LEC004 Demand Forecasting

VG441 SS2021

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Ensemble Learning

"The wisdom of the crowd is the collective opinion of
a group of individuals rather than that of a single expert."

"A group of predictors is called an ensemble. Therefore this Machine Learning technique is known as Ensemble Learning. Voilá!"

"Ensemble methods work best when the predictors are as independent of one another as possible. One way to get diverse classifiers is to train them using very different algorithms. This increases the chance that they will make very different types of errors, improving the ensemble's accuracy."

Ensemble Learning Techniques

- Hard voting classifier (for classification)

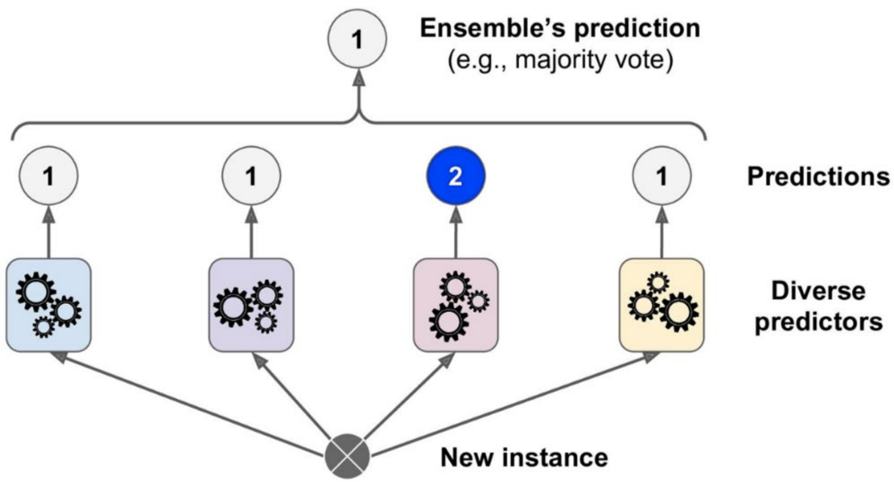
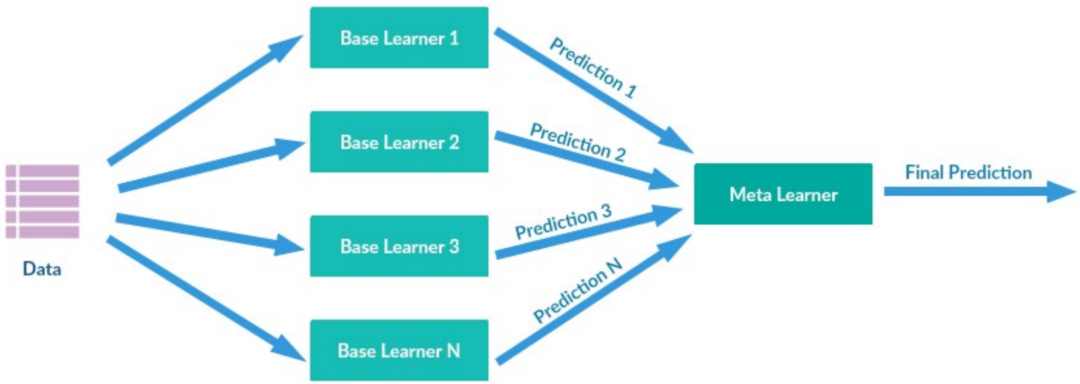


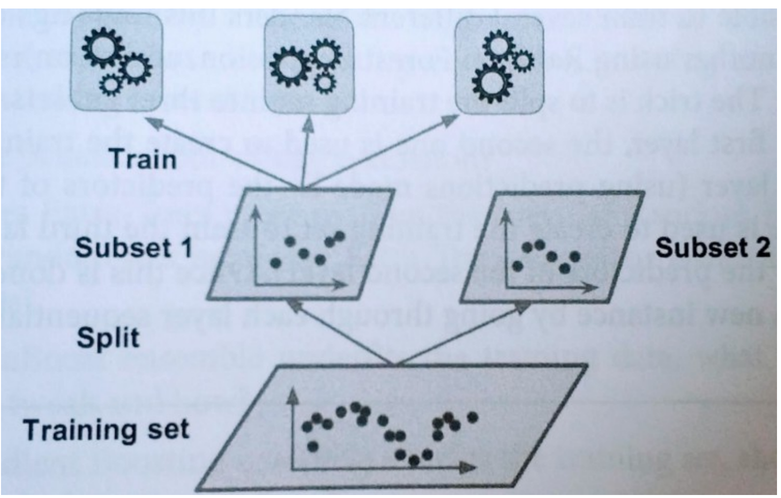
Figure 7-2. Hard voting classifier predictions

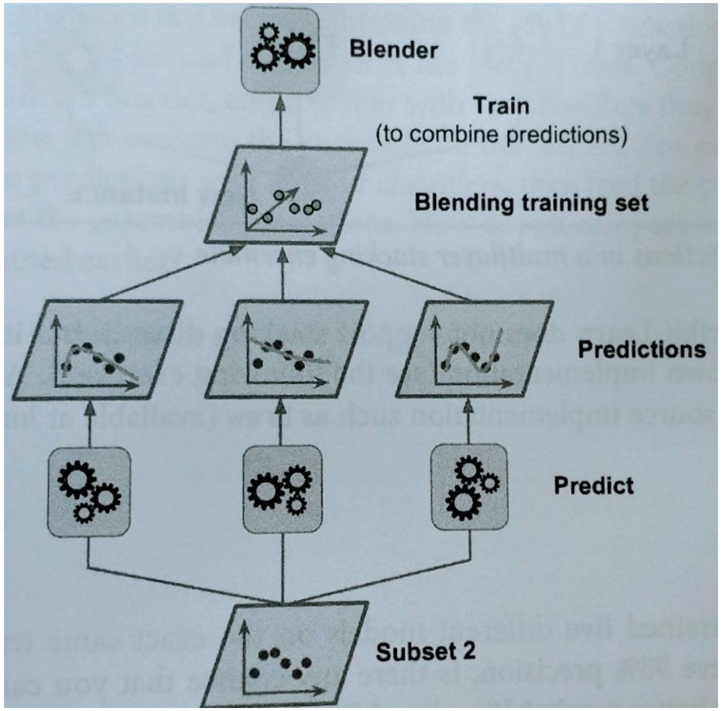
- Averaging or weighted averaged (for regression)

Ensemble Learning Techniques

- Stacking

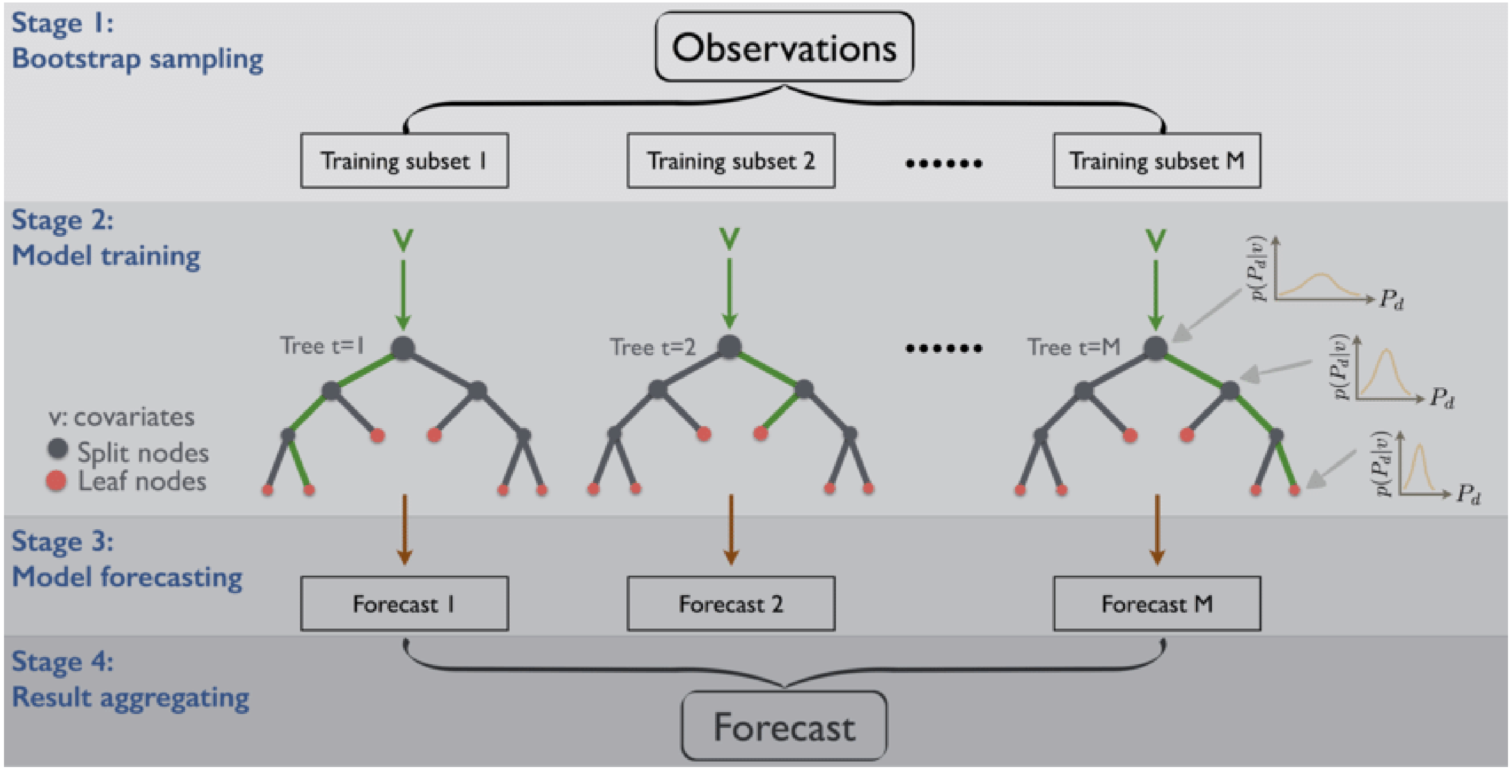






Ensemble Learning Techniques

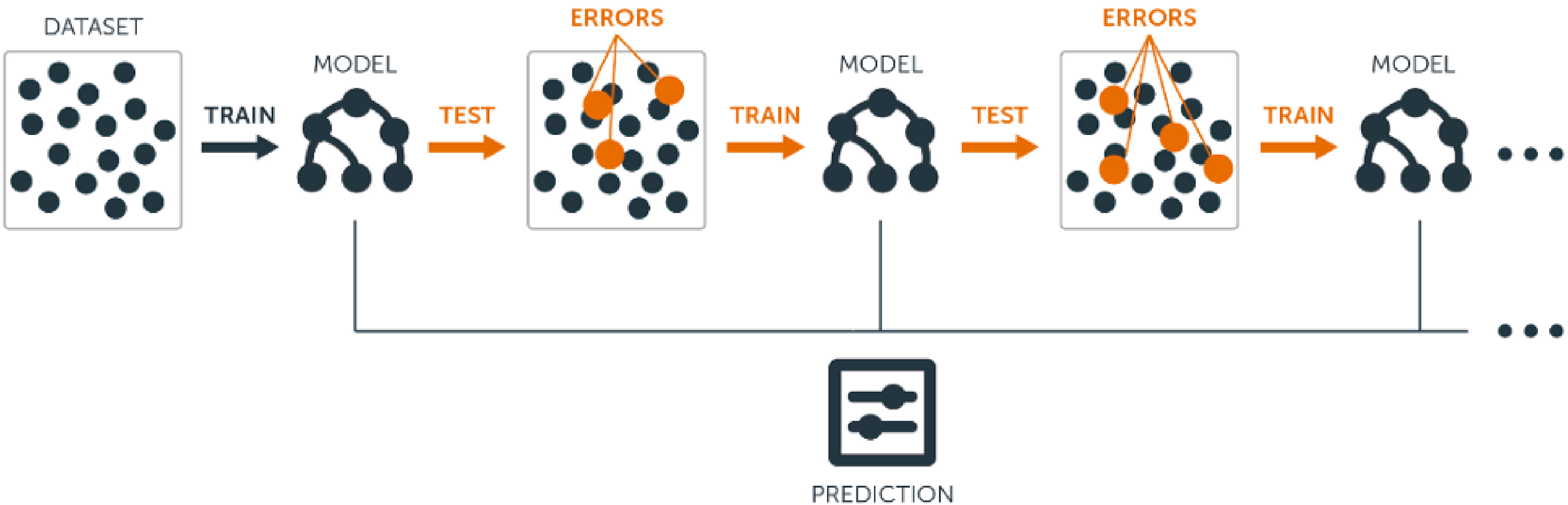
- Bagging



Random Forest

Ensemble Learning Techniques

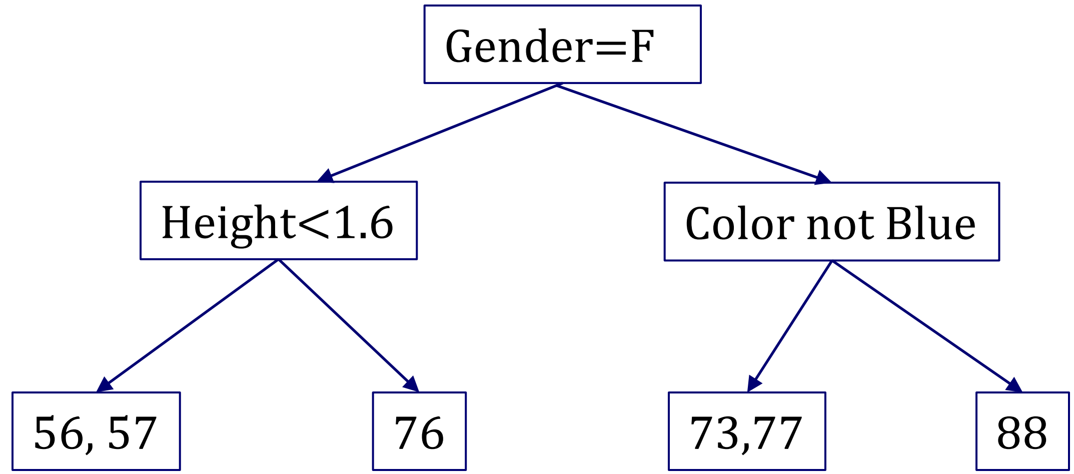
- Boosting



AdaBoost, Gradient Boosting, XGBoost

Decision Tree

Height (m)	Favorite Color	Gender	Weight (kg)
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



Question 1: How do we determine the next node (starting from root)?

Question 2: Should we split at the current node?

How to determine and split a node?

Measure of impurity (for regression) is deviance

Height (m)	Favorite Color	Gender	Weight (kg)
1.6	Blue	Male	88
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1.5	Blue	Female	56
1.8	Red	Male	73
1.5	Green	Male	77
1.4	Blue	Female	57

88, 76, 56, 73, 77, 57

Deviance = 774.83

Gender=F

76, 56, 57

88, 73, 77

Deviance = 254 + 120.67 = 374.67

Height<1.6

56, 77, 57

88, 76, 73

Deviance = 280.67 + 126 = 406.67

Not Blue

76, 73, 77

88, 56, 57

Deviance = 8.67 + 662 = 670.67

Gradient Boosting

F0 = Initial Model = Taking the mean

Height (m)	Favorite Color	Gender	Weight (kg)
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

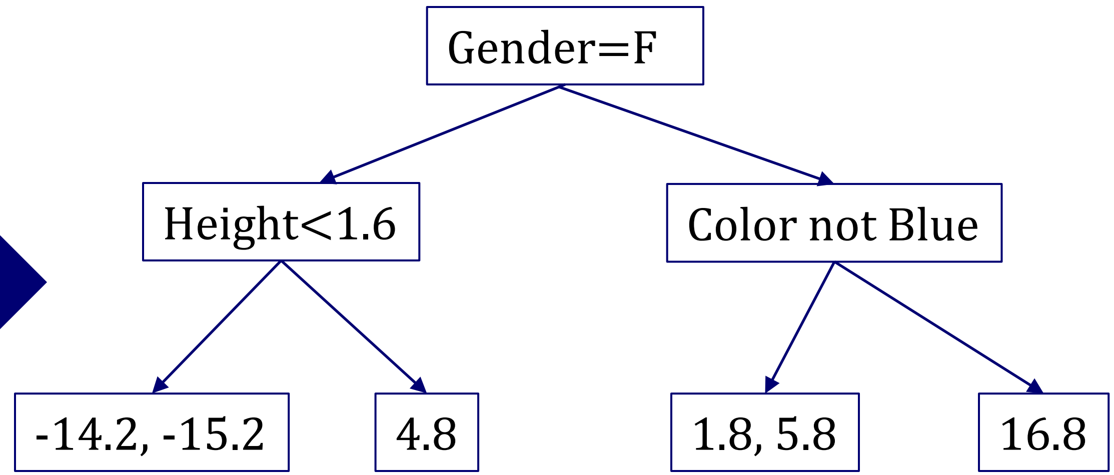
Height (m)	Favorite Color	Gender	Weight (kg)	F0	PR0
1.6	Blue	Male	88	71.2	16.8
1.6	Green	Female	76	71.2	4.8
1.5	Blue	Female	56	71.2	-15.2
1.8	Red	Male	73	71.2	1.8
1.5	Green	Male	77	71.2	5.8
1.4	Blue	Female	57	71.2	-14.2

Pseudo Residual (PR) = True Value – Predicted Value

Gradient Boosting

Fit PR0 into a decision tree (up to four leaves)

Height (m)	Favorite Color	Gender	PR0
1.6	Blue	Male	16.8
1.6	Green	Female	4.8
1.5	Blue	Female	-15.2
1.8	Red	Male	1.8
1.5	Green	Male	5.8
1.4	Blue	Female	-14.2

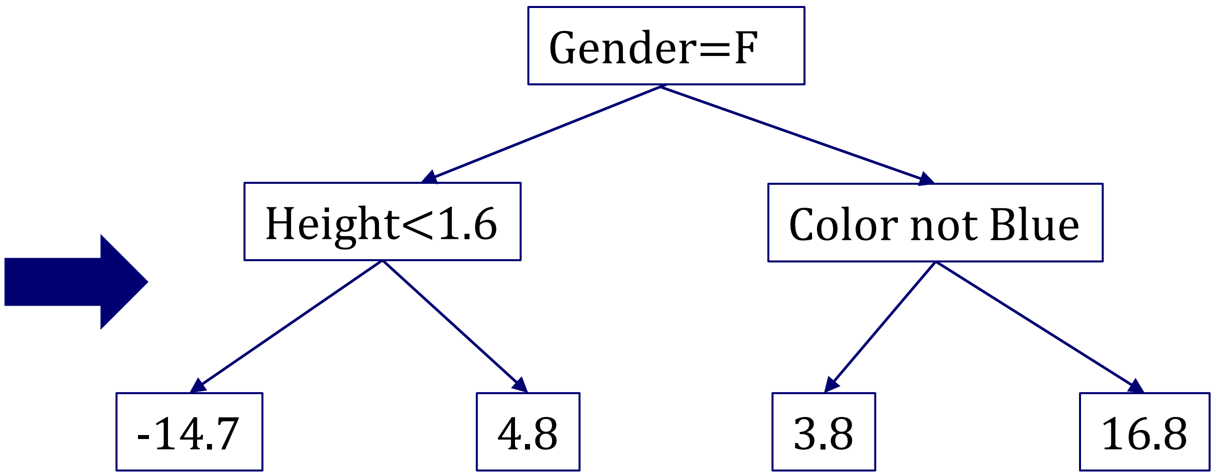


Pseudo Residual (PR) = True Value – Predicted Value

Gradient Boosting

Fit PR0 into a decision tree (up to four leaves)

Height (m)	Favorite Color	Gender	PR0
1.6	Blue	Male	16.8
1.6	Green	Female	4.8
1.5	Blue	Female	-15.2
1.8	Red	Male	1.8
1.5	Green	Male	5.8
1.4	Blue	Female	-14.2



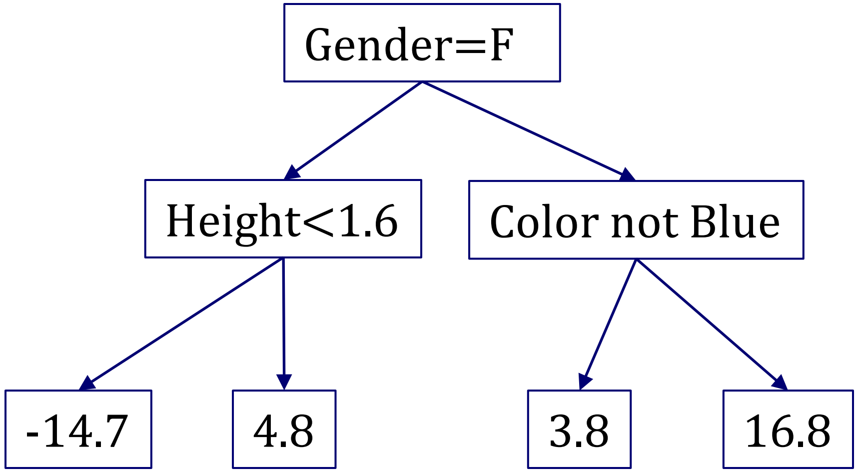
Averaging the residuals on each leaf…

Gradient Boosting

Learning rate = 0.1

$$F1(x) = F0(x) + \gamma_1 \times \text{Output of DT}(x)$$

Height (m)	Favorite Color	Gender	Weight (kg)	F0
1.6	Blue	Male	88	71.2
1.6	Green	Female	76	71.2
1.5	Blue	Female	56	71.2
1.8	Red	Male	73	71.2
1.5	Green	Male	77	71.2
1.4	Blue	Female	57	71.2



F1((1.6, Blue, Male)) = 71.2 + 0.1 × 16.8 = 72.9
F1((1.6, Green, Female)) = 71.2 + 0.1 × 4.8 = 71.7
F1((1.5, Blue, Female)) = 71.2 + 0.1 × -14.7 = 69.7
F1((1.8, Red, Male)) = 71.2 + 0.1 × 3.8 = 71.6
F1((1.5, Green, Male)) = 71.2 + 0.1 × 3.8 = 71.6
F1((1.4, Blue, Female)) = 71.2 + 0.1 × -14.7 = 69.7

Gradient Boosting

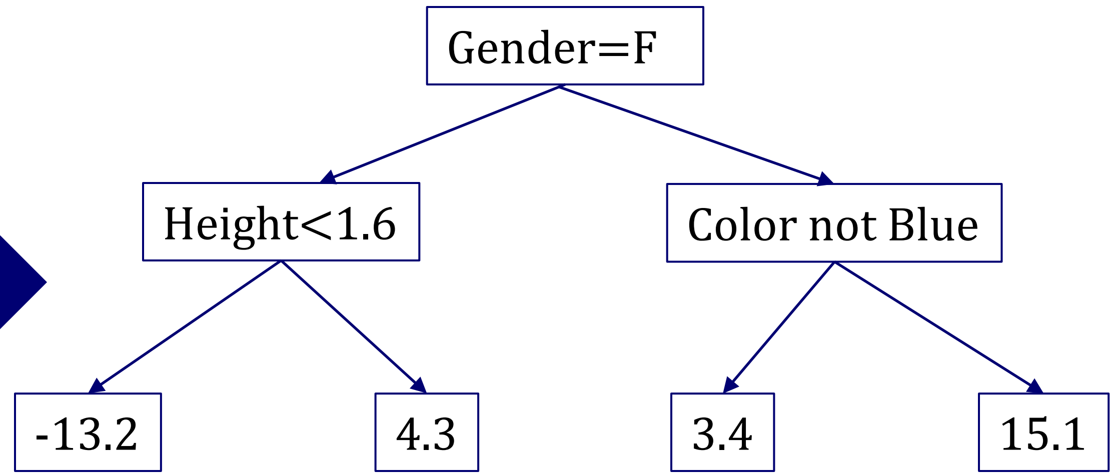
So after building the first DT, we obtain…

Height (m)	Favorite Color	Gender	Weight (kg)	F0	PR0	F1	PR1
1.6	Blue	Male	88	71.2	16.8	72.9	15.1
1.6	Green	Female	76	71.2	4.8	71.7	4.3
1.5	Blue	Female	56	71.2	-15.2	69.7	-13.7
1.8	Red	Male	73	71.2	1.8	71.6	1.4
1.5	Green	Male	77	71.2	5.8	71.6	5.4
1.4	Blue	Female	57	71.2	-14.2	69.7	-12.7

Gradient Boosting

Fit PR1 into a decision tree (up to four leaves)

Height (m)	Favorite Color	Gender	PR1
1.6	Blue	Male	15.1
1.6	Green	Female	4.3
1.5	Blue	Female	-13.7
1.8	Red	Male	1.4
1.5	Green	Male	5.4
1.4	Blue	Female	-12.7

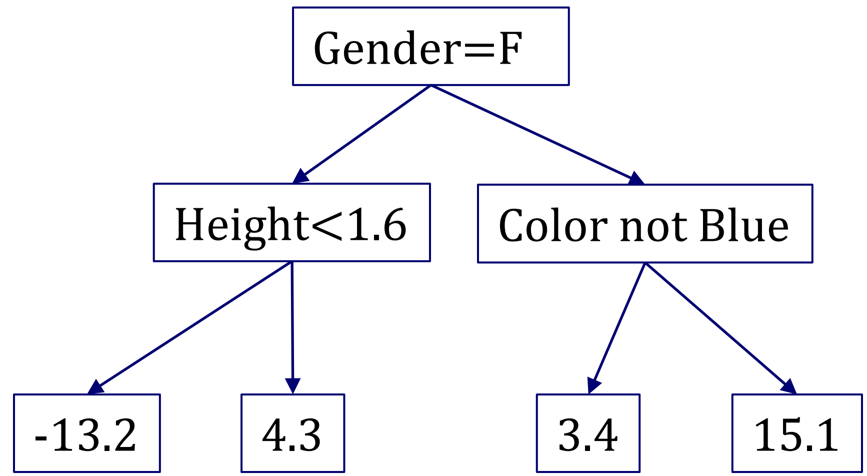


Gradient Boosting

Learning rate = 0.1

$$F2(x) = F1(x) + \gamma_2 \times \text{Output of DT}(x)$$

Height (m)	Favorite Color	Gender	Weight (kg)	F1
1.6	Blue	Male	88	72.9
1.6	Green	Female	76	71.7
1.5	Blue	Female	56	69.7
1.8	Red	Male	73	71.6
1.5	Green	Male	77	71.6
1.4	Blue	Female	57	69.7



F2((1.6, Blue, Male)) = 72.9 + 0.1 × 15.1 = 74.4
F2((1.6, Green, Female)) = 71.7 + 0.1 × 4.3 = 72.1
F2((1.5, Blue, Female)) = 69.7 + 0.1 × -13.2 = 68.4
F2((1.8, Red, Male)) = 71.6 + 0.1 × 3.4 = 71.9
F2((1.5, Green, Male)) = 71.6 + 0.1 × 3.4 = 71.9
F2((1.4, Blue, Female)) = 69.7 + 0.1 × -13.2 = 68.4

Gradient Boosting

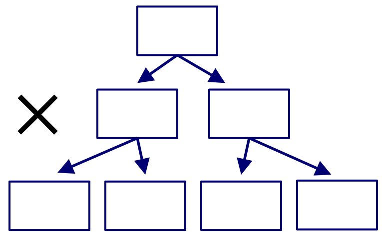
So after building the second DT, we obtain…

Height (m)	Favorite Color	Gender	Weight (kg)	F0	PR0	F1	PR1	F2	PR2
1.6	Blue	Male	88	71.2	16.8	72.9	15.1	74.4	13.6
1.6	Green	Female	76	71.2	4.8	71.7	4.3	72.1	3.9
1.5	Blue	Female	56	71.2	-15.2	69.7	-13.7	68.4	-12.4
1.8	Red	Male	73	71.2	1.8	71.6	1.4	71.9	1.1
1.5	Green	Male	77	71.2	5.8	71.6	5.4	71.9	5.1
1.4	Blue	Female	57	71.2	-14.2	69.7	-12.7	68.4	-11.4

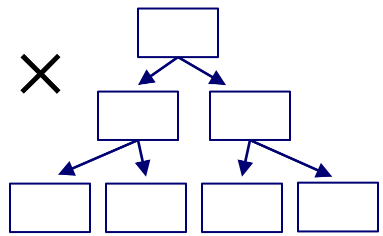
Notice the PR’s are shrinking: Small steps towards the right direction!

Gradient Boosting

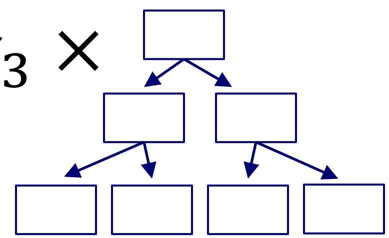
$Fm = F0 + \gamma_1 \times$



$+ \gamma_2 \times$



$+ \gamma_3 \times$



$+ \dots$

Fit the new PR into DT

Stop until the pre-specified #DTs or the PR stops improving!

Python Time!

- from sklearn import ensemble

Some Mathematics...

Input: training set $\{(x_i, y_i)\}_{i=1}^n$, a differentiable loss function $L(y, F(x))$, number of iterations M.

Algorithm:

1. Initialize model with a constant value:

$$F_0(x) = \arg\min_{\gamma} \sum_{i=1}^{n} L(y_i, \gamma).$$

2. For m = 1 to M:

    1. Compute so-called *pseudo-residuals*:

    $$r_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)} \quad \text{for } i = 1, \ldots, n.$$

    2. Fit a base learner (or weak learner, e.g. tree) $h_m(x)$ to pseudo-residuals, i.e. train it using the training set $\{(x_i, r_{im})\}_{i=1}^n$.
    3. Compute multiplier γ_m by solving the following one-dimensional optimization problem:

    $$\gamma_m = \arg\min_{\gamma} \sum_{i=1}^{n} L\left(y_i, F_{m-1}(x_i) + \gamma h_m(x_i)\right).$$

    4. Update the model:

    $$F_m(x) = F_{m-1}(x) + \gamma_m h_m(x).$$

3. Output $F_M(x)$.

Gradient Boosting

- Works exceptionally well in practice
- Won a series of Kaggle competitions
- More robust and explainable