boosting

Bagging

Multiple independent trees

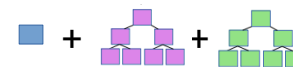
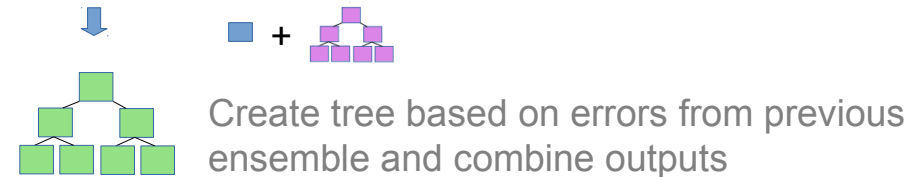
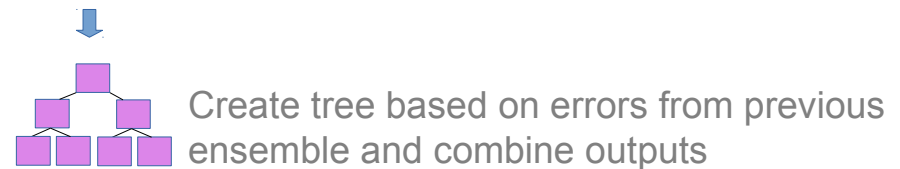


$$(p1 + p2 + p3)/3 = \text{val}$$

Build trees in parallel
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Boosting

Start with average target value

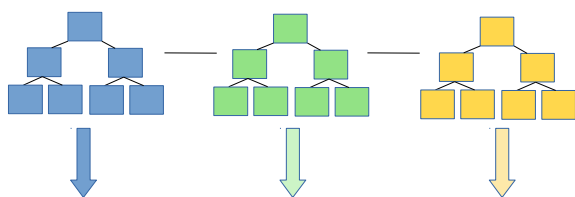


Continue until build number trees requested
Or additional trees fail to improve prediction

Bagging versus Boosting

Bagging

Multiple independent trees



p1

p2

p3

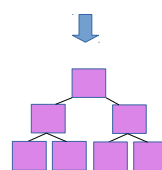
For Regression just Average results

$$(p1 + p2 + p3)/3 = \text{val}$$

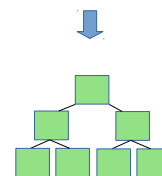
Build trees in parallel
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Boosting

Start with average target value



Create tree based on errors from previous ensemble and combine outputs



Create tree based on errors from previous ensemble and combine outputs



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

Build trees sequentially so slow.
But more accurate than bagged methods like
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

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

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
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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 this for All rows

Example

Height	Color	Gender	Weight	Residuals
1.6	Blue	Male	88	16.8
1.6	Green	Female	76	4.8
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1.5	Green	Male	77	5.8
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Average weight

71.2

Now build a tree to predict the Residuals. Use Height, Color and Gender. 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

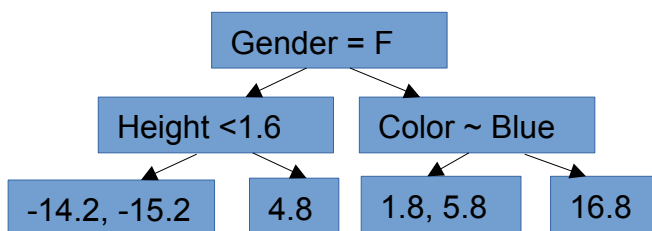
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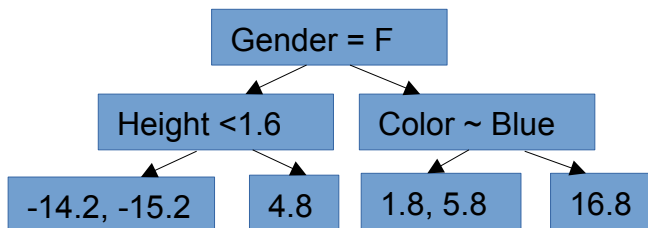
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But can have a max of only 4 leaf nodes

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

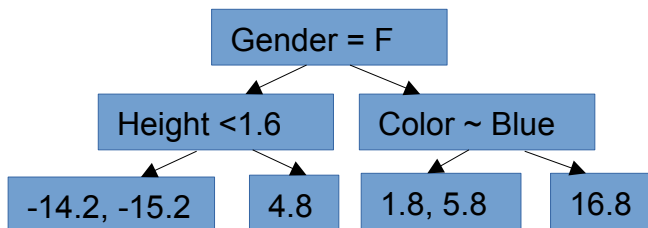
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So average the leaf nodes with more than 2 values
 $(-14.2 + -15.2) / 2 = -14.7$
 $(1.8 + 5.8) / 2 = 3.8$

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

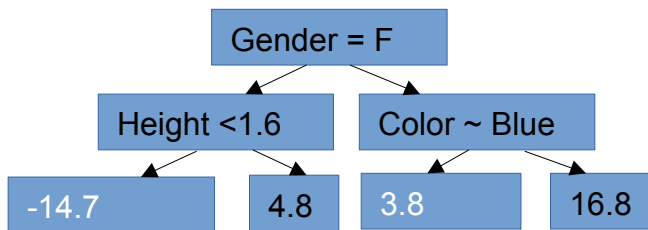
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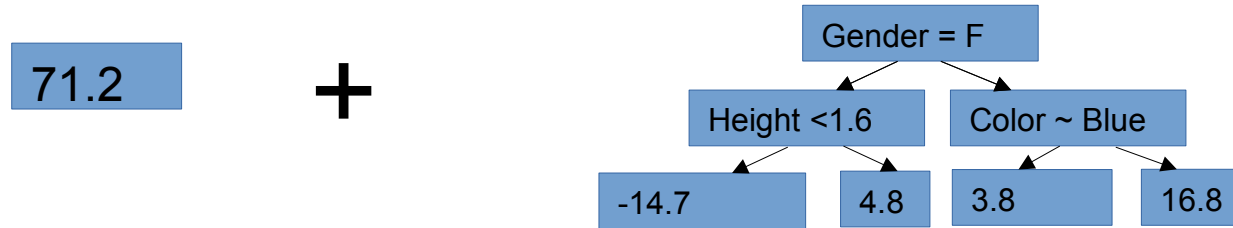
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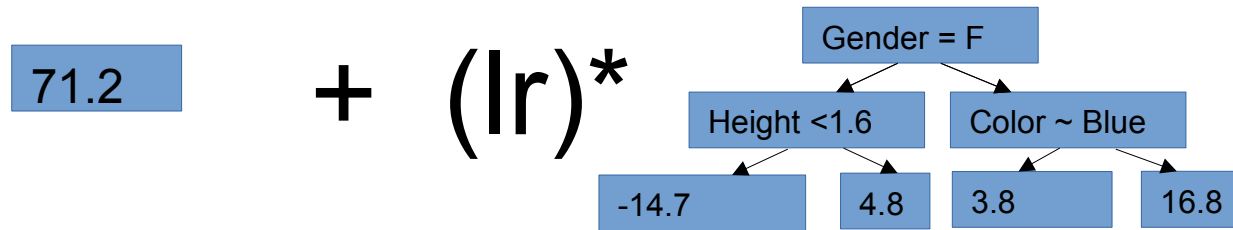
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Example



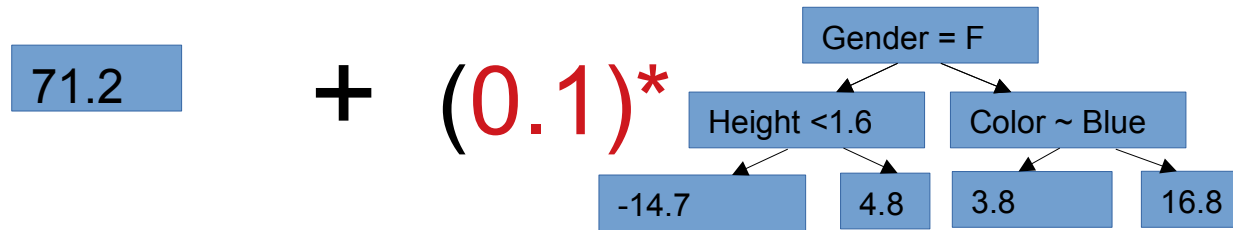
Combine new tree with
Original leaf and use to
calculate new residuals

Example



Use only part of the new trees
prediction to prevent overfitting (low bias, high variance) by
Multiplying it's output by learning rate < 1

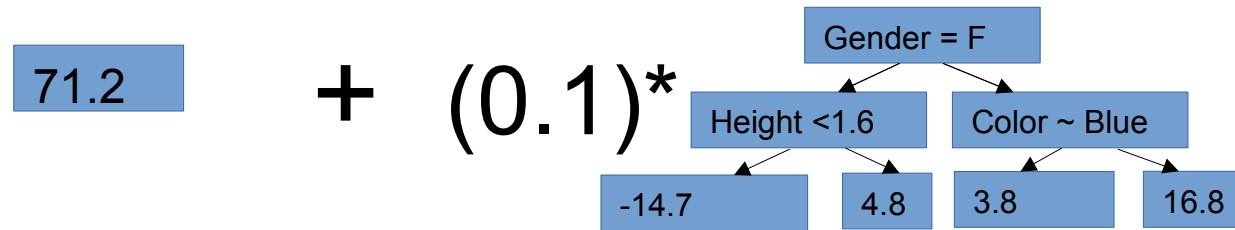
Example



Use only part of the new trees
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Multiplying it's output by learning rate <1

Lr=0.1

Example

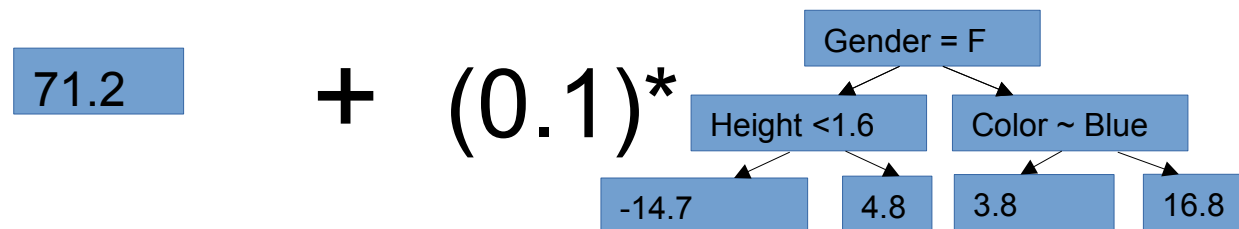


Calculate predicted weight (for row 0)
 $71.2 + 0.1 * 16.8 = 72.9$

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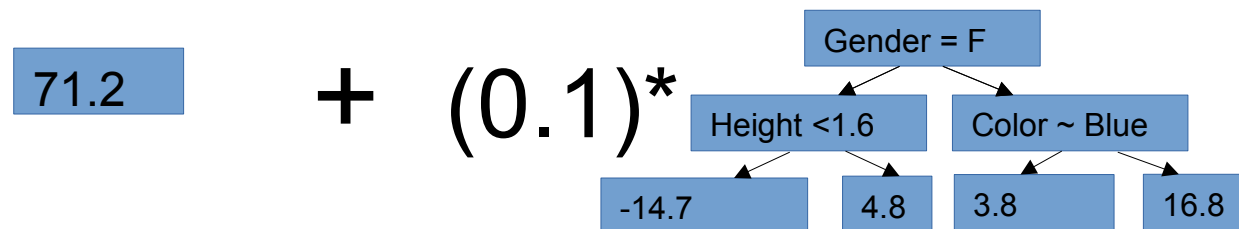


Calculate predicted weight (for row 0)
 $71.2 + 0.1 * 16.8 = 72.9$

Which is a little better than 71.2 (the original average estimate)

Height	Color	Gender	Weight
1.6	Blue	Male	88
1.6	Green	Female	76
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Example



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

Which is a little better than 71.2

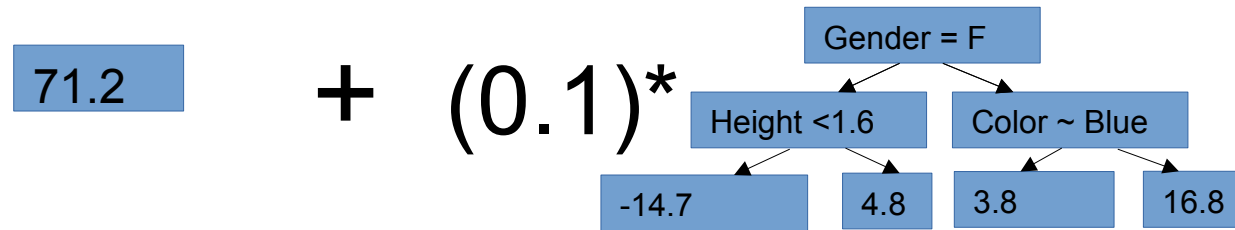
Calculate the new residuals (first row)
 $88 - 72.9 = 15.1$

We are getting closer to the true weight

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	

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

Example



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

Which is a little better than 71.2

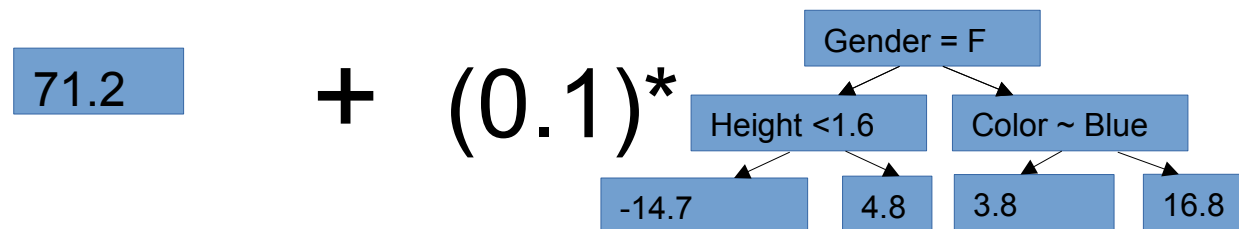
Calculate the new residuals (first row)
 $88 - 72.9 = 15.1$

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
1.5	Green	Male	77	5.4
1.4	Blue	Female	57	-12.7

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

Example



Original
residuals

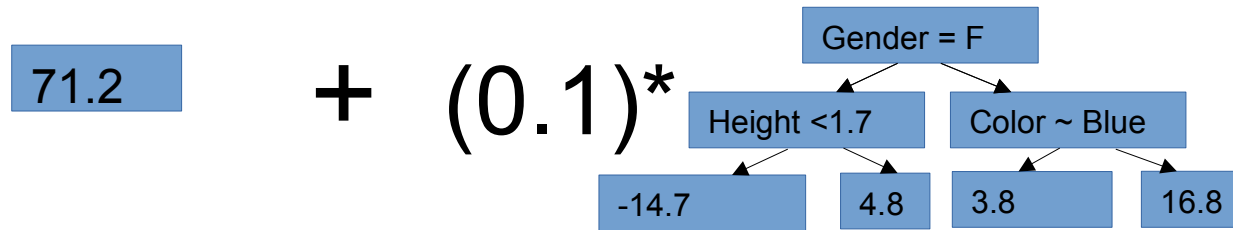
Residuals
16.8
4.8
-15.2
1.8
5.8
-14.2

New
residuals

Residuals
15.1
4.3
-13.7
1.4
5.4
-12.7

Note that the New Residuals are lower Than the originals. We are reducing the Error as we add more trees.

Example



Original
residuals

Residuals
16.8
4.8
-15.2
1.8
5.8
-14.2

New
residuals

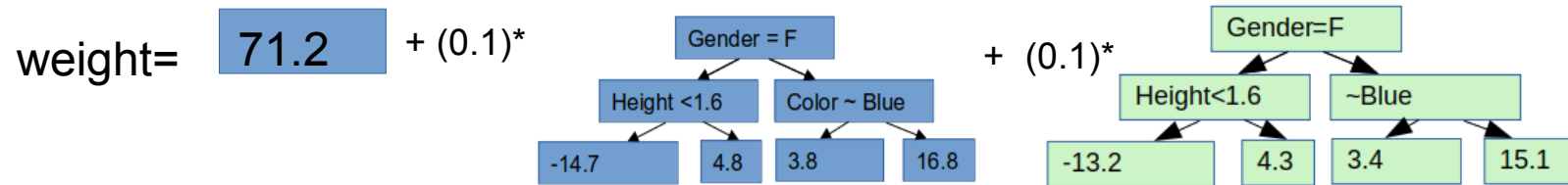
Residuals
15.1
4.3
-13.7
1.4
5.4
-12.7

Note that the New Residuals are lower Than the originals. We are reducing the Error as we add more trees.

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

Example

When we have enough trees, we can predict weight



Example

When we have enough trees, we can predict weight

$$\text{weight} = 71.2 + (0.1)^* \left(\begin{array}{c} \text{Gender} = F \\ \swarrow \quad \searrow \\ \text{Height} < 1.6 \quad \text{Color} \sim \text{Blue} \\ \swarrow \quad \searrow \quad \swarrow \quad \searrow \\ -14.7 \quad 4.8 \quad 3.8 \quad 16.8 \end{array} \right) + (0.1)^* \left(\begin{array}{c} \text{Gender} = F \\ \swarrow \quad \searrow \\ \text{Height} < 1.6 \quad \sim \text{Blue} \\ \swarrow \quad \searrow \quad \swarrow \quad \searrow \\ -13.2 \quad 4.3 \quad 3.4 \quad 15.1 \end{array} \right)$$

Height	Color	Gender	Weight
1.6	Blue	Male	88



$$\begin{aligned} \text{Weight} &= 71.2 + 0.1 * 16.8 + 0.1 * (15.1) \\ &= 74.39 \end{aligned}$$

Example

When we have enough trees, we can predict weight

$$\text{weight} = 71.2 + (0.1) * \left(\begin{array}{c} \text{Gender} = F \\ \swarrow \quad \searrow \\ \text{Height} < 1.6 \quad \text{Color} \sim \text{Blue} \\ \swarrow \quad \searrow \quad \swarrow \quad \searrow \\ -14.7 \quad 4.8 \quad 3.8 \quad 16.8 \end{array} \right) + (0.1) * \left(\begin{array}{c} \text{Gender} = F \\ \swarrow \quad \searrow \\ \text{Height} < 1.6 \quad \sim \text{Blue} \\ \swarrow \quad \searrow \quad \swarrow \quad \searrow \\ -13.2 \quad 4.3 \quad 3.4 \quad 15.1 \end{array} \right)$$

Height	Color	Gender	Weight
1.6	Blue	Male	88



$$\begin{aligned} \text{Weight} &= 71.2 + 0.1 * 16.8 + 0.1 * (15.1) \\ &= 74.39 \end{aligned}$$

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

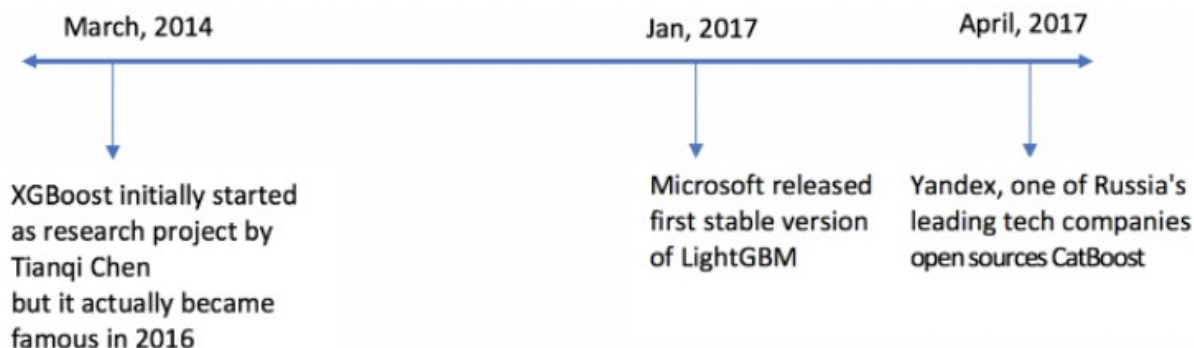
- Reducing residual approach lets trees push wrong answers in the 'right' direction.
- Each tree tries to improve the overall model by reducing residuals. Trees work together.
- More accurate than random forest, where each tree makes an independent estimate.

Drawbacks

- Trees calculated serially. Much slower than Random Forest which is calculated in parallel.
- More hyperparameters to tune (learning rate, max_tree_depth, max_leaf_nodes etc.)

Packages

- LightGBM: by Microsoft, gradient boosted trees
- Catboost: by Yandex, more gradient boosted trees
- Sklearn: GradientBoostingClassifier and GradientBoostingRegressor, **not covered here since LightGBM and Catboost are faster, more accurate and support sklearn's default model training procedure**
- XGBoost: still more gradient boosted trees, **not covered here because they take MUCH longer to train than catboost or 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
- Built into scikitlearn
- Harder to tune (more hyperparameters)
- Longer to train