Boosting

Adaboost, Gradient Boost, XGBoost

Seunghan Lee

20.03.18 (Wed)

Contents

1. What is Boosting?

1) Ensemble method
2) Bagging vs Boosting

(1) Ensemble

*In statistics and machine learning, **ensemble methods** use **multiple learning algorithms** to obtain better predictive performance than could be obtained from any of the constituent learning algorithms alone. (Wikipedia)*

- Use "**multiple models**" to predict the output
(both regression & classification)

- Several Weak learner > One Strong learner

- ex) Bagging & Boosting

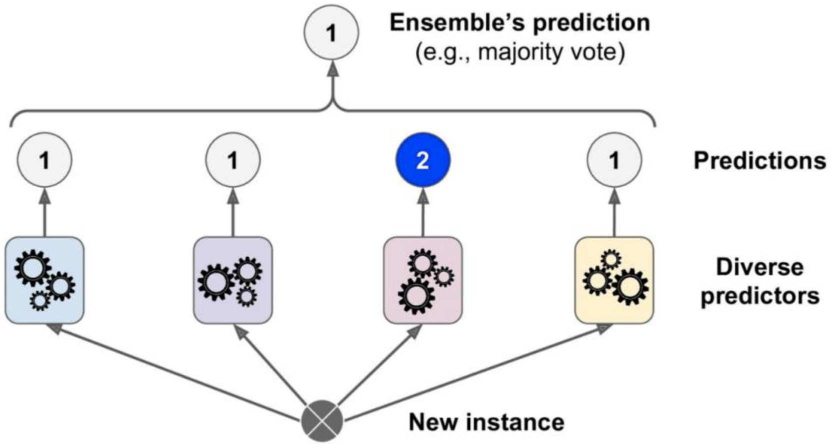


Figure 7-2. Hard voting classifier predictions

https://miro.medium.com/max/2454/0*c0Eg6-UArkslgviw.png

(2) Bagging vs Boosting

Steps of Bagging

1) Random sampling with replacement (= Bootstrapping)

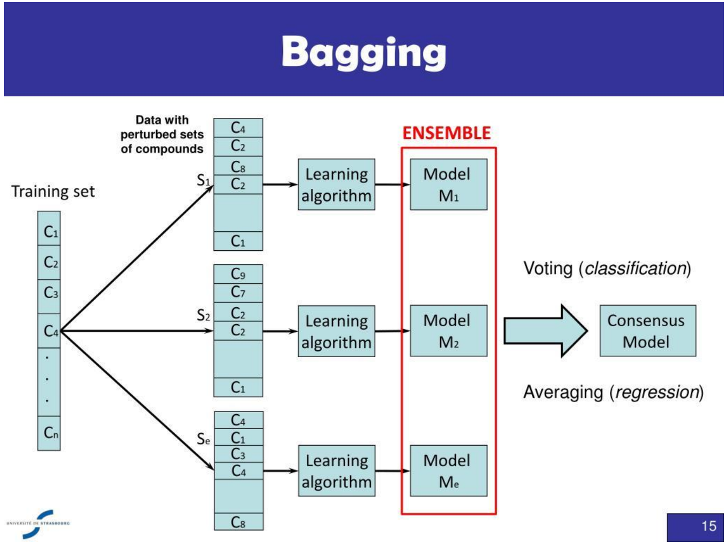
2) Select subset of features randomly

3) Grow the tree to the largest

4) Repeat 1)~3) N times (total of N models)

   -> make prediction based on these N models

https://www.slideserve.com/tarala/short-overview-of-weka



(2) Bagging vs Boosting

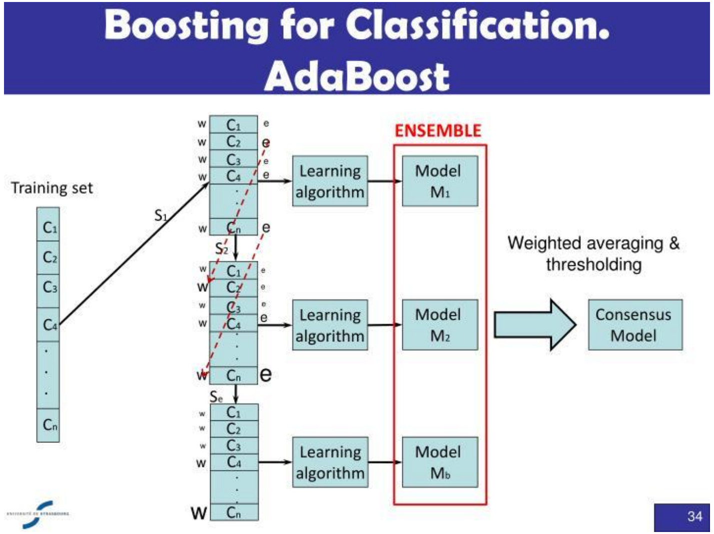
Steps of Boosting

1) First random sample (d1) without replacement
 -> train a weak learner C1

2) Second random sample (d2) without replacement, considering the misclassified sample in learner C1
-> train a weak learner C2

3) Third random sample (d2) without replacement, considering the misclassified sample in learner C1,C2
-> train a weak learner C3

4) Combine all the weak learners(C1~Cn) via majority voting.

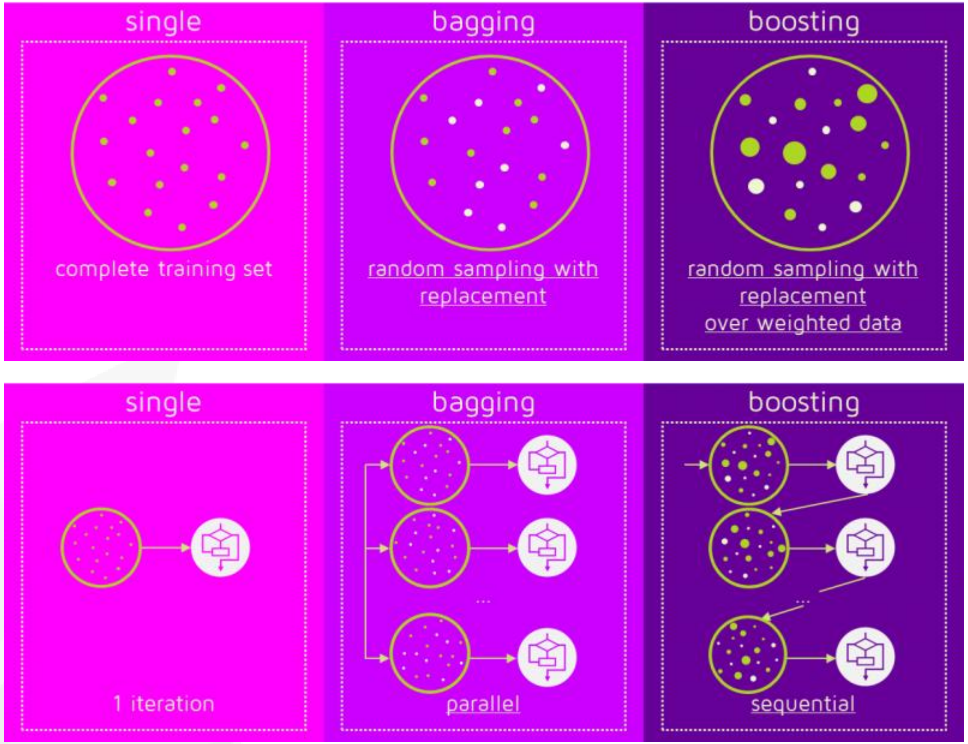


https://www.slideserve.com/tarala/short-overview-of-weka

(2) Bagging vs Boosting

	Bagging	Boosting
	Parallel Ensemble (Each model is independent)	Sequential Ensemble (Next Model is dependent to the previous model)
Sampling	Random sample (Bootstrapping)	Higher vote to misclassified sample
Goal	Reduce Variance	Reduce Bias
Base Learner	Unstable Learner (ex. Decision Tree)	Stable Leaner (ex. Stump)
Example)	Random Forest	XGBoost, LightGBM

(2) Bagging vs Boosting



way of sampling

way of making models

2-a. Adaboost

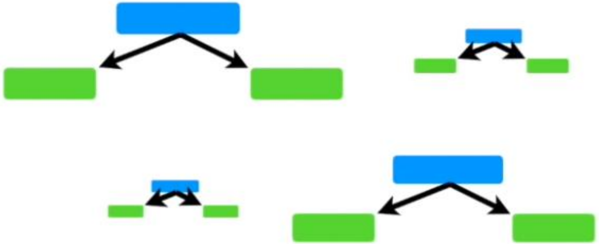
What is Adaboost?

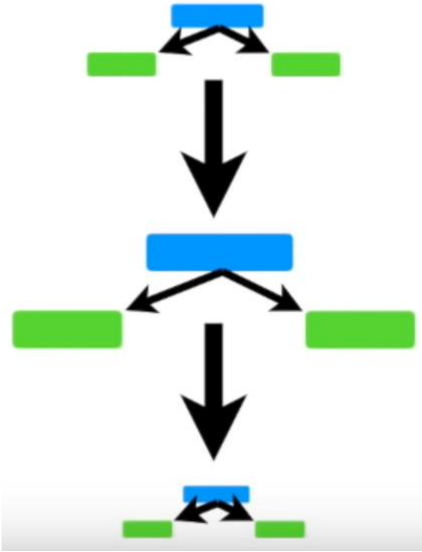
- Adaboost = **Adaptive Boosting**
 (Adaptive? “more likely to choose the misclassified samples” from the previous learners)

- base learner : **weak learners** (not very accurate)
 ex) **Stump** (= a tree with 1 node & 2 leaves)

- **weighted sum** of the output of weak learners
 (= unlike RF, learners get different vote to the final output!)

- weak learners are **dependent** to each other! (made **sequentially**)





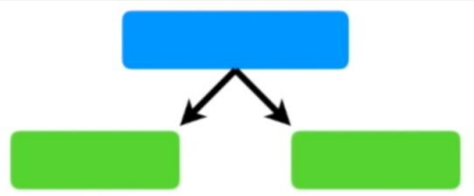
StatQuest with Josh Starmer

How does Adaboost work?

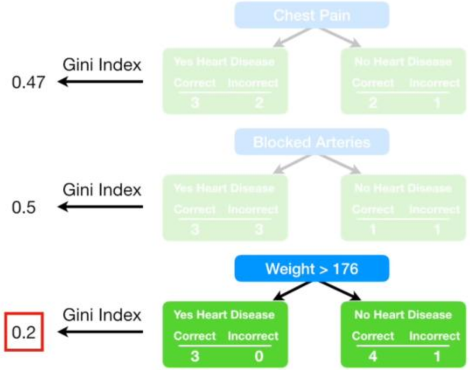
Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	1/8
No	Yes	180	Yes	1/8
Yes	No	210	Yes	1/8
Yes	Yes	167	Yes	1/8
No	Yes	156	No	1/8
No	Yes	125	No	1/8
Yes	No	168	No	1/8
Yes	Yes	172	No	1/8

(How each data is important to be correctly classified) -> will be updated!

1) Make a Stump



with the variable which makes the best classification



In this example,
“weight > 176” will be chosen

2-a. Adaboost

How does Adaboost work?

“How much say” does each stump has?

$$\text{Amount of Say} = \frac{1}{2}\log\left(\frac{1 - \text{Total Error}}{\text{Total Error}}\right)$$

Example)

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	1/8
No	Yes	180	Yes	1/8
Yes	No	210	Yes	1/8
Yes	Yes	167	Yes	1/8

$$\text{Amount of Say} = \frac{1}{2}\log(7) = 0.97$$

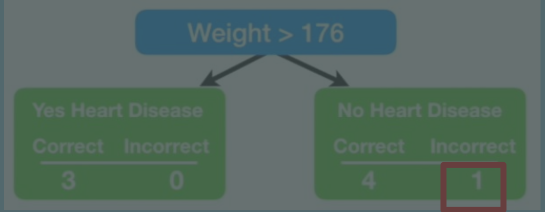
How does Adaboost work?

"How much say" does each stump has?

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	1/8
No	Yes	180	Yes	1/8
Yes	No	210	Yes	1/8
Yes	Yes	167	Yes	1/8

Need to update!
(to a SMALLER value)

Need to update!
(to a LARGER value)



Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
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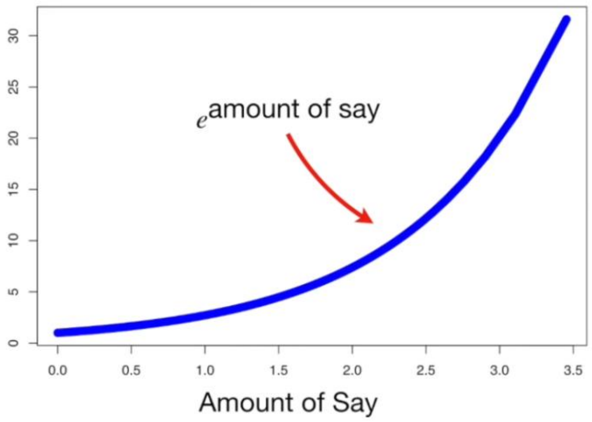
No	Yes	180	Yes	1/8
Yes	No	210	Yes	1/8
Yes	Yes	167	Yes	1/8

$$\text{Amount of Say} = \frac{1}{2}\log(7) = 0.97$$

How does Adaboost work?

< for the "Misclassified" sample >

$$\text{New Sample Weight} = \text{sample weight} \times e^{\text{amount of say}}$$



(increase the weight for the "incorrectly classified" sample!)

Example)

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	1/8
No	Yes	180	Yes	1/8
Yes	No	210	Yes	1/8
Yes	Yes	167	Yes	$\boxed{1/8}$

$$\text{Amount of Say} = \frac{1}{2}\log(7) = 0.97$$

$$\frac{1}{8}e^{0.97} = \frac{1}{8} \times 2.64 \boxed{= 0.33}$$

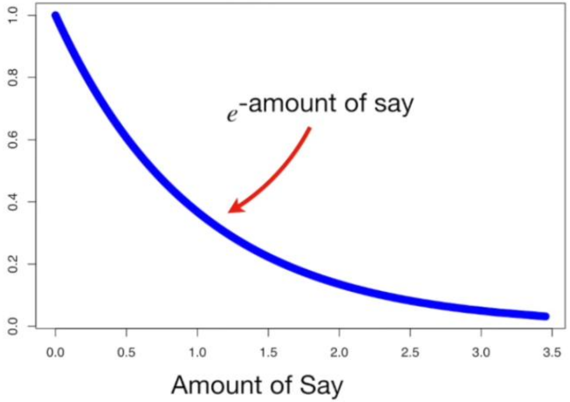
Before) 0.125

After) 0.33

How does Adaboost work?

< for the "Correctly classified" sample >

$$\text{New Sample Weight} = \text{sample weight} \times e^{-\text{amount of say}}$$



(decrease the weight for the "correctly classified" sample!)

Example)

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	1/8
No	Yes	180	Yes	1/8
Yes	No	210	Yes	1/8
Yes	Yes	167	Yes	1/8

$$\text{Amount of Say} = \frac{1}{2}\log(7) = 0.97$$

$$\frac{1}{8}e^{-0.97} = \frac{1}{8} \times 0.38 \boxed{= 0.05}$$

Before) 0.125

After) 0.05

How does Adaboost work?

After updating the weight
(+ normalization)

New Weight	Norm. Weight
0.05	0.07
0.05	0.07
0.05	0.07
0.33	0.49
0.05	0.07
0.05	0.07
0.05	0.07
0.05	0.07

→

This becomes the new sample weight!

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	0.07
No	Yes	180	Yes	0.07
Yes	No	210	Yes	0.07
Yes	Yes	167	Yes	0.49
No	Yes	156	No	0.07
No	Yes	125	No	0.07
Yes	No	168	No	0.07
Yes	Yes	172	No	0.07

How does Adaboost work?

Make the next stump,
with the “new sample weight”

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
Yes	Yes	205	Yes	0.07
No	Yes	180	Yes	0.07
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Yes	Yes	167	Yes	0.49
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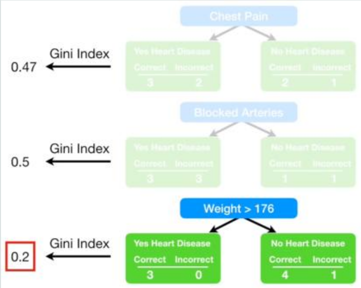
Option 1)

Use “weighted Gini index” to select the feature to make new stump



Option 2)

Duplicate copies of the samples

(bigger ‘sample weight’ ->

more likely to be selected)

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease
No	Yes	156	No
Yes	Yes	167	Yes
No	Yes	125	No
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Yes	Yes	167	Yes
Yes	Yes	172	No
Yes	Yes	205	Yes
Yes	Yes	167	Yes

2-a. Adaboost

How does Adaboost work?

Make the next stump,
with the “new sample weight”

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease	Sample Weight
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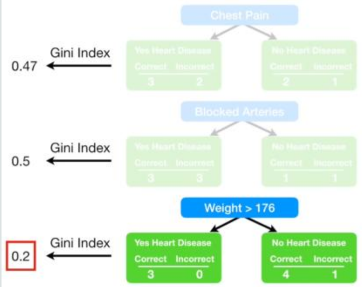

Option 2)

Duplicate copies of the samples

(bigger ‘sample weight’ ->

more likely to be selected)

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease
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How does Adaboost work?

Chest Pain	Blocked Arteries	Patient Weight	Heart Disease
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Yes	Yes	167	Yes
Yes	Yes	167	Yes
Yes	Yes	172	No
Yes	Yes	205	Yes
Yes	Yes	167	Yes

Sample Weight
1/8
1/8
1/8
1/8
1/8
1/8
1/8
1/8

Same sample weights doesn’t mean same importance to every sample!

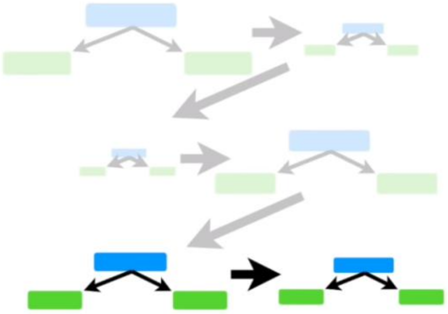
(important samples are duplicated!)

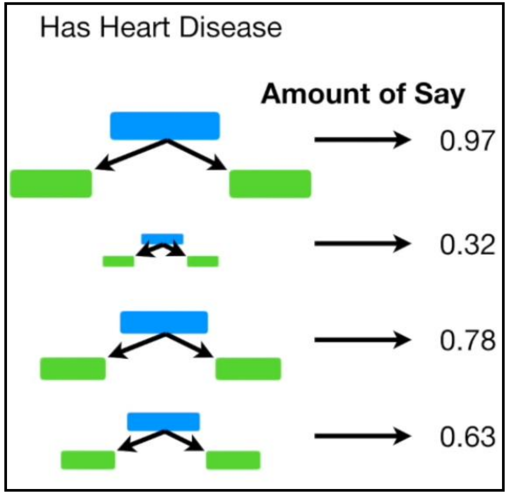
Give equal weight to all the samples!

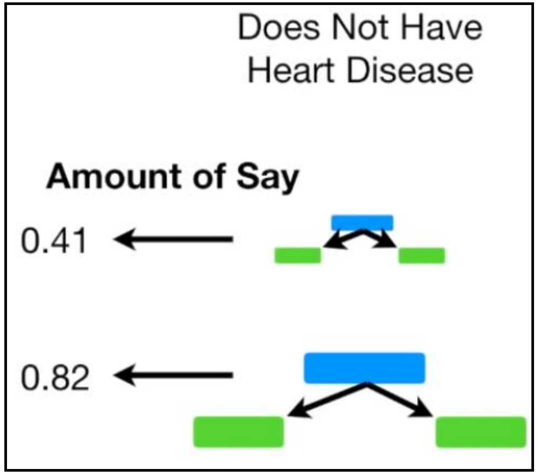
2-a. Adaboost

How does Adaboost work?

Make models(stumps) sequentially







Total Sum : 2.7 **>** **Total Sum : 1.23**

How to predict the final output?

Result : “Has Heart Disease”

2-a. Adaboost

How does Adaboost work?

Lecture 11: Boosting (I) AdaBoost (Draft: version 0.9.2) Seoul National University, Hyeong In Choi

binary

Binary AdaBoost
Input:

- Data: $\mathfrak{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$, where $x^{(i)} \in \mathfrak{X}$ and $y^{(i)} \in \mathfrak{Y} = \{-1, 1\}$ for $i = 1, \cdots, N$
- Total number of rounds: T

Initialize: Define the initial probability distribution $D_1(i) = \dfrac{1}{N}$ for $i = 1, \cdots, N$.
Do for $t = 1, \cdots, T$:

- Train using the probability distribution D_t on $\{1, \cdots, N\}$.
- Get a hypothesis (classifier) $h_t : \mathfrak{X} \to \mathfrak{Y}$ that has a training error rate ε_t (with respect to D_t) given by

$$\varepsilon_t = \sum_{i:h_t(x^{(i)}) \neq y^{(i)}} D_t(i).$$

- If $\varepsilon_t > \dfrac{1}{2}$, then set $T = t - 1$ and abort the loop.
- Set $\alpha_t = \dfrac{1}{2} \log \left(\dfrac{1 - \varepsilon_t}{\varepsilon_t} \right)$.
- Define the new probability distribution D_{t+1} by setting

$$\begin{aligned} D_{t+1}(i) &= \frac{D_t(i)}{Z_t} \cdot \begin{cases} e^{-\alpha_t} & \text{if } y^{(i)} = h_t(x^{(i)}) \\ e^{\alpha_t} & \text{if } y^{(i)} \neq h_t(x^{(i)}) \end{cases} \\ &= \frac{D_t(i)}{Z_t} \exp(-\alpha_t y^{(i)} h_t(x^{(i)})), \end{aligned}$$

where

$$Z_t = \sum_{i=1}^N D_t(i) \exp(-\alpha_t y^{(i)} h_t(x^{(i)})).$$

Output: Define $g(x) = \sum_{t=1}^T \alpha_t h_t(x)$. The final hypothesis (classifier) $H(x)$ is

$$H(x) = \operatorname{sgn}(g(x)).$$

Extend to multi-class

Multi-class

AdaBoost.M1
Input:

- Data: $\mathfrak{D} = \{(x^{(i)}, y^{(i)})\}_{i=1}^N$, where $x^{(i)} \in \mathfrak{X}$ and $y^{(i)} \in \mathfrak{Y}$ for $i = 1, \cdots, N$. Here $\mathfrak{Y}$ is a set of K elements, which, as usual, is identified with $\{1, \cdots, K\}$
- Total number of rounds: T

Initialize: Define the initial probability $D_1(i) = \dfrac{1}{N}$ for $i = 1, \cdots, N$.
Do for $t = 1, 2, \cdots, T$:

- Train using the probability distribution D_t on $\{1, \cdots, N\}$.
- Get a hypothesis (classifier) $h_t : \mathfrak{X} \to \mathfrak{Y}$ that has a training error rate ε_t (with respect to D_t) given by

$$\varepsilon_t = \sum_{i:h_t(x^{(i)}) \neq y^{(i)}} D_t(i).$$

- If $\varepsilon_t > \dfrac{1}{2}$, then set $T = t - 1$ and abort the loop.
- Set $\alpha_t = \dfrac{1}{2} \log \left(\dfrac{1 - \varepsilon_t}{\varepsilon_t} \right)$.
- Define the new probability distribution D_{t+1} by setting

$$\begin{aligned} D_{t+1(i)} &= \frac{D_t(i)}{Z_t} \cdot \begin{cases} e^{-\alpha_t} & \text{if } y^{(i)} = h_t(x^{(i)}) \\ e^{\alpha_t} & \text{if } y^{(i)} \neq h_t(x^{(i)}) \end{cases} \\ &= \frac{D_t(i)}{Z_t} \exp(-\alpha_t S(h_t(x^{(i)}), y^{(i)})), \end{aligned}$$

where $Z_t = \sum_{i=1}^N D_t(i) \exp(-\alpha_t S(h_t(x^{(i)}), y^{(i)}))$, and $S(a, b) = \mathbb{I}(a = b) - \mathbb{I}(a \neq b)$ so that $S(a, b) = 1$ if $a = b$ and $S(a, b) = -1$ if $a \neq b$.

Output: the final hypothesis (classifier)

$$H(x) = \underset{y \in \mathfrak{Y}}{\operatorname{argmax}} \sum_{t:h_t(x)=y} \alpha_t.$$

Adaboost Summary

1) Combine weak learners to make classifications

2) Some learners have more say than over learners

3) Each learner is made by considering the result of the previous learner's mistake

2-b. Gradient Boost

2-b. Gradient Boost

What is Gradient Boost?

- not so much different with Adaboost

1) Combine weak learners to make classifications
2) Some learners have more say than over learners
3) Each learner is made by considering the result of the previous learner's mistake

- difference?

Can be expressed in more general terms! (by using "**gradient**")

+ use trees larger than stumps as base learners

Minimizing the cost(loss) function

1. Gradient Boosting Regression

2. Gradient Boosting Classification

$$y = f(x) + \underline{e1}$$

$$\underline{e1} = g(x) + \underline{e2}$$

$$\underline{e2} = h(x) + e3$$

$$Y = f(x) + g(x) + h(x) + \ldots$$

1. Gradient Boost Regression

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

1

First, make a “leaf (= guess for the y value)”

(initial leaf : average of all the y values) Average Weight 71.2

(= first predicted y)

1. Gradient Boost Regression

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)	Residual
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

1

First, make a "leaf (= guess for the y value)"

(initial leaf : average of all the y values)

Average Weight
71.2

(= first predicted y)

2

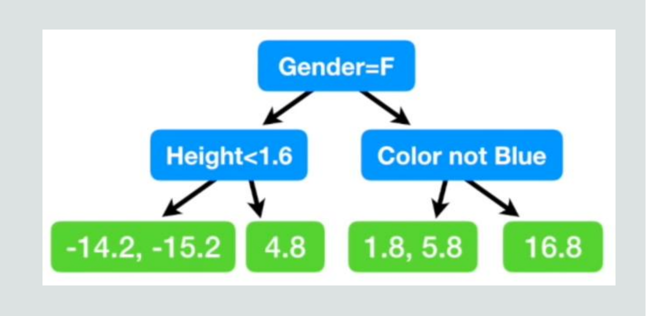
Then, predict the "residual"

(build the next model (tree) predicting the residuals)

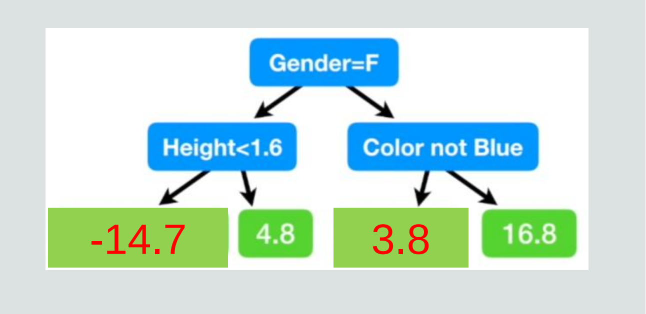
1. Gradient Boost Regression

Height (m)	Favorite Color	Gender	Weight (kg)	Residual
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

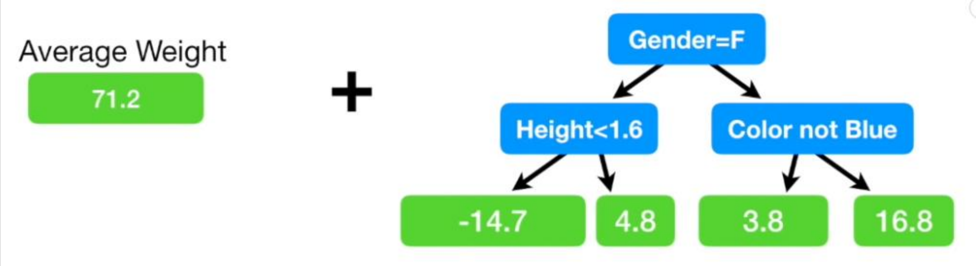
(usually 8~32 leaves)



Replace the residuals into their average



1. Gradient Boost Regression



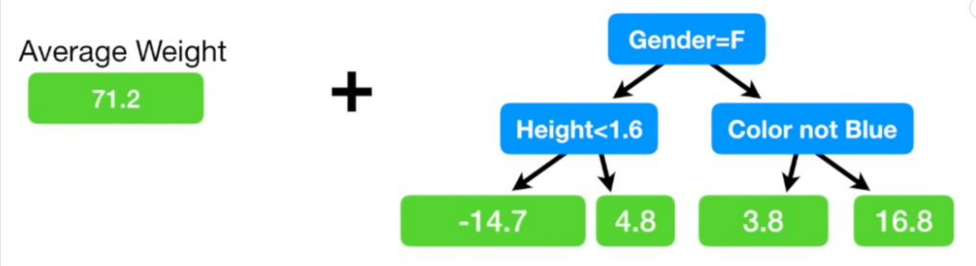
Height (m)	Favorite Color	Gender	Weight (kg)
1.6	Blue	Male	88

100% correct (no error)

Overfitting!

2-b. Gradient Boost

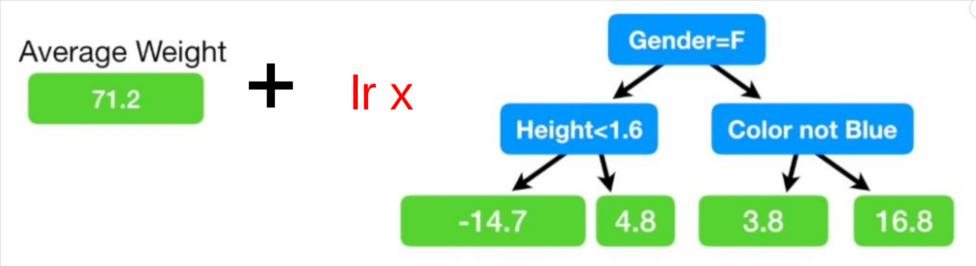
1. Gradient Boost Regression



Height (m)	Favorite Color	Gender	Weight (kg)
1.6	Blue	Male	88

100% correct (no error)

Overfitting!



Height (m)	Favorite Color	Gender	Weight (kg)
1.6	Blue	Male	72.9

(If learning rate = 0.1)

$71.2 + (0.1 \times 16.8) = 72.9$

1. Gradient Boost Regression

new residuals
(becomes smaller)

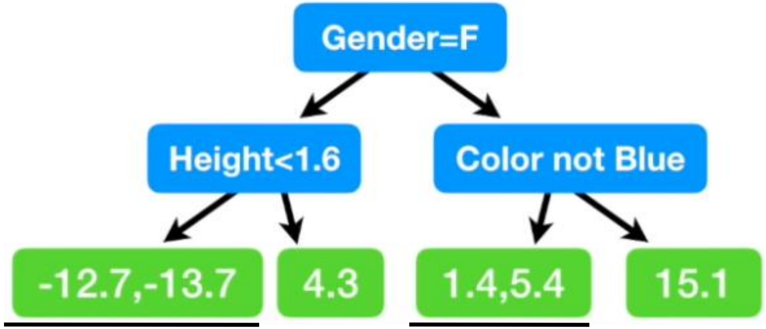
$88 - (71.2 + 0.1 \times 16.8) =$

Height (m)	Favorite Color	Gender	Weight (kg)	Residual
1.6				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

1. Gradient Boost Regression

new residuals
(becomes smaller)

Height (m)	Favorite Color	Gender	Weight (kg)	Residual
1.6	88 – (71.2 + 0.1x16.8) =			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



into -13.2

Into 3.4

3

Then, predict the "residual's residual"

(build the next model (tree) predicting the residuals)

1. Gradient Boost Regression

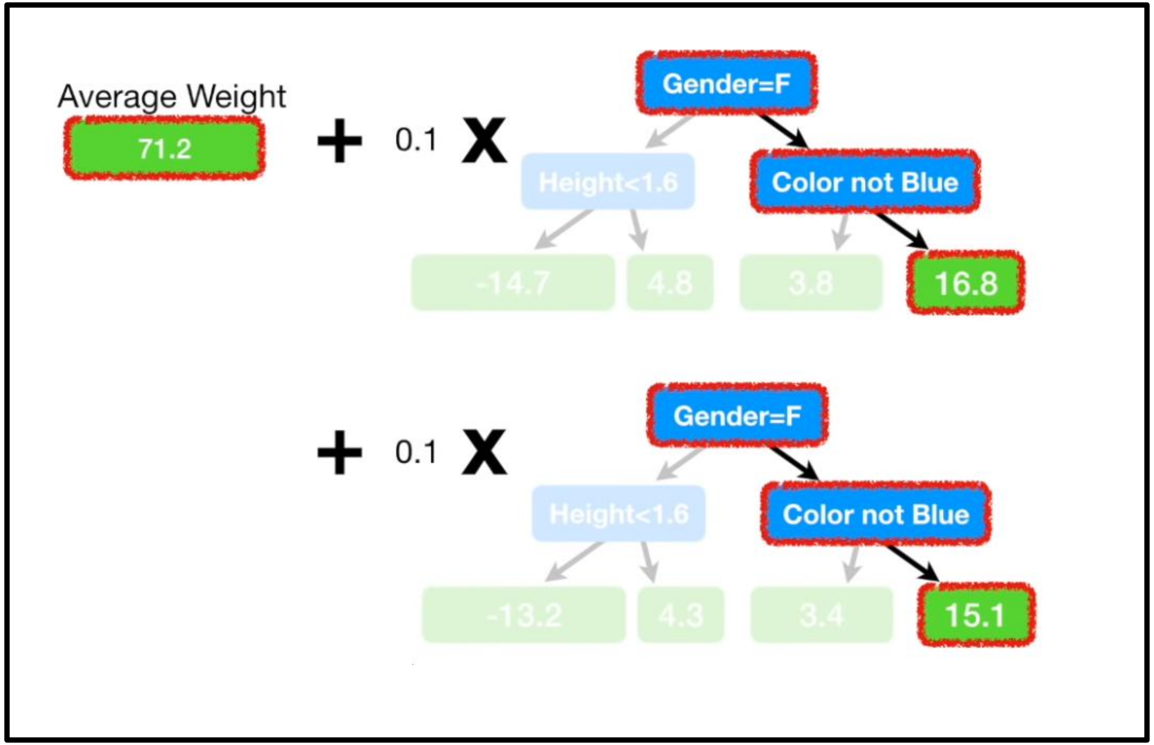
Height (m)	Favorite Color	Gender	Weight (kg)
1.6	Blue	Male	74.4

71.2 + (0.1 x 16.8) + (0.1 x 15.1) = 74.4

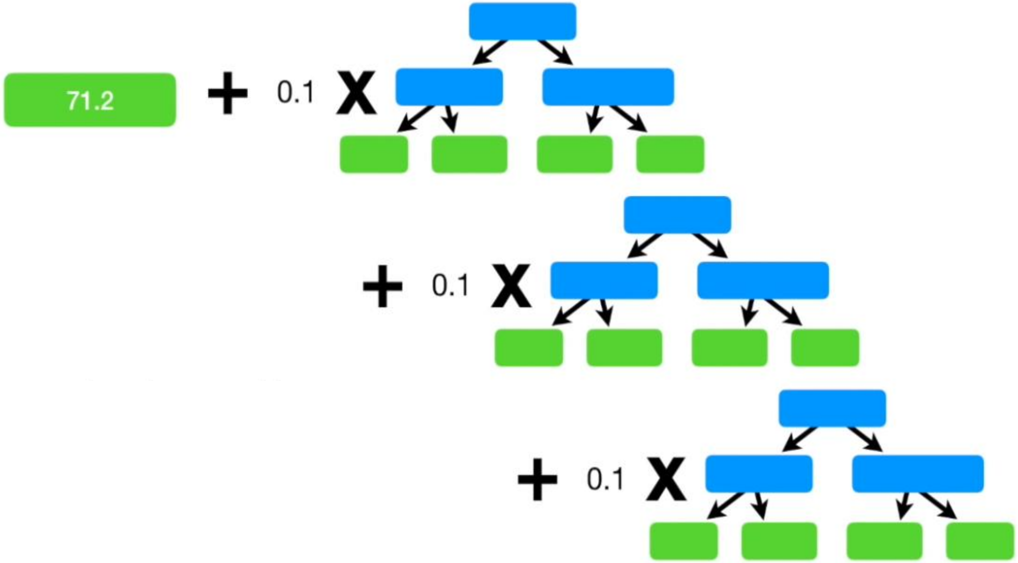
y = f(x) + e1

e1 = $\boxed{g(x)}$ + e2

e2 = $\boxed{h(x)}$ + e3



1. Gradient Boost Regression



Keep making the sequential trees!

(until specified level, or until the residuals doesn’t significantly drops)

1. Gradient Boost Regression

Mathematical Expression

$$\text{Loss Function} = \frac{1}{2}(\text{Observed} - \text{Predicted})^2$$

To minimize this loss function

$$\frac{d}{d\,\text{Predicted}}\frac{1}{2}(\text{Observed} - \text{Predicted})^2 = -(\text{Observed} - \text{Predicted}) = 0$$

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

$$\frac{d}{d\,\text{Predicted}}:\quad \frac{1}{2}(88 - \text{Predicted})^2 + \frac{1}{2}(76 - \text{Predicted})^2 + \frac{1}{2}(56 - \text{Predicted})^2$$

$$\longrightarrow -(88 - \text{Predicted}) + -(76 - \text{Predicted}) + -(56 - \text{Predicted}) = 0$$

1. Gradient Boost Regression

Mathematical Expression

$$\text{Loss Function} = \frac{1}{2}(\text{Observed} - \text{Predicted})^2$$

To minimize this loss function

$$\frac{d}{d\,Predicted}\frac{1}{2}(\text{Observed} - \text{Predicted})^2 = -(\text{Observed} - \text{Predicted}) = 0$$

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

$\frac{1}{2}(88 - \text{Predicted})^2 + \rightarrow -(88 - \text{Predicted}) +$

$-(76 - \text{Predicted}) +$

$-(56 - \text{Predicted})$

$= 0$

$\frac{d}{d\,Predicted}$

That is why we kept making the predicted value as the "AVERAGE" value!

1. Gradient Boost Regression

https://ascelibrary.org/cms/asset/

Gradient Boosted Regression Tree

Input: $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}, \theta, \gamma$

Output: $F(\mathrm{x}) = \sum_{i=0}^{M} F_i(x)$

Initialize $F_0(x) = \arg min_\beta \sum_{i=0}^{N} L(y_i, \beta)$

While $(m < M)$

$d_i = -[\partial L(y_i, F(x_i))/\partial F(x_i)]_{F(x_i)=F_{m-1}(x_i)}$

$\vartheta = \{(x_i, d_i)\}, i = 1, N$

$g(\mathrm{x}) = \mathrm{FITREGRETREE}(\vartheta, \theta)$

$\rho_m = \arg min_\rho \sum_{i=1}^{N} L(y_i, F_{m-1}(x) + \rho g(x))$

$F_m(x) = F_{m-1}(x) + \gamma \rho_m g(x)$

End while

Done!

2-b. Gradient Boost

1. Gradient Boost Regression

Gradient Boosted Regression Tree

1. **Input:** $D = \{(x_1, y_1), \dots, (x_N, y_N)\}, \theta, \gamma$
2. **Output:** $F(\mathrm{x}) = \sum_{i=0}^{M} F_i(x)$
3. Initialize $F_0(x) = \arg min_\beta \sum_{i=0}^{N} L(y_i, \beta)$
4. **While** $(m < M)$
5. $d_i = -[\partial L(y_i, F(x_i))/\partial F(x_i)]_{F(x_i)=F_{m-1}(x_i)}$
6. $\vartheta = \{(x_i, d_i)\}, i = 1, N$
7. $g(\mathrm{x}) = \mathrm{FITREGRETREE}(\vartheta, \theta)$
8. $\rho_m = \arg min_\rho \sum_{i=1}^{N} L(y_i, F_{m-1}(x) + \rho g(x))$
9. $F_m(x) = F_{m-1}(x) + \gamma \rho_m g(x)$

13. **End while**

Loss Function : MSE

y = f(x) + e1

e1 = g(x) + e2

e2 = h(x) + e3

Y = f(x) + g(x) + h(x) + …

First prediction = “average” of all y values

Height (m)	Favorite Color	Gender	Weight	Residual
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

Y = f(x) + g(x) + e2

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2
Yes	12	Blue	Yes
Yes	87	Green	Yes
No	44	Blue	No
Yes	19	Red	No
No	32	Green	Yes
No	14	Blue	Yes

➡

4 Yes, 2 No

Odds ratio (of yes): 4/2 = 2

Odds ratio (of no) : 2/4 = 0.5

Log(2) = **0.7**

Log(0.5) = -0.7

Log Odds Ratio?

1

First, make a "leaf (= guess for the y value)"

(initial leaf : log odds ratio of the highest value)

log(4/2) = 0.7 (= first predicted y)

2. Gradient Boost Classification

1) Log Odds Ratio (= Logit)

$$\operatorname{logit}(p) = \log\left(\frac{p}{1-p}\right)$$

If p is a probability, then $p/(1 - p)$ is the corresponding odds

2. Gradient Boost Classification

1) Log Odds Ratio (= Logit)

$$\mathrm{logit}(p) = \log\left(\frac{p}{1-p}\right)$$

If *p* is a probability, then *p*/(1 − *p*) is the corresponding odds

Example)

Chance of winning?

DSL	YBIGTA
5	2

$$\frac{5}{2}$$

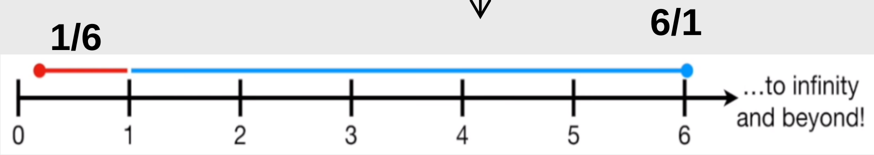
(5/7) / (2/7) = 5/2

Odds are 2.5
that DSL will win!

(probability (p) = 5/7)

log(5/2) = 0.916

Why log?



2. Gradient Boost Classification

2) Logistic Function (= Sigmoid)

$$f(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$$

As a method to turn 'log odds ratio' back to 'probability'

2. Gradient Boost Classification

2) Logistic Function (= Sigmoid)

$$f(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$$

As a method to turn 'log odds ratio' back to 'probability'

Example)

(The probability was 5/7)

log(5/2) = 0.916 ➡ **f(log(5/2)) = 5/7**

```
>>> 5/7
0.7142857142857143
>>>
>>> 1/(1+np.exp(-np.log(5/2)))
0.7142857142857143
```

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2
Yes	12	Blue	Yes
Yes	87	Green	Yes
No	44	Blue	No
Yes	19	Red	No
No	32	Green	Yes
No	14	Blue	Yes

4 Yes, 2 No

Odds ratio (of yes): 4/2 = 2

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Log(2) = **0.7**

Log(0.5) = -0.7

1

First, make a "leaf (= guess for the y value)"

(initial leaf : log odds ratio of the highest value)

log(4/2) = 0.7 (= first predicted y)

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2
Yes	12	Blue	Yes
Yes	87	Green	Yes
No	44	Blue	No
Yes	19	Red	No
No	32	Green	Yes
No	14	Blue	Yes

4 Yes, 2 No

Odds ratio (of yes): 4/2 = 2

Odds ratio (of no) : 2/4 = 0.5

Log(2) = **0.7**

Log(0.5) = -0.7

1

First, make a “leaf (= guess for the y value)”

(initial leaf : log odds ratio of the highest value)

log(4/2) = 0.7 (= first predicted y)

Put log odds ratio into sigmoid function

$$\frac{1}{1+e^{-log(4/2)}} = 0.7$$

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2
Yes	12	Blue	Yes
Yes	87	Green	Yes
No	44	Blue	No
Yes	19	Red	No
No	32	Green	Yes
No	14	Blue	Yes

4 Yes, 2 No

Odds ratio (of yes): 4/2 = 2

Odds ratio (of no) : 2/4 = 0.5

Log(2) = **0.7**

Log(0.5) = -0.7

Therefore, every sample will be classified 'Yes' for the initial guess!

1

First, make a "leaf (= guess for the y value)"

(initial leaf : log odds ratio of the highest value)

log(4/2) = 0.7 (= first predicted y)

Put log odds ratio into sigmoid function

$$\frac{1}{1+e^{-log(4/2)}} = 0.7$$

(threshold : 0.5)

Bigger than 0.5

-> classify into 'Yes'

Smaller than 0.5

-> classify into 'No'

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2	Residual
Yes	12	Blue	Yes	0.3
Yes	87	Green	Yes	0.3
No	44	Blue	No	-0.7
Yes	19	Red	No	-0.7
No	32	Green	Yes	0.3
No	14	Blue	Yes	0.3

(Yes = 1, No = 0)

(= 1(actual) – 0.7(predicted))

(= 0(actual) – 0.7(predicted))

2

Calculate Error based on the first prediction

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2	Residual
Yes	12	Blue	Yes	0.3
Yes	87	Green	Yes	0.3
No	44	Blue	No	-0.7
Yes	19	Red	No	-0.7
No	32	Green	Yes	0.3
No	14	Blue	Yes	0.3

(Yes = 1, No = 0)

(= 1(actual) – 0.7(predicted))

(= 0(actual) – 0.7(predicted))

Don't get confused!

0.7 is not "log odds ratio"!

It is "probability"

2

Calculate Error based on the first prediction

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2	Residual
Yes	12	Blue	Yes	0.3
Yes	87	Green	Yes	0.3
No	44	Blue	No	-0.7
Yes	19	Red	No	-0.7
No	32	Green	Yes	0.3
No	14	Blue	Yes	0.3

(Yes = 1, No = 0)

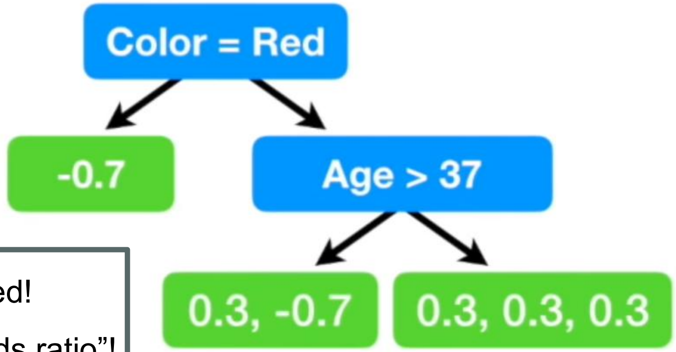
(= 1(actual) – 0.7(predicted))

(= 0(actual) – 0.7(predicted))

Don't get confused!

0.7 is not "log odds ratio"!

It is "probability"



2

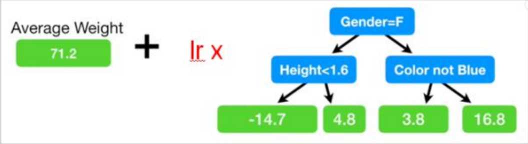
Calculate Error based on the first prediction

3

Make a tree, predicting the "residuals"

2. Gradient Boost Classification

(in Regression)



Height (m)	Favorite Color	Gender	Weight (kg)
1.6	Blue	Male	72.9

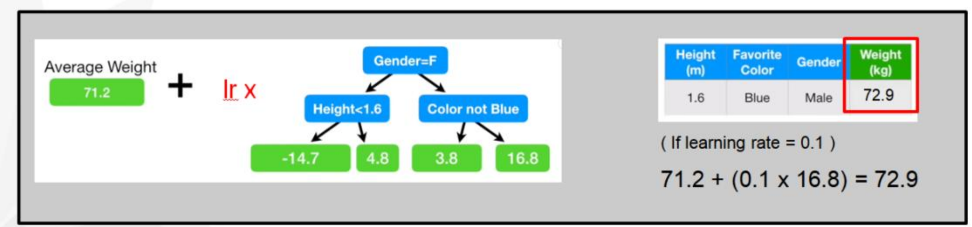
(If learning rate = 0.1)

71.2 + (0.1 x 16.8) = 72.9

A bit different in Classification

2. Gradient Boost Classification

(in Regression)



A bit different in Classification

(in Classification)

$$\frac{\sum \text{Residual}_i}{\sum [\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)]}$$

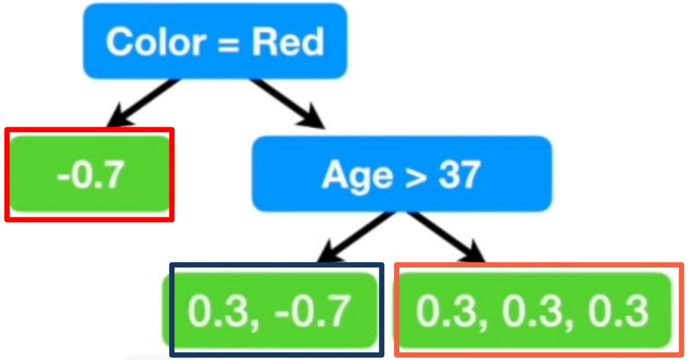
Log odds ratio

Probability

MISMATCH! Can't just add them together!

How to make 'probability' compatible with 'log odds ratio'?

2. Gradient Boost Classification



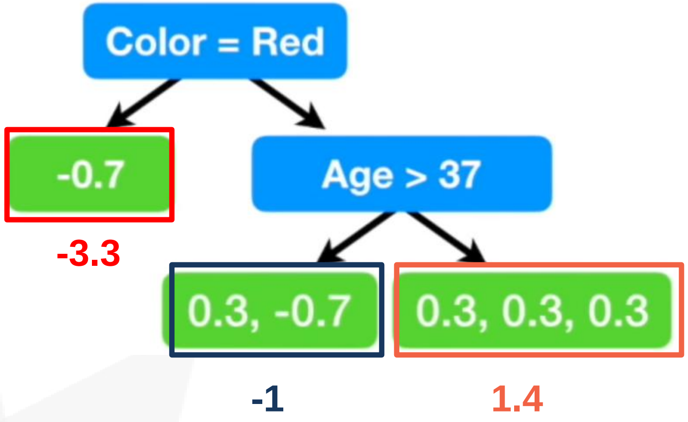
$$\frac{\sum \text{Residual}_i}{\sum [\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)]}$$

$$\frac{-0.7}{0.7 \times (1 - 0.7)} \quad (= -3.3)$$

$$\frac{0.3 + -0.7}{(0.7 \times (1 - 0.7)) + (0.7 \times (1 - 0.7))} \quad (= -1)$$

With this formula, we can change the value of terminal node (which is probability) to be expressed in log odds ratio!

2. Gradient Boost Classification



$$\frac{\sum \text{Residual}_i}{\sum \left[\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)\right]}$$

$$\boxed{\frac{-0.7}{0.7 \times (1 - 0.7)} \quad (= -3.3)}$$

$$\boxed{\frac{0.3 + -0.7}{(0.7 \times (1 - 0.7)) + (0.7 \times (1 - 0.7))} \quad (= -1)}$$

Replace the value!
(to be compatible with ‘log odds ratio’)

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2
Yes	12	Blue	Yes
Yes	87	Green	Yes
No	44	Blue	No
Yes	19	Red	No

Prediction (before) : **0.7**

Prediction (after) : **0.7 + (0.8x1.4)** = 1.82

convert 1.82 (log odds ratio) into 0.9 (probability)

Make a new prediction! (considering the tree newly made)

2. Gradient Boost Classification

Likes Popcorn	Age	Favorite Color	Loves Troll 2	Predicted Prob.	Residual
Yes	12	Blue	Yes	0.9	0.1
Yes	87	Green	Yes	0.5	0.5
No	44	Blue	No	0.5	-0.5
Yes	19	Red	No	0.1	-0.1
No	32	Green	Yes	0.9	0.1
No	14	Blue	Yes	0.9	0.1

(= 1(actual) – 0.9(predicted))

(= 1(actual) – 0.5(predicted))

4

Calculate error, based on the second prediction!

2. Gradient Boost Classification

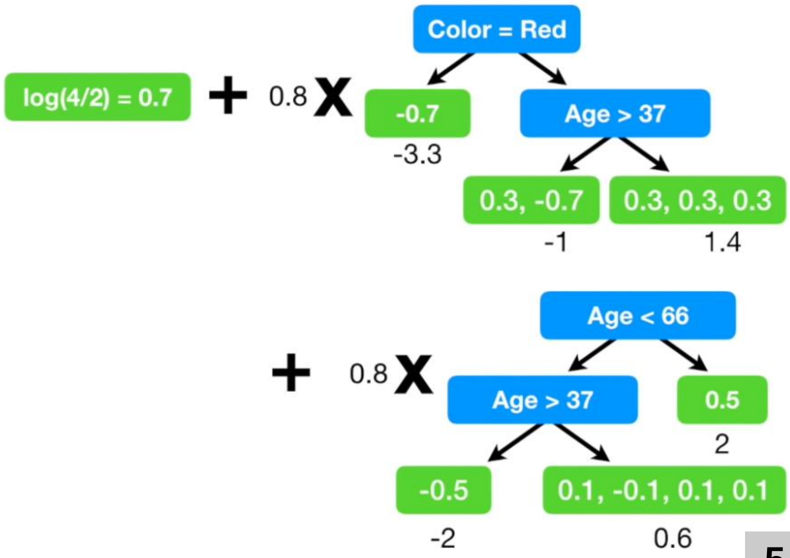
Likes Popcorn	Age	Favorite Color	Loves Troll 2	Predicted Prob.	Residual
Yes	12	Blue	Yes	0.9	0.1
Yes	87	Green	Yes	0.5	0.5
No	44	Blue	No	0.5	-0.5
Yes	19	Red	No	0.1	-0.1
No	32	Green	Yes	0.9	0.1
No	14	Blue	Yes	0.9	0.1

(= 1(actual) – 0.9(predicted))

(= 1(actual) – 0.5(predicted))

4

Calculate error, based on the second prediction!



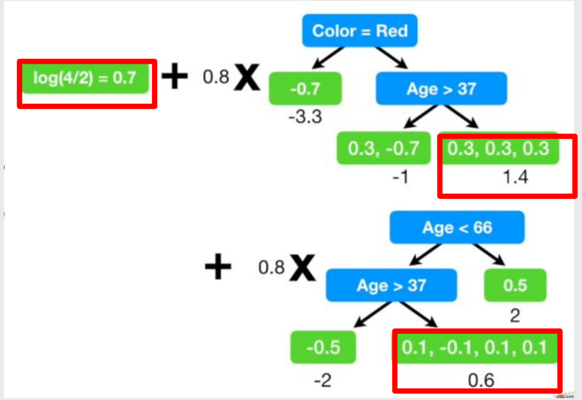
5

Keep making **sequential trees**!

2. Gradient Boost Classification

Ex) How would the person like below be classified?

Likes Popcorn	Age	Favorite Color	Loves Troll 2
Yes	25	Green	???



0.7 + (0.8x1.4) + (0.8x0.6) = 2.3

(into Logistic function)

f(2.3) = exp(2.3) / (1+exp(2.3)) = 0.9

Therefore, it will be classified as ‘Yes’

2. Gradient Boost Classification

Mathematical Expression

Loss Function : $LogLoss = -\frac{1}{n}\sum_{i=0}^{n}[y_i log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i)]$

(also called binary-cross entropy)

2. Gradient Boost Classification

Mathematical Expression

Loss Function : $LogLoss = -\frac{1}{n}\sum_{i=0}^{n}[y_i log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i)]$

(also called binary-cross entropy)

$$-\left[\textbf{Observed} \times \log(\boldsymbol{p}) + (1 - \textbf{Observed}) \times \log(1 - \boldsymbol{p}) \right]$$

Case 1) Actual(=Observed) = 1, Predicted = 1 $\longrightarrow$ Log loss : 0

Case 2) Actual(=Observed) = 1, Predicted = 0.5 $\longrightarrow$ Log loss : 0.69

Case 3) Actual(=Observed) = 1, Predicted = 0 $\longrightarrow$ Log loss : infinity

2-b. Gradient Boost

2. Gradient Boost Classification

Gradient Boosted Regression Tree

1. **Input:** $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}, \theta, \gamma$
2. **Output:** $F(\mathrm{x}) = \sum_{i=0}^{M} F_i(x)$
3. Initialize $F_0(x) = \arg min_\beta \sum_{i=0}^{N} L(y_i, \beta)$
4. **While** $(m < M)$
5. $\quad d_i = -[\partial L(y_i, F(x_i))/\partial F(x_i)]_{F(x_i)=F_{m-1}(x_i)}$
6. $\quad \vartheta = \{(x_i, d_i)\}, i = 1, N$
7. $\quad g(\mathrm{x}) = \mathrm{FITREGRETREE}(\vartheta, \theta)$
8. $\quad \rho_m = \arg min_\rho \sum_{i=1}^{N} L(y_i, F_{m-1}(x) + \rho g(x))$
9. $\quad F_m(x) = F_{m-1}(x) + \gamma \rho_m g(x)$

13. **End while**

2. Gradient Boost Classification

Gradient Boosted Classification Tree

Input: $D = \{(x_1, y_1), \dots, (x_N, y_N)\}, \theta, \gamma$

Output: $F(\mathrm{x}) = \sum_{i=0}^{M} F_i(x)$

Initialize $F_0(x) = \arg min_\beta \sum_{i=0}^{N} L(y_i, \beta)$

While $(m < M)$

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$\quad \rho_m = \arg min_\rho \sum_{i=1}^{N} L(y_i, F_{m-1}(x) + \rho g(x))$

$\quad F_m(x) = F_{m-1}(x) + \gamma \rho_m g(x)$

End while

Almost the same as the Regression Model!

2-b. Gradient Boost

2. Gradient Boost Classification

Gradient Boosted Regression Tree

1. **Input:** $D = \{(x_1, y_1), \dots, (x_N, y_N)\}, \theta, \gamma$
2. **Output:** $F(\mathrm{x}) = \sum_{i=0}^{M} F_i(x)$
3. Initialize $F_0(x) = \arg min_\beta \sum_{i=0}^{N} L(y_i, \beta)$
4. **While** $(m < M)$
5. $d_i = -[\partial L(y_i, F(x_i))/\partial F(x_i)]_{F(x_i)=F_{m-1}(x_i)}$
6. $\vartheta = \{(x_i, d_i)\}, i = 1, N$
7. $g(\mathrm{x}) = \mathrm{FITREGRETREE}(\vartheta, \theta)$
8. $\rho_m = \arg min_\rho \sum_{i=1}^{N} L(y_i, F_{m-1}(x) + \rho g(x))$
9. $F_m(x) = F_{m-1}(x) + \gamma \rho_m g(x)$

13. **End while**

Loss Function : MSE

y = f(x) + e1

e1 = g(x) + e2

e2 = h(x) + e3

Y = f(x) + g(x) + h(x) + …

First prediction = "average" of all y values

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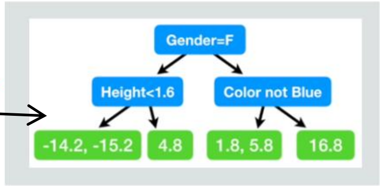
1.8	Red	Male	73	1.8
1.5	Green	Male	77	5.8
1.4	Blue	Female	57	-14.2



Y = f(x) + g(x) + e2

2-b. Gradient Boost

2. Gradient Boost Classification

Gradient Boosted Classification Tree

1. **Input:** $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}, \theta, \gamma$
2. **Output:** $F(x) = \sum_{i=0}^{M} F_i(x)$
3. Initialize $F_0(x) = \arg min_\beta \sum_{i=0}^{N} L(y_i, \beta)$
4. **While** $(m < M)$
5. $d_i = -[\partial L(y_i, F(x_i))/\partial F(x_i)]_{F(x_i)=F_{m-1}(x_i)}$
6. $\vartheta = \{(x_i, d_i)\}, i = 1, N$
7. $g(x) = \text{FITREGRETREE}(\vartheta, \theta)$
8. $\rho_m = \arg min_\rho \sum_{i=1}^{N} L(y_i, F_{m-1}(x) + \rho g(x))$
9. $F_m(x) = F_{m-1}(x) + \gamma \rho_m g(x)$

13. **End while**

y = f(x) + e1

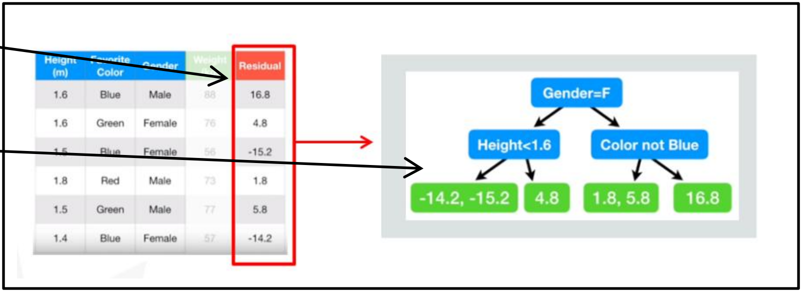
e1 = g(x) + e2

e2 = h(x) + e3

Y = f(x) + g(x) + h(x) + …

First prediction = "log odds ratio" of the mode

Loss Function : Log Loss



Y = f(x) + g(x) + e2

2-c. XGBoost

1. Characteritics of XGBoost

XGBoost (eXtreme Gradient Boost)

Consists of lots of parts!

1) Gradient Boost
2) Regularization
3) Unique Regression Tree
4) Approximate Greedy Algorithm
5) Weighted Quantile Sketch
6) Sparsity-Aware Split Finding
7) Parallel Learning
8) Cache-Aware Access
9) Blocks for Out-of-Core Computation

1. XGBoost Regression

2. XGBoost Classification

2. XGBoost Regression

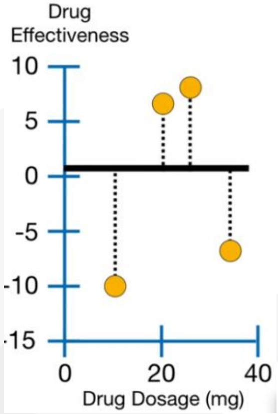
2. XGBoost Regression

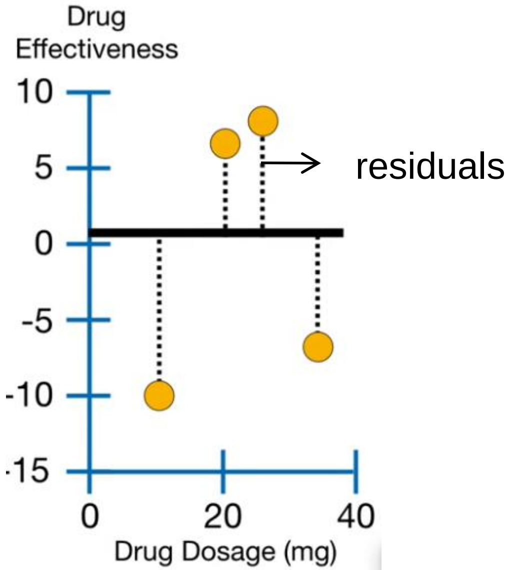
Unique Regression Tree!

Example with simple data)

X : drug dosage

Y : drug Effectiveness

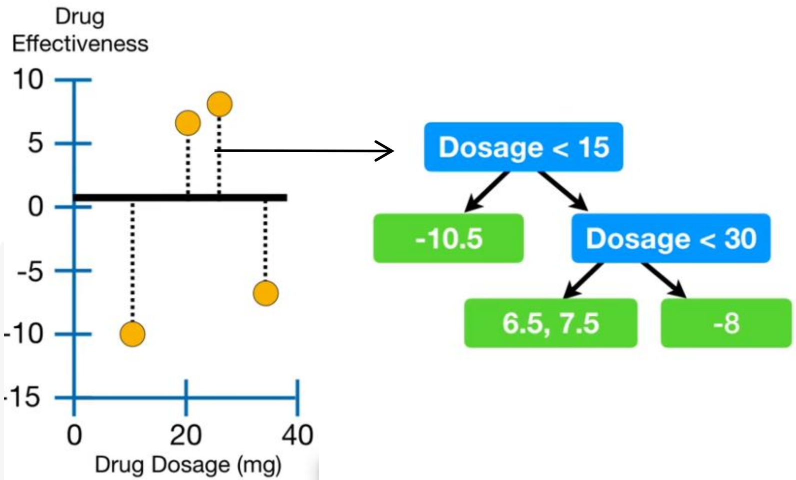




1

Initial Prediction : 0.5 (default)
(both in Regression & Classification)

2. XGBoost Regression

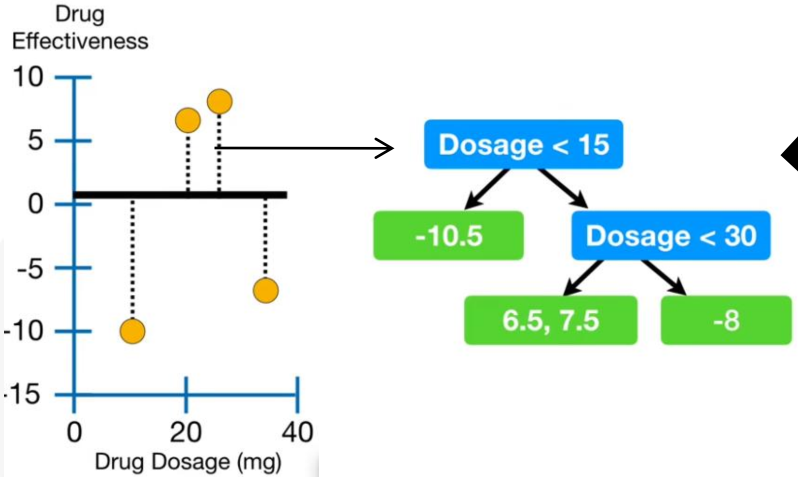


(same as non-extreme GB) **2**

Then, predict the "residual"

(build the next model (tree) predicting the residuals)

2. XGBoost Regression



(same as non-extreme GB) **2**

Then, predict the "residual"

(build the next model (tree) predicting the residuals)

HOW?

Step 1.

Put all the residuals to the same leaf

-10.5, 6.5, 7.5, -7.5

And calculate a "**similarity score**"

$$\text{Similarity Score} = \frac{\text{Sum of Residuals, Squared}}{\text{Number of Residuals} + \lambda}$$

(lambda : regularization term)

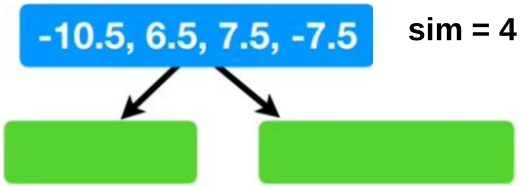
$$\frac{(-10.5 + 6.5 + 7.5 + -7.5)^2}{4 + 0} = 4$$

2. XGBoost Regression

HOW?

Step 2.

Split the leaf, which gives the most **"Gain"**



sim = 4

1 Drug Dosage < 15

2 Drug Dosage < 22.5

3 Drug Dosage < 15

Which split criterion should we choose?

2. XGBoost Regression

HOW?

Step 2.

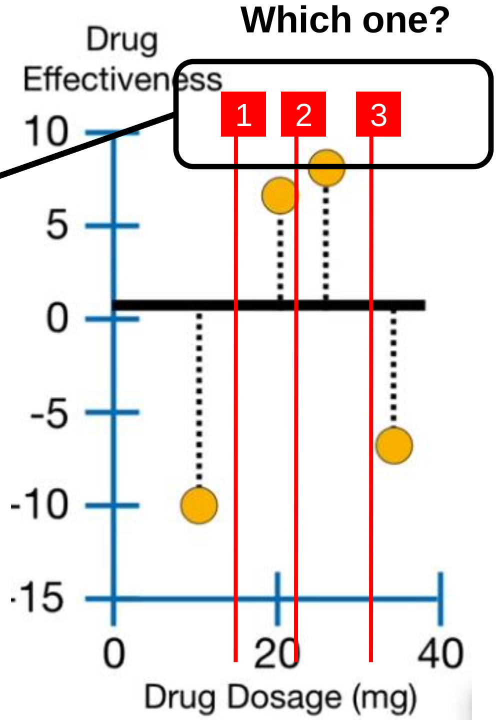
Split the leaf, which gives the most **"Gain"**

1 Drug Dosage < 15

2 Drug Dosage < 22.5

3 Drug Dosage < 15

Which split criterion should we choose?



2. XGBoost Regression

1 Drug Dosage < 15

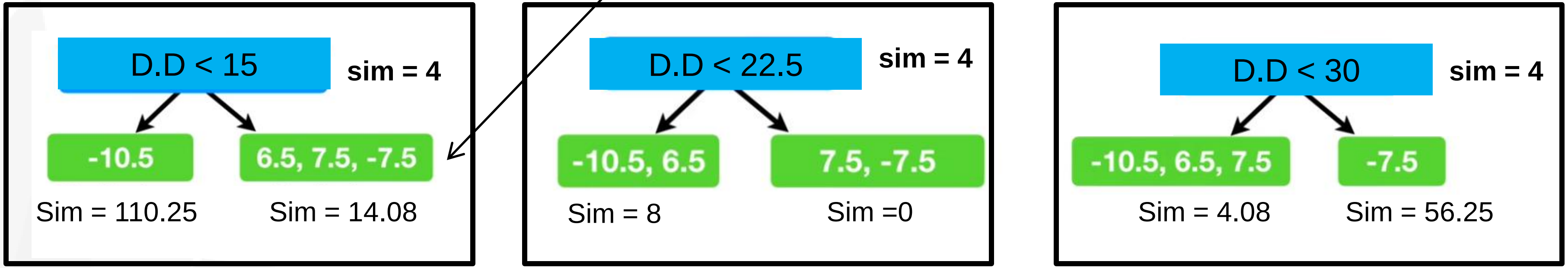
2 Drug Dosage < 22.5

3 Drug Dosage < 30

Which split criterion should we choose?

Example)

$$14.08 = \frac{(6.5 + 7.5 + -7.5)^2}{3 + 0}$$



2. XGBoost Regression

1 Drug Dosage < 15

2 Drug Dosage < 22.5

3 Drug Dosage < 30

Which split criterion should we choose?

Example)

$$14.08 = \frac{(6.5 + 7.5 + -7.5)^2}{3 + 0}$$

D.D < 15 sim = 4

-10.5 | 6.5, 7.5, -7.5

Sim = 110.25 | Sim = 14.08

D.D < 22.5 sim = 4

-10.5, 6.5 | 7.5, -7.5

Sim = 8 | Sim =0

D.D < 30 sim = 4

-10.5, 6.5, 7.5 | -7.5

Sim = 4.08 | Sim = 56.25

Gain

(110.25 + 14.08) - 4 = 120.33

Gain

(8 + 0) - 4 = 4

Gain

(4.08 + 56.25) – 4 = 56.33

2. XGBoost Regression

1 Drug Dosage < 15

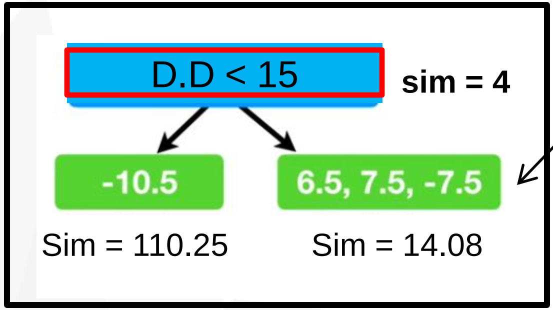
2 Drug Dosage < 22.5

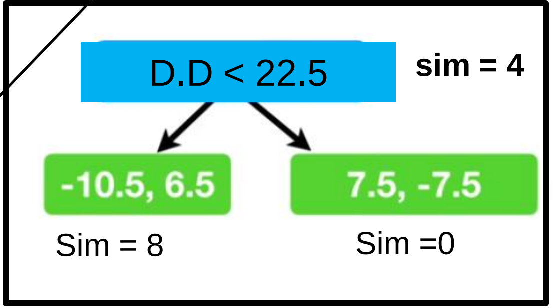
3 Drug Dosage < 30

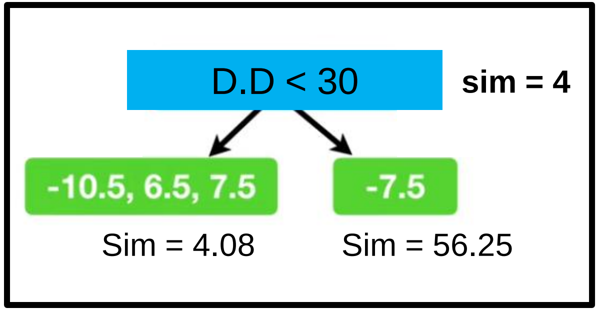
Which split criterion should we choose?

Example)

$$14.08 = \frac{(6.5 + 7.5 + -7.5)^2}{3 + 0}$$







Gain

(110.25 + 14.08) - 4 = **120.33**

Gain

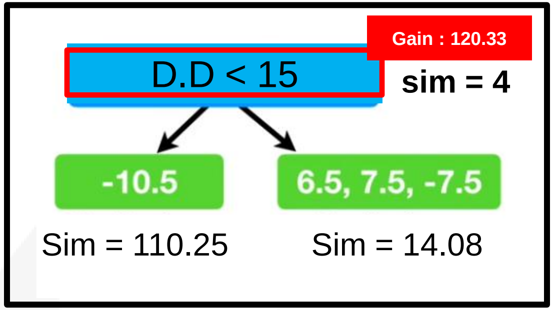
(8 + 0) - 4 = 4

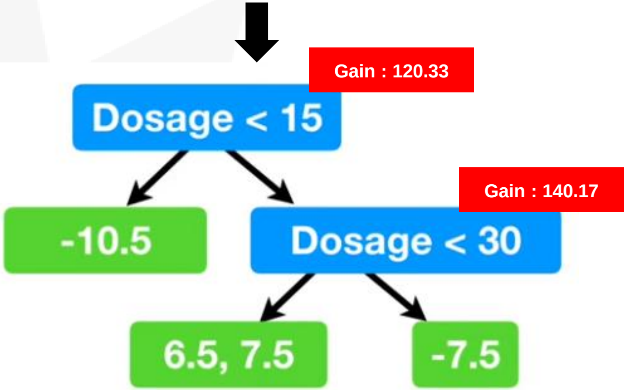
Gain

(4.08 + 56.25) – 4 = 56.33

2. XGBoost Regression

choose “D.D<15” as the criterion

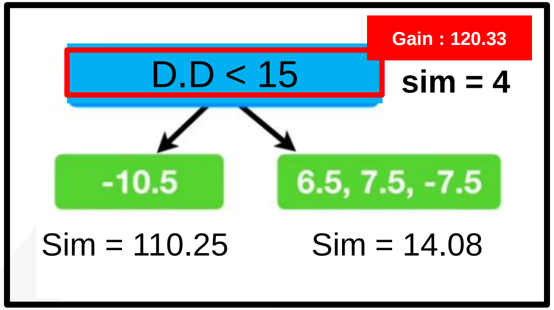


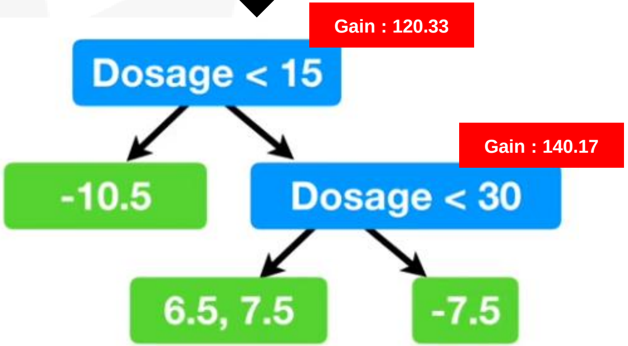


2-c. XGBoost

2. XGBoost Regression

choose “D.D<15” as the criterion



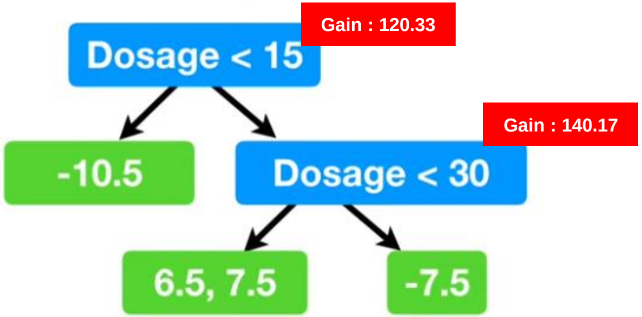


HOW?

Step 3.

Prune the tree (if necessary)

To Prevent Overfitting!



New parameter : **‘gamma’**

If gamma = 130 :

(140.17 > 130) -> Prune X

If gamma = 150 :

(140.17 < 150) -> Prune O -> (120.33 < 150) -> Prune O

NO GAIN,
NO PRUNE

2. XGBoost Regression

Another method for preventing overfitting (regularization)

$$\text{Similarity Score} = \frac{\text{Sum of Residuals, Squared}}{\text{Number of Residuals} + \boxed{\lambda}}$$

2. XGBoost Regression

Another method for preventing overfitting (regularization)

$$\text{Similarity Score} = \frac{\text{Sum of Residuals, Squared}}{\text{Number of Residuals} + \boxed{\lambda}}$$

What happens if lambda gets larger?

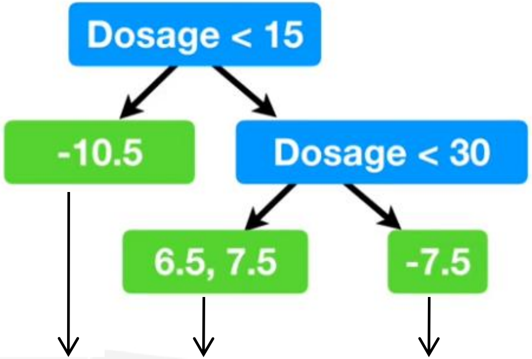
lambda ↑ -> similarity score ↓ -> **More chance of getting pruned**

2. XGBoost Regression

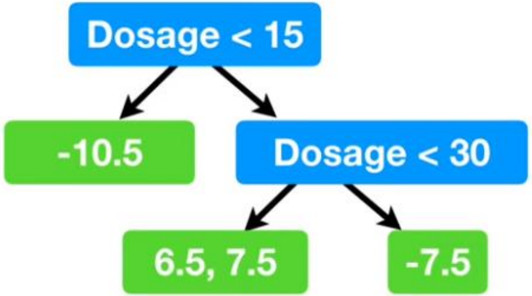
Step 4.

Predict output values of each leaf !

$$\text{Output Value} = \frac{\text{Sum of Residuals}}{\text{Number of Residuals} + \lambda}$$



these are all RESIDUALS, not output values!



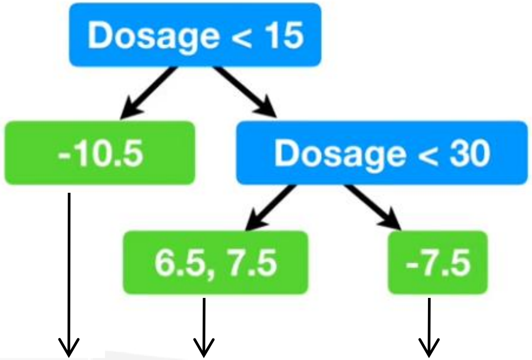
How will these values (of leaves) change?

2. XGBoost Regression

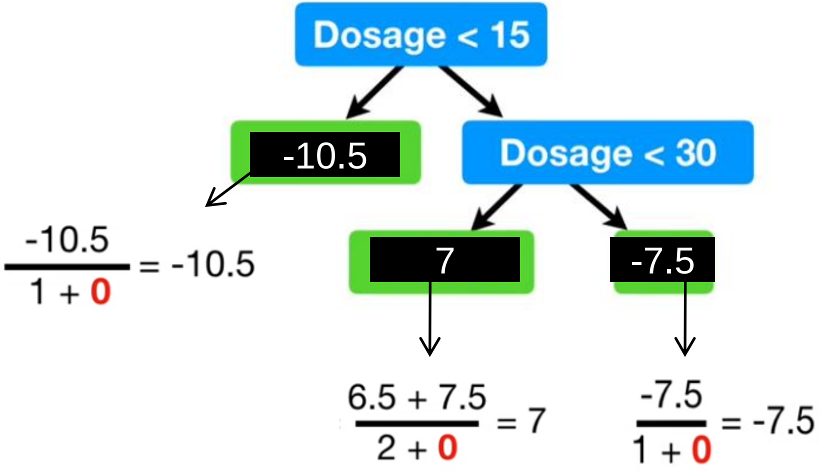
Step 4.

Predict output values of each leaf !

$$\text{Output Value} = \frac{\text{Sum of Residuals}}{\text{Number of Residuals} + \lambda}$$



these are all RESIDUALS, not output values!



2. XGBoost Regression

Step 5.

Predict the final outcome!

...

...

...

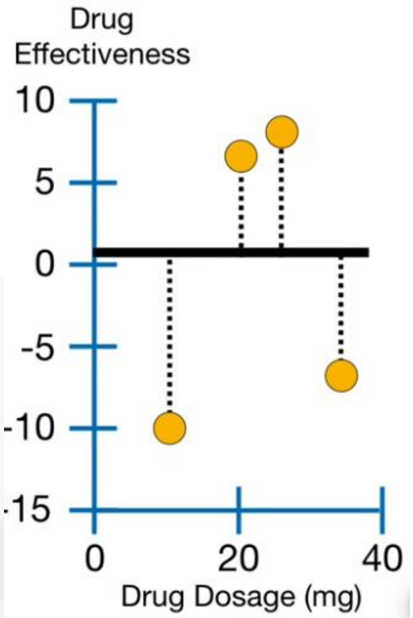
2. XGBoost Regression

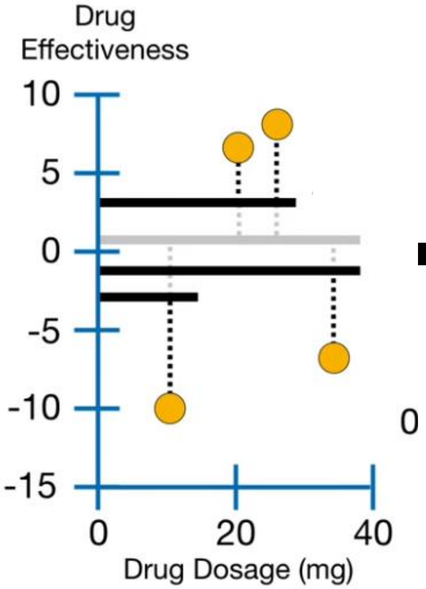
Step 5.

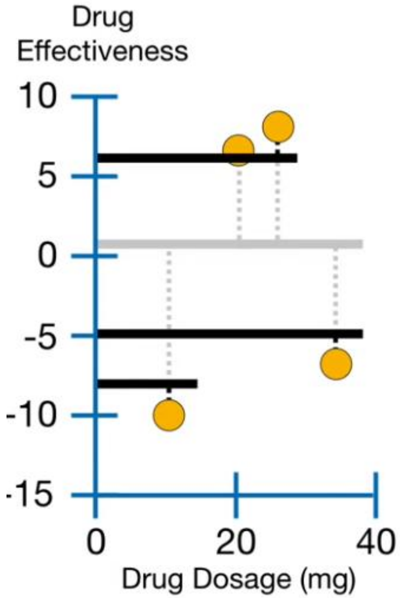
Predict the final outcome!

Getting a more precise prediction as the model is made!

(But be careful of overfitting!)







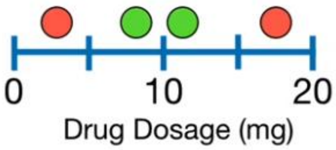
3. XGBoost Classification

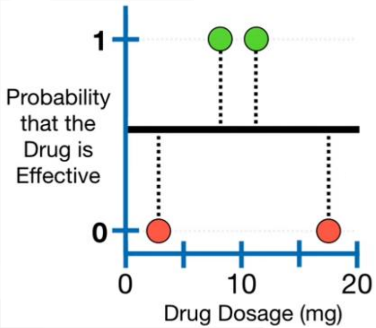
3. XGBoost Classification

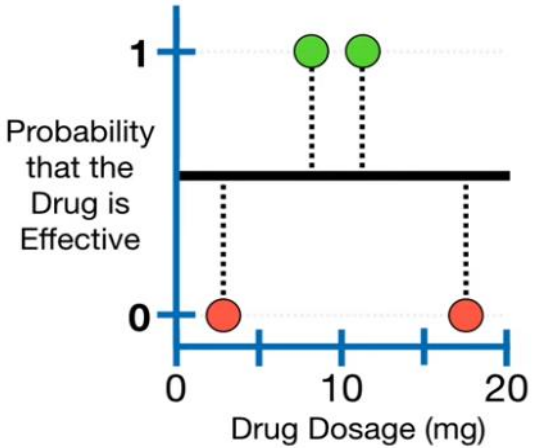
Example with simple data)

X : drug dosage

Y : Effective / Not Effective



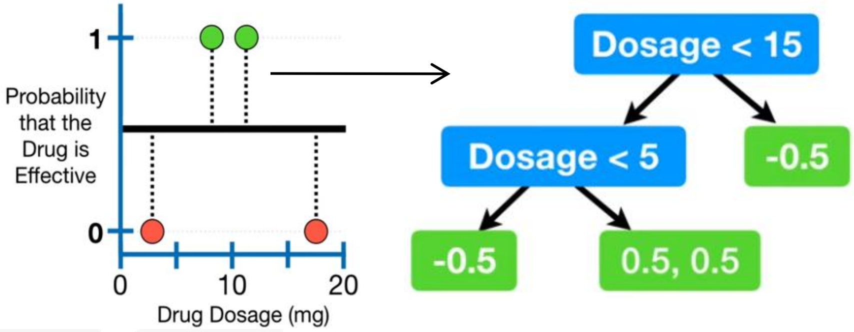




1

Initial Prediction : 0.5 (default)
(both in Regression & Classification)

3. XGBoost Classification



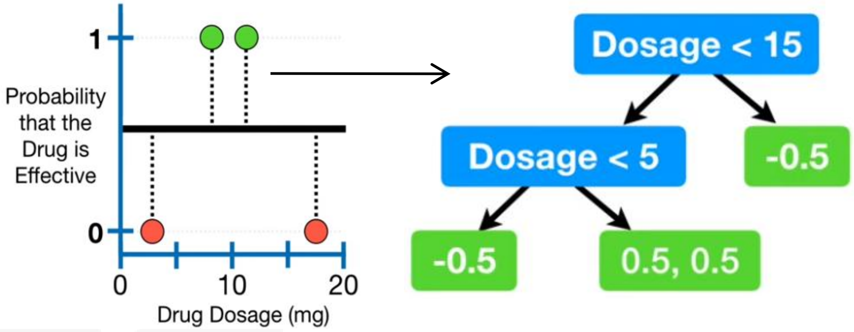
(same as non-extreme GB)

2

Then, predict the "residual"

(build the next model (tree) predicting the residuals)

3. XGBoost Classification



(same as non-extreme GB) **2**

Then, predict the "residual"

(build the next model (tree) predicting the residuals)

HOW?

Step 1.

Put all the residuals to the same leaf

-0.5, 0.5, 0.5, -0.5

And calculate a "**similarity score**"

$$\frac{(\sum \text{Residual}_i)^2}{\sum [\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)] + \lambda}$$

(lambda : regularization term)

$$\frac{(-0.5 + 0.5 + 0.5 + -0.5)^2}{4 \text{ x } (0.5\text{x}(1-0.5))} = 0$$

3. XGBoost Classification

Nothing is different from XGBoost Regression,

except the "similarity score"

(in Regression)

$$\text{Similarity Score} = \frac{\text{Sum of Residuals, Squared}}{\text{Number of Residuals} + \boldsymbol{\lambda}}$$

(in Classification)

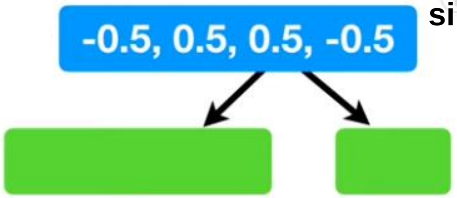
$$\frac{\left(\sum \text{Residual}_i\right)^2}{\sum \left[\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)\right] + \boldsymbol{\lambda}}$$

2. XGBoost Regression

HOW?

Step 2.

Split the leaf, which gives the most **"Gain"**



sim = 0

1 Drug Dosage < 15

2 Drug Dosage < 22.5

3 Drug Dosage < 15

Which split criterion should we choose?

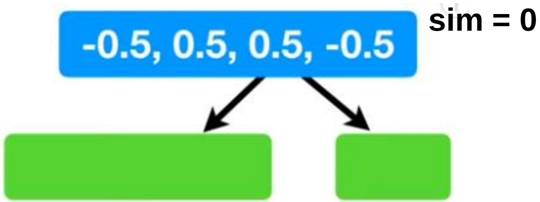
2-c. XGBoost

2. XGBoost Regression

HOW?

Step 2.

Split the leaf, which gives the most **"Gain"**



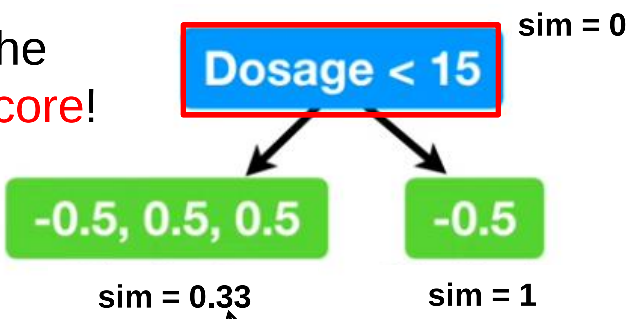
1 Drug Dosage < 15

2 Drug Dosage < 22.5

3 Drug Dosage < 15

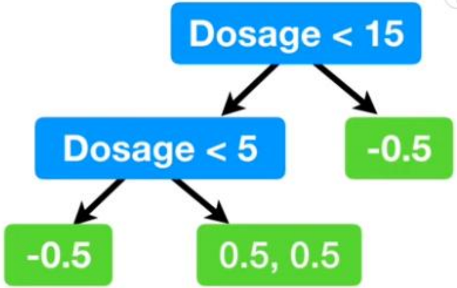
Which split criterion should we choose?

Calculate the similarity score!



$$\frac{(0.5)^2}{(0.5 \times (1-0.5)) + (0.5 \times (1-0.5)) + (0.5 \times (1-0.5)) + 0}$$

Repeat this for the next leaf



3. XGBoost Classification

Step 3.

Pruning the tree

- parameter 'gamma'

  (minimum gain to make a split!)

- parameter 'lambda'

  (regularization term)

3. XGBoost Classification

Step 3.

Pruning the tree

- parameter 'gamma'

(minimum gain to make a split!)

- parameter 'lambda'

(regularization term)

- **minimum number of residuals in each leaf**

(new term, 'cover')

3. XGBoost Classification

Step 3.

Pruning the tree

- parameter 'gamma'
  (minimum gain to make a split!)

- parameter 'lambda'
  (regularization term)

- **minimum number of residuals in each leaf**
  (new term, 'cover')

$$\frac{(\sum \text{Residual}_i)^2}{\boxed{\sum [\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)]} + \lambda}$$

(in regression)

$$\text{Similarity Score} = \frac{\text{Sum of Residuals, Squared}}{\text{Number of Residuals} + \lambda}$$

- cover can be defined as 'number of residuals'
- default value : 1 -> means that it has no affect on the growth of tree

3. XGBoost Classification

Step 3.

Pruning the tree

- parameter ‘gamma’

(minimum gain to make a split!)

- parameter ‘lambda’

(regularization term)

- **minimum number of residuals in each leaf**

(new term, ‘cover’)

$$\frac{(\sum \text{Residual}_i)^2}{\boxed{\sum [\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)]} + \lambda}$$

(in regression)

$$\text{Similarity Score} = \frac{\text{Sum of Residuals, Squared}}{\text{Number of Residuals} + \lambda}$$

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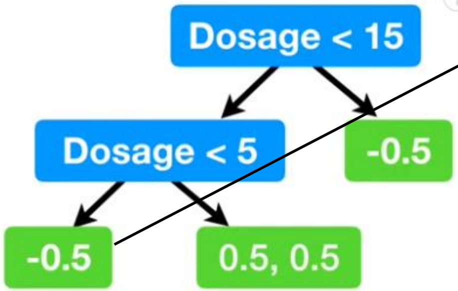
Example)



‘cover’ for this leaf is

1 x (0.5 x (1-0.5)) = 0.25

3. XGBoost Classification

Step 3.

Pruning the tree

- parameter 'gamma'
  (minimum gain to make a split!)

- parameter 'lambda'
  (regularization term)

- **minimum number of residuals in each leaf**
  (new term, 'cover')

we call this parameter 'cover' as "**min_child_weight**"

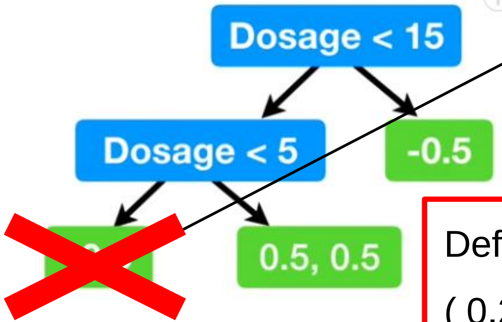
$$\frac{\left(\sum \text{Residual}_i\right)^2}{\boxed{\sum \left[\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)\right]} + \lambda}$$

(in regression)

$$\text{Similarity Score} = \frac{\text{Sum of Residuals, Squared}}{\text{Number of Residuals} + \lambda}$$

- cover can be defined as 'number of residuals'
- default value : 1 -> means that it has no affect on the growth of tree

Example)



'cover' for this leaf is

1 x (0.5 x (1-0.5)) = 0.25

Default value for cover : 1

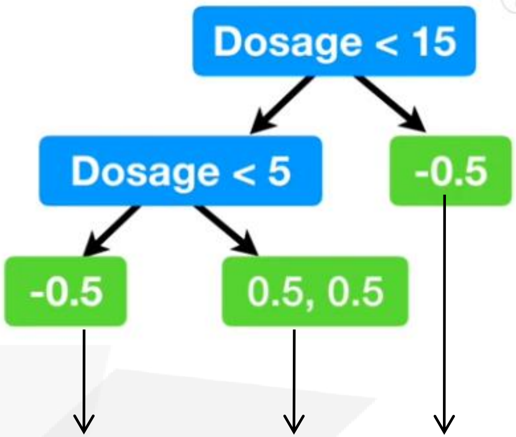
(0.25 < 1) -> get pruned!

3. XGBoost Classification

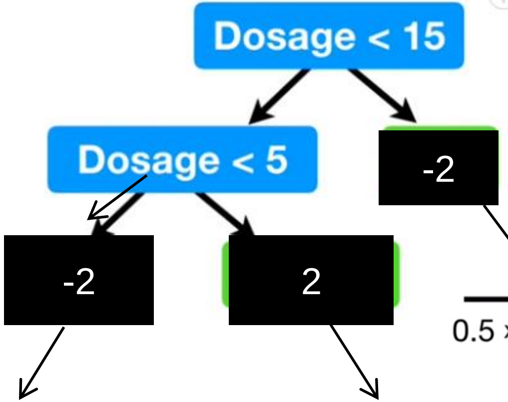
Step 4.

Predict the output values of each leaf

$$\text{Output value} = \frac{\left(\sum \text{Residual}_i\right)}{\sum \left[\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)\right] + \lambda}$$



these are all RESIDUALS, not output values!



$$\frac{-0.5}{0.5 \times (1 - 0.5) + 0} = -2$$

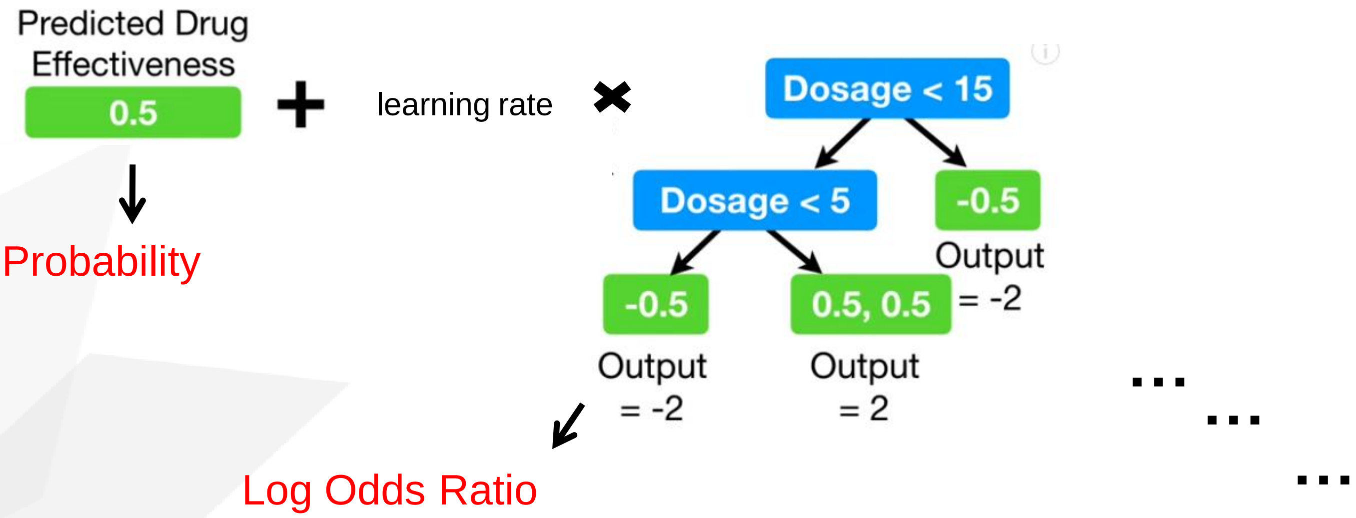
$$\frac{-0.5}{0.5 \times (1 - 0.5) + 0} = -2$$

$$\frac{0.5 + 0.5}{0.5 \times (1 - 0.5) + 0.5 \times (1 - 0.5) + 0} = 2$$

3. XGBoost Classification

Step 5.

Predict the final outcome

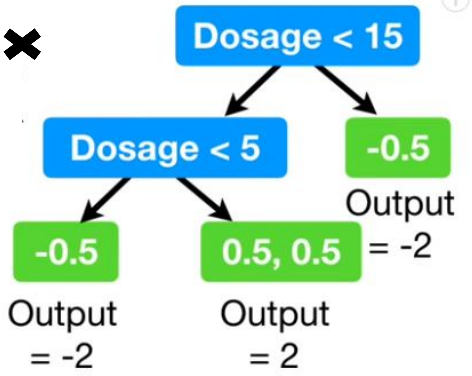


3. XGBoost Classification

Step 5.

Predict the final outcome

Predicted Drug Effectiveness 0.5 + learning rate ✖



… … …

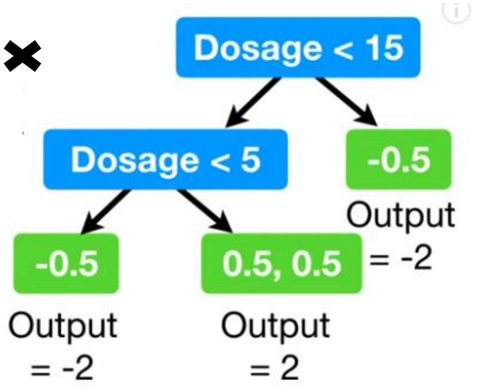
0.5 is "probability", so we have to convert this into "log odds ratio"

3. XGBoost Classification

Step 5.

Predict the final outcome

+ learning rate ×



log(odds) = log(0.5 / (1-0.5)) = 0

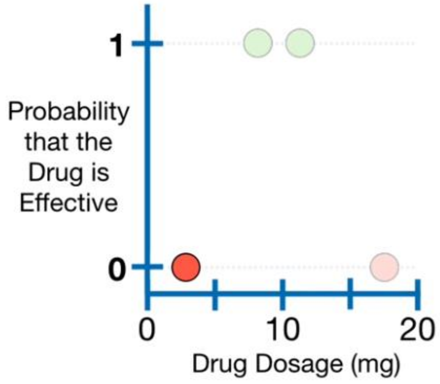
…

…

…

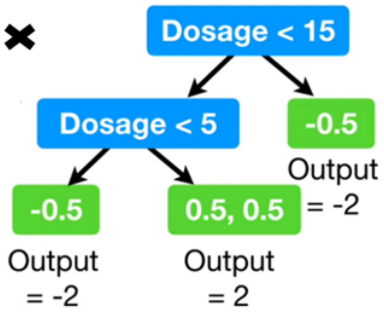
3. XGBoost Classification

Ex) What is the predicted class for the sample below, with the red color? (let learning rate = 0.3)



Predicted Drug Effectiveness

0.5 + learning rate ×



log(odds) = log(0.5 / (1-0.5)) = 0

Answer :

1) 0 + (0.3 x (-2)) = - 0.6

(this is in terms of 'log(odds)' ! Have to convert into probability)

2) Probability = $\dfrac{e^{-0.6}}{1 + e^{-0.6}}$ = 0.35 -> Predicted as 'NO EFFECT'

3. XGBoost Classification

Gradient Boosting Classification

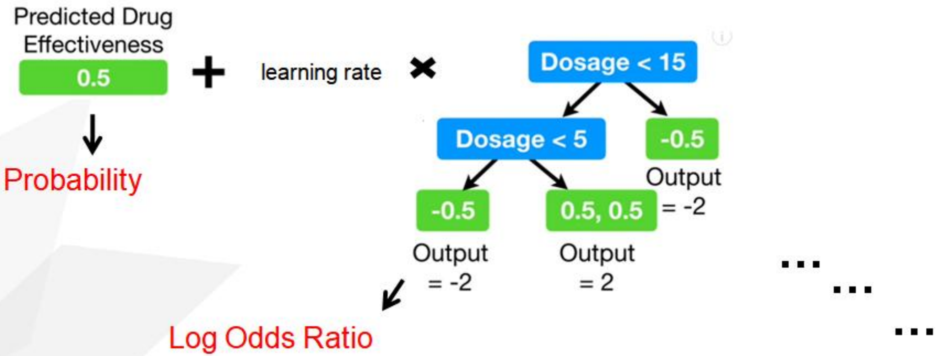
(in Classification)

$$\frac{\sum \text{Residual}_i}{\sum [\text{Previous Probability}_i \times (1 - \text{Previous Probability}_i)]}$$

Log odds ratio   Probability

MISMATCH! Can't just add them together!
How to make 'probability' compatible with 'log odds ratio'?

XGBoost Classification



3. XGBoost Classification

Parameters of XGBoost

Parameter	Description	Default Value
max_depth	controls the maximum depth of each tree (used to control over-fitting)	6
subsample	specifies the fraction of observations to be randomly sampled at each tree (adds randomness)	1
eta	the learning rate	0.3
nrounds	the number of trees to be produced (similar to ntree)	100–1000
gamma	controls the minimum loss reduction required to make a node split (used to control over-fitting)	0
min_child_weight	Specifies the minimum sum of instance weight of all the observations required in a child (used to control over-fitting)	1
colsample_bytree	Specifies the number of features to consider when searching for the best node split (adds randomness)	1

https://www.researchgate.net/figure/Key-parameters-used-for-XGBoost-classification_tbl1_322791200

3. XGBoost Classification

Mathematical Expressions

https://brunch.co.kr/@snobberys/137

- Model: assuming we have K trees

$$\hat{y}_i = \sum_{k=1}^{K} f_k(x_i), \quad f_k \in \mathcal{F}$$

- Objective

$$Obj = \sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k)$$

Training loss

Complexity of the Trees

3. XGBoost Classification

Mathematical Expressions

- Goal $Obj^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + constant$
  - Seems still complicated except for the case of square loss
- Take Taylor expansion of the objective
  - Recall $f(x + \Delta x) \simeq f(x) + f'(x)\Delta x + \frac{1}{2} f''(x)\Delta x^2$
  - Define $g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial^2_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$

$$Obj^{(t)} \simeq \sum_{i=1}^{n} \left[l(y_i, \hat{y}_i^{(t-1)}) + g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t) + constant$$

3. XGBoost Classification

Mathematical Expressions

$$\Omega(f_t) = \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} w_j^2$$

Number of leaves

L2 norm of leaf scores

$$Obj^{(t)} \simeq \sum_{i=1}^{n} \left[l(y_i, \hat{y}_i^{(t-1)}) + g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \underline{\Omega(f_t)} + constant$$

At time 't'

$$\sum_{i=1}^{n} \left[g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t)$$

- where $g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial^2_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$

3. XGBoost Classification

Mathematical Expressions

- Define the instance set in leaf j as $I_j = \{i | q(x_i) = j\}$
- Regroup the objective by each leaf

$$
\begin{aligned}
Obj^{(t)} &\simeq \sum_{i=1}^{n} \left[g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t) \\
&= \sum_{i=1}^{n} \left[g_i w_{q(x_i)} + \frac{1}{2} h_i w_{q(x_i)}^2 \right] + \gamma T + \lambda \frac{1}{2} \sum_{j=1}^{T} w_j^2 \\
&= \sum_{j=1}^{T} \left[(\sum_{i \in I_j} g_i) w_j + \frac{1}{2} (\sum_{i \in I_j} h_i + \lambda) w_j^2 \right] + \gamma T
\end{aligned}
$$

- This is sum of T independent quadratic functions

3. XGBoost Classification

G : sum of g

H : sum of h

Mathematical Expressions

$$argmin_x \; Gx + \frac{1}{2}Hx^2 = -\frac{G}{H}, \; H > 0 \qquad \min_x \; Gx + \frac{1}{2}Hx^2 = -\frac{1}{2}\frac{G^2}{H}$$

$$w_j^* = -\frac{G_j}{H_j+\lambda} \qquad Obj = -\frac{1}{2}\sum_{j=1}^{T}\frac{G_j^2}{H_j+\lambda} + \gamma T$$

This measures how good a tree structure is!

Make a tree that makes the best split according to the following gain!

$$\boxed{Gain = \frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{(G_L+G_R)^2}{H_L+H_R+\lambda} - \gamma}$$

3. Boosting with Python

1) Adaboost
2) Gradient Boosting
3) XGBoost

4. Homework

Homework

HW1) Classification

HW2) Regression

- Choose any two of the ten datasets below

https://machinelearningmastery.com/standard-machine-learning-datasets/

Make a prediction using the models below (5-fold Cross Validation)

(Gradient Boosting, XGBoost, LightGBM + Stacking (next week))

Reference

[1] Josh Starmer(2019). *StatQuest with Josh Starmer*

[2] Seoul National University, Hyeong In Choi (2017). *Lecture 11: Boosting (I) AdaBoost (Draft: version 0.9.2)*

[3] Chongchong Qi, S.M.ASCE, Andy Fourie, Xu Zhao (2018). *Back-Analysis Method for Stope Displacements Using Gradient-Boosted Regression Tree and Firefly Algorithm*

[4] T.Chen (2016). *XGBoost : A Scalable Tree Boosting System*

Thank you