Boosting

Adaboost, Gradient Boost, XGBoost

Seunghan Lee

Contents

What is Boosting?

1) Ensemble method / 2) Bagging vs Boosting

2

- 1. Adaboost
- 2. Gradient Boost
- 3. XGBoost

Boosting with Python







- 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

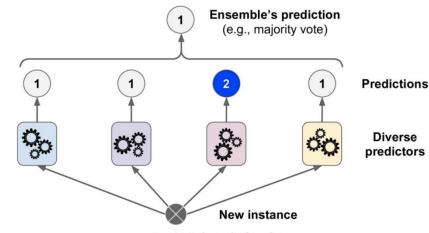


Figure 7-2. Hard voting classifier predictions

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

(2) Bagging vs Boosting

Steps of Bagging

- 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 **Bagging ENSEMBLE** perturbed sets of compounds C2 Learning Model Training set Mı Voting (classification) Model Learning Consensus M₂ Model algorithm Averaging (regression) Learning Model algorithm

(2) Bagging vs Boosting

Steps of Boosting

- First random sample (d1) without replacement
 train a weak learner C1
- Second random sample (d2) without replacement, considering the misclassified sample in learner C1
 train a weak learner C2
- 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.

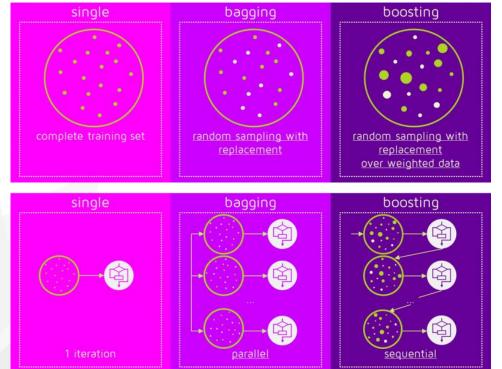
Training set Si W Ca Boosting for Classification. AdaBoost ENSEMBLE W Ca Boosting for Classification. W Ca Boosting for Classification. Weighted averaging & thresholding Weighted averaging & thresholding Work Ca W Ca W

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

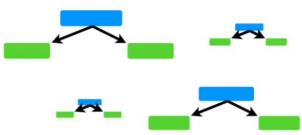


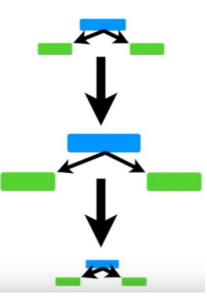




What is Adaboost?

- 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**)



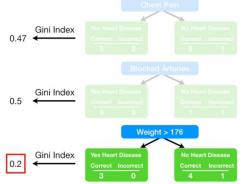


StatQuest with Josh Starmer

How does Adaboost work?

Yes Yes	1/8
Yes	1/8
Yes	1/8
Yes	1/8
No	1/8
	No No





In this example,

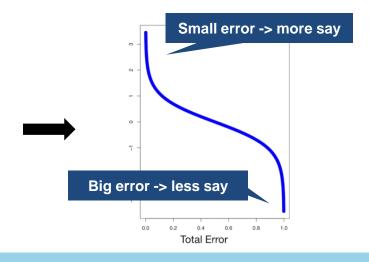
"weight > 176" will be chosen

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

How does Adaboost work?

"How much say" does each stump has?

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

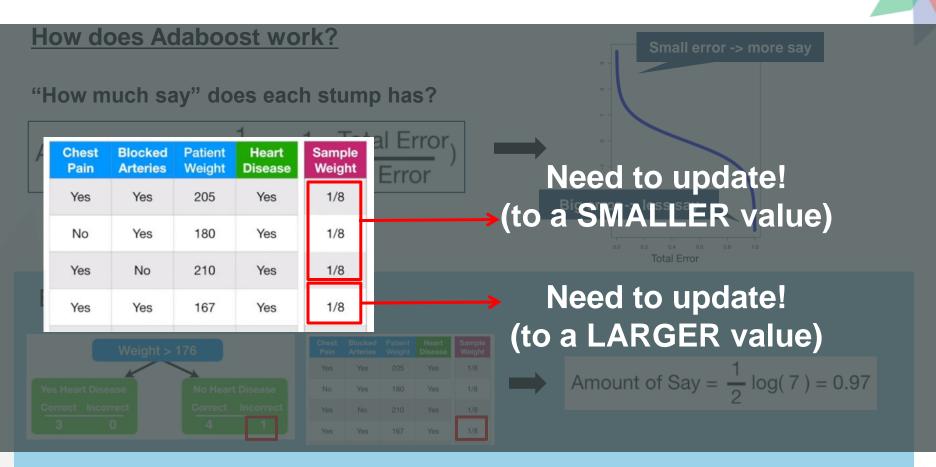


Example)



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

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



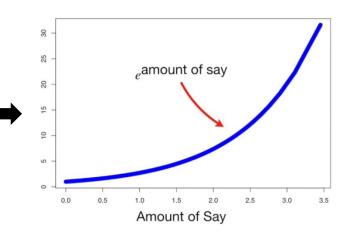
How does Adaboost work?

< for the "Misclassified" sample >

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

Weight

(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	1/8

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

Before) 0.125

After) 0.33

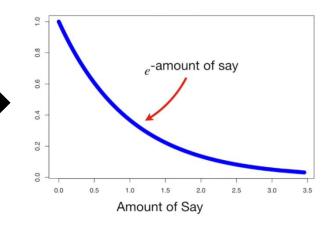
Amount of Say =
$$\frac{1}{2}$$
 log(7) = 0.97

How does Adaboost work?

< for the "Correctly classified" sample >

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

(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

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

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

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

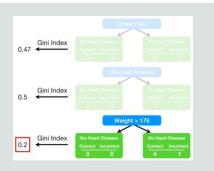
How does Adaboost work?

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
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

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
Yes	Yes	167	Yes
Yes	Yes	167	Yes
Yes	Yes	172	No
Yes	Yes	205	Yes
Yes	Yes	167	Yes

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
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No	Yes	125	No	0.07
Yes	No	168	No	0.07
Yes	Yes	172	No	0.07

Option 1)

Use "weighted Gini index" to select the feature to make new stump



Option 2)

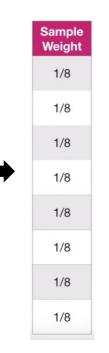
Duplicate copies of the samples (bigger 'sample weight' ->

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
Yes	Yes	167	Yes
Yes	Yes	167	Yes
Yes	Yes	172	No
Yes	Yes	205	Yes
Yes	Yes	167	Yes

How does Adaboost work?





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

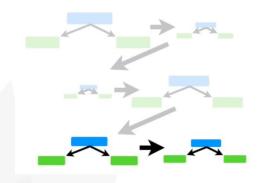
(important samples are duplicated!)

Give equal weight to all the samples!

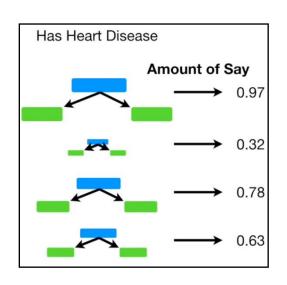
Amount of Say

How does Adaboost work?

Make models(stumps) sequentially



How to predict the final output?



Total Sum: 2.7

Does Not Have Heart Disease

Result: "Has Heart Disease"

How does Adaboost work?

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

Binary AdaBoost Input:

binary

- 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 $D_1(i) = \frac{1}{N}$ for $i = 1, \dots, N$.

Do for $t = 1, \dots, T$:

- Train using the probability distribution D_t on $\{1, \dots, N\}$.
- 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 $\varepsilon_t > \frac{1}{2}$, then set T = t 1 and abort the loop.
- Set $\alpha_t = \frac{1}{2} \log \left(\frac{1 \varepsilon_t}{\varepsilon_t} \right)$.
- Define the new probability distribution D_{t+1} by setting

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

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

Extend to multi-class

AdaBoost.M1 Input:

Multi-class

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

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

- Train using the probability distribution D_t on $\{1, \dots, N\}$.
- 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 $\varepsilon_t > \frac{1}{2}$, then set T = t 1 and abort the loop.
- Set $\alpha_t = \frac{1}{2} \log \left(\frac{1 \varepsilon_t}{\varepsilon_t} \right)$.
- Define the new probability distribution D_{t+1} by setting

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

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

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











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

1. Gradient Boosting Regression

2. Gradient Boosting Classification

$$y = f(x) + e1$$

 $e1 = g(x) + e2$
 $e2 = h(x) + e3$

$$Y = f(x) + g(x) + h(x) + ...$$

Residual

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

1.6 16.8 Blue Male 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 -14.2 Blue Female

Gender

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)

Then, predict the "residual"

Height

(m)

Favorite

Color

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

)

1. Gradient Boost Regression

(usually 8~32 leaves)

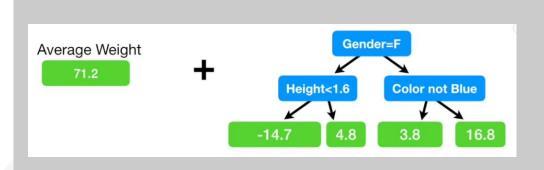




Replace the residuals into their average



1. Gradient Boost Regression



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

100% correct (no error)

Overfitting!



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

(If learning rate = 0.1)

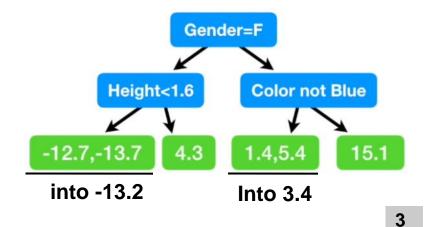
$$71.2 + (0.1 \times 16.8) = 72.9$$

1. Gradient Boost Regression

new residuals

(becomes smaller)

Height (m)	Favorite Color	Gender	Weight (kg)	Residual
1.6	88 – (7	'1.2 + 0.1x	(16.8) =	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



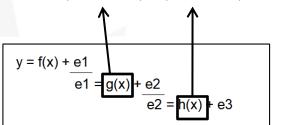
Then, predict the "residual's residual"

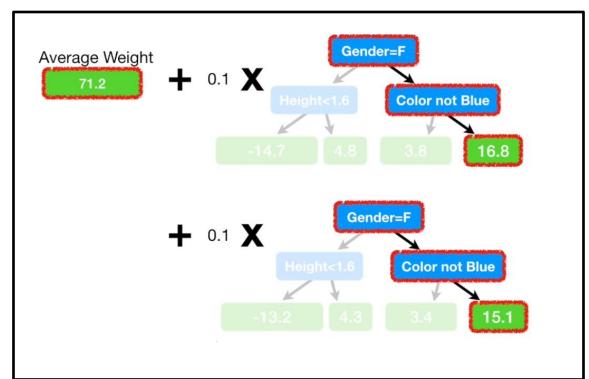
(build the next model (tree) predicting the residuals)

1. Gradient Boost Regression

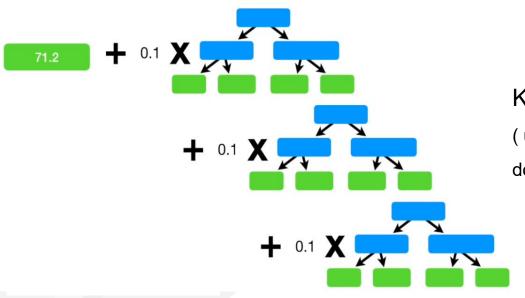
Height	Favorite	Gender	Weight
(m)	Color		(kg)
1.6	Blue	Male	74.4

$$71.2 + (0.1 \times 16.8) + (0.1 \times 15.1) = 74.4$$





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

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



To minimize this loss function

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

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

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

$$\frac{1}{2}(76 - \text{Predicted})^2 + \longrightarrow -(76 - \text{Predicted}) +$$

$$\frac{1}{2}(56 - \text{Predicted})^2 \longrightarrow -(56 - \text{Predicted})$$

1. Gradient Boost Regression

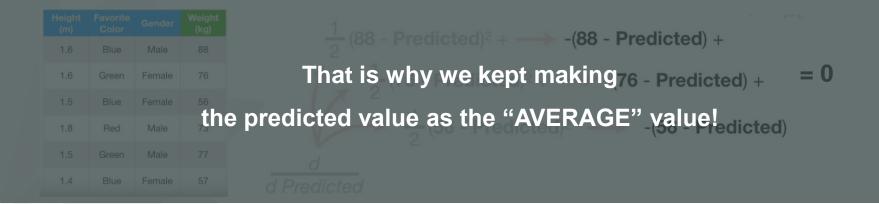
Mathematical Expression

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



To minimize this loss function

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



1. Gradient Boost Regression

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

Gradient Boosted Regression Tree

- 1. **Input:** $D = \{(x_1, y_1), ..., (x_N, y_N)\}, \theta, \gamma$
- 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. $\theta = \{(x_i, d_i)\}, i = 1, N$
- 7. $g(x) = FITREGRETREE(\vartheta, \theta)$
- 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

Done!

1. Gradient Boost Regression

Gradient Boosted Regression Tree

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

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
$$(m < M)$$
 Loss Function : MSE

5.
$$d_i = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x_i) = F_{m-1}(x_i)}$$

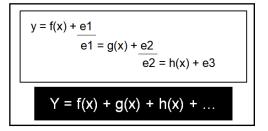
6.
$$\theta = \{(x_i, d_i)\}, i = 1, N$$

7.
$$g(x) = FITREGRETREE(\vartheta, \theta)$$

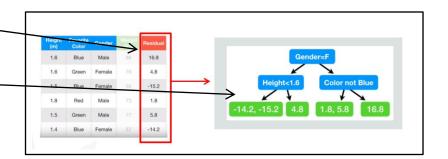
8.
$$\rho_m = \arg\min_{\rho} \sum_{i=1}^{N} L(y_i, F_{m-1}(x) + \rho g(x))$$

9.
$$F_m(x) = F_{m-1}(x) + \gamma \rho_m g(x)$$

13. End while



First prediction = "average" of all y values



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

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)

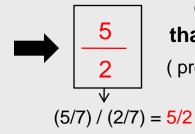
$$\operatorname{logit}(p) = \operatorname{log}\!\left(rac{p}{1-p}
ight)$$

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

Example)

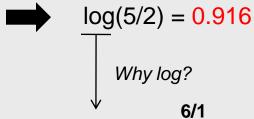
Chance of winning?

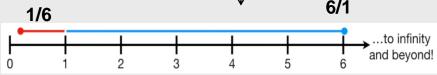
DSL YBIGTA
5 2



Odds are 2.5 that DSL will win!

(probability (p) = 5/7)





2. Gradient Boost Classification

2) Logistic Function (= Sigmoid)

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

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

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



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)

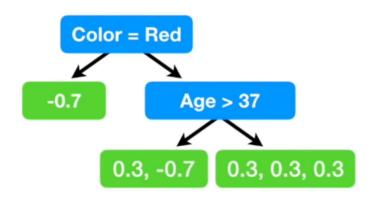
(threshold: 0.5)

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 = 1, No = 0)
Yes	12	Blue	Yes	0.3	
Yes	87	Green	Yes	0.3	(= 1(actual) - 0.7(predicted))
No	44	Blue	No	-0.7	(=0(actual)-0.7(predicted))
Yes	19	Red	No	-0.7	
No	32	Green	Yes	0.3	
No	14	Blue	Yes	0.3	



2

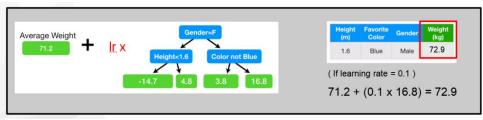
Calculate Error based on the first prediction

Make a tree, predicting the "residuals"

3

2. Gradient Boost Classification

(in Regression)



A bit different in Classification

(in Classification)



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

2. Gradient Boost Classification

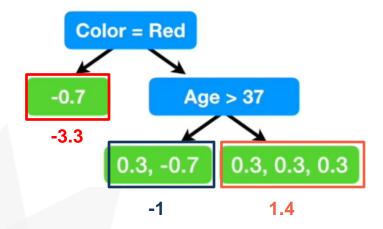


$$\frac{\sum \mathsf{Residual}_i}{\sum \left[\mathsf{Previous\ Probability}_i \times (1 - \mathsf{Previous\ Probability}_i)\right]}$$

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

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

2. Gradient Boost Classification



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

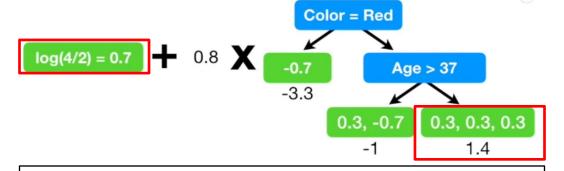
$$\frac{\sum \mathsf{Residual}_i}{\sum \left[\mathsf{Previous\ Probability}_i \times (1 - \mathsf{Previous\ Probability}_i)\right]}$$

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

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

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)

3

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

Color = Red

2. Gradient Boost Classification

					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

Calculate error, based on the second prediction!

4

Keep making sequential trees!

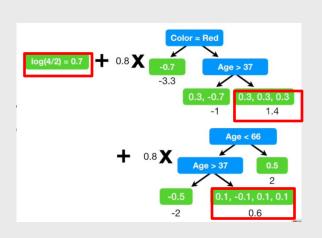
0.6

-2

2. Gradient Boost Classification

Ex) How would the person like below be classified?

Likes	Age	Favorite	Loves	
Popcorn		Color	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:
$$LogLoss = -\frac{1}{n}\sum_{i=0}^{n}[y_ilog(\hat{y}_i) + (1-y_i)log(1-\hat{y}_i)]$$

(also called binary-cross entropy)

- Observed
$$\times \log(\mathbf{p}) + (1 - \mathbf{Observed}) \times \log(1 - \mathbf{p})$$

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

2. Gradient Boost Classification

Gradient Boosted Regression Tree

- 1. **Input:** $D = \{(x_1, y_1), ..., (x_N, y_N)\}, \theta, \gamma$
- 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. $\theta = \{(x_i, d_i)\}, i = 1, N$
- 7. $g(x) = FITREGRETREE(\vartheta, \theta)$
- 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

2. Gradient Boost Classification

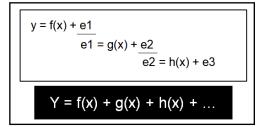
Gradient Boosted Classification Tree **Input:** $D = \{(x_1, y_1), ..., (x_N, y_N)\}, \theta, \gamma$ **Output:** $F(x) = \sum_{i=0}^{M} F_i(x)$ Initialize $F_0(x) = \arg\min_{\beta} \sum_{i=0}^{N} L(y_i, \beta)$ While (m < M) $| d_i = -[\partial L(y_i, F(x_i))/\partial F(x_i)]_{F(x_i) = F_{m-1}(x_i)}$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

Almost the same as the Regression Model!

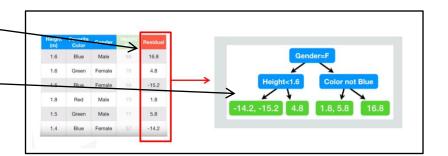
2. Gradient Boost Classification

Gradient Boosted Regression Tree

- 1. **Input:** $D = \{(x_1, y_1), ..., (x_N, y_N)\}, \theta, \gamma$
- 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) Loss Function : MSE
- 5. $d_i = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x_i) = F_{m-1}(x_i)}$
- 6. $\theta = \{(x_i, d_i)\}, i = 1, N$
- 7. $g(x) = FITREGRETREE(\vartheta, \theta)$
- 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



First prediction = "average" of all y values

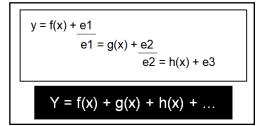


$$Y = f(x) + g(x) + e2$$

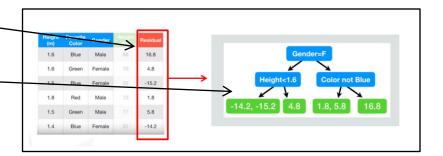
2. Gradient Boost Classification

Gradient Boosted Classification Tree

- 1. **Input:** $D = \{(x_1, y_1), ..., (x_N, y_N)\}, \theta, \gamma$
- 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) Loss Function : Log Loss
- 5. $d_i = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x_i) = F_{m-1}(x_i)}$
- 6. $\theta = \{(x_i, d_i)\}, i = 1, N$
- 7. $g(x) = FITREGRETREE(\vartheta, \theta)$
- 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

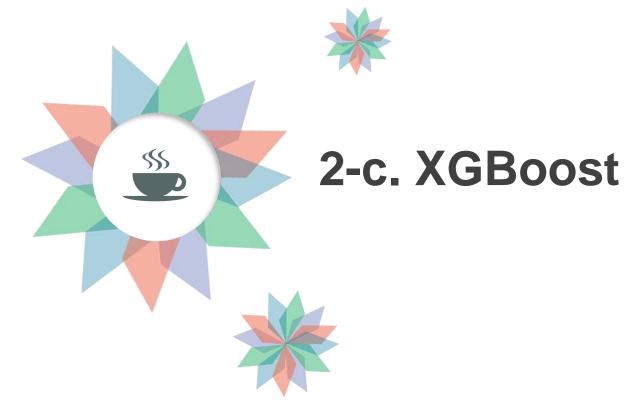


First prediction = "log odds ratio" of the mode



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







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

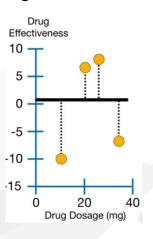
2. XGBoost Regression

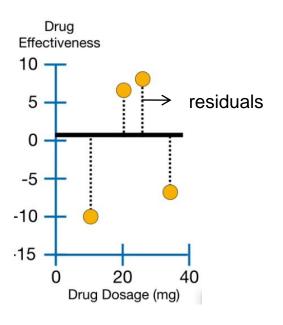
Unique Regression Tree!

Example with simple data)

X : drug dosage

Y: drug Effectiveness

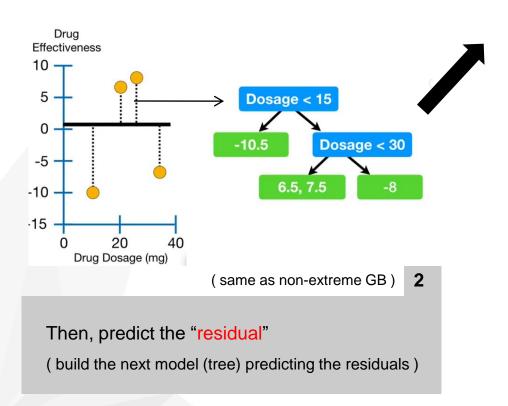




•

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

2. XGBoost Regression



HOW?

Step 1.

Put all the residuals to the same leaf

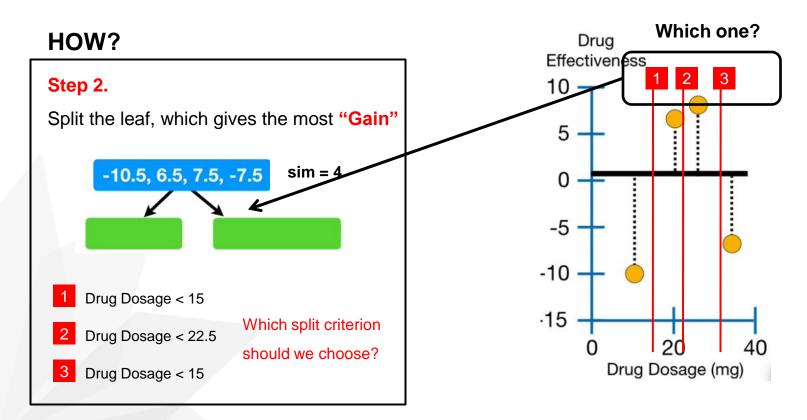
And calculate a "similarity score"

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



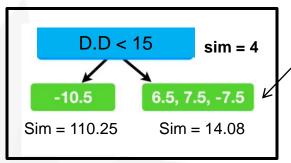
2. XGBoost Regression

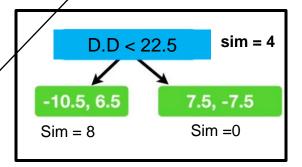
Which split criterion

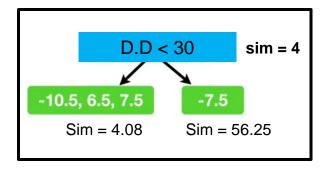
should we choose?

- 1 Drug Dosage < 15
- 2 Drug Dosage < 22.5
- 3 Drug Dosage < 30

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







$$(8 + 0) - 4 = 4$$

Gain

$$(4.08 + 56.25) - 4 = 56.33$$

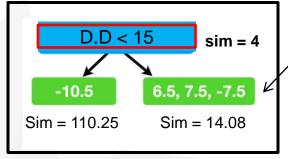
Gain

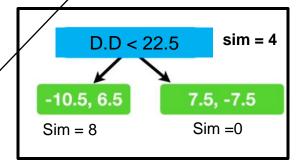
2. XGBoost Regression

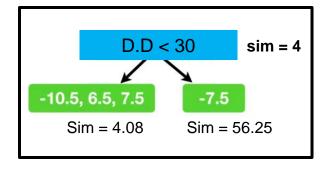
- 1 Drug Dosage < 15
- 2 Drug Dosage < 22.5
- 3 Drug Dosage < 30

Example)

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







$$(8+0)-4=4$$

Gain

Which split criterion

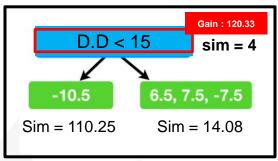
should we choose?

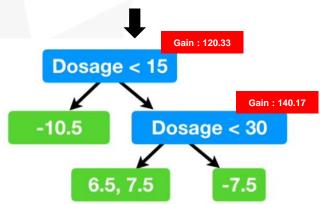
(4.08 + 56.25) - 4 = 56.33

Gain

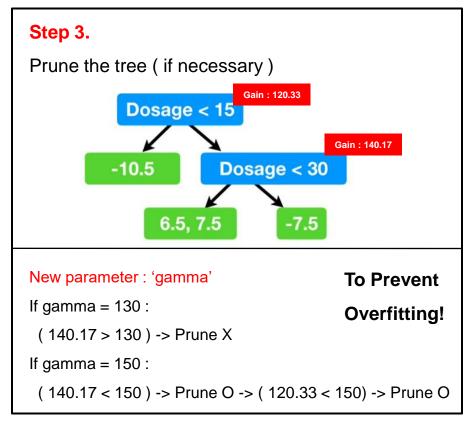
2. XGBoost Regression

choose "D.D<15" as the criterion





HOW?



2. XGBoost Regression

Another method for preventing overfitting (regularization)

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

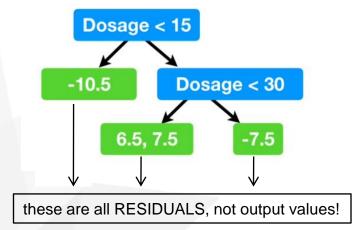
What happens if lambda gets larger?

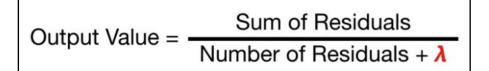
lambda ↑ -> similarity score ↓ -> More chance of getting pruned

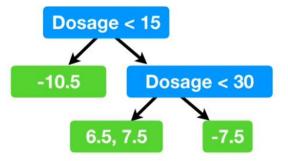
2. XGBoost Regression

Step 4.

Predict output values of each leaf!





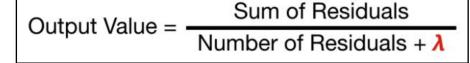


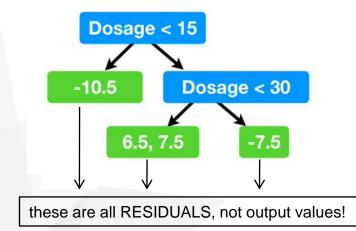
How will these values (of leaves) change?

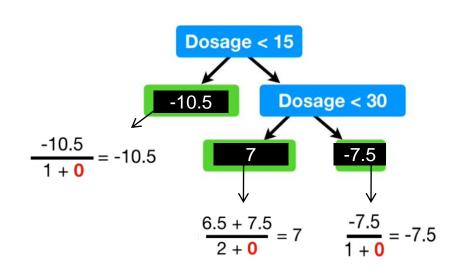
2. XGBoost Regression

Step 4.

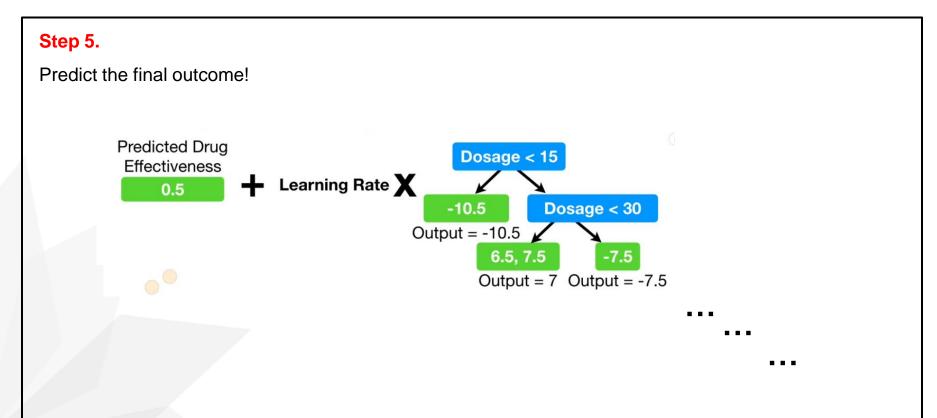
Predict output values of each leaf!



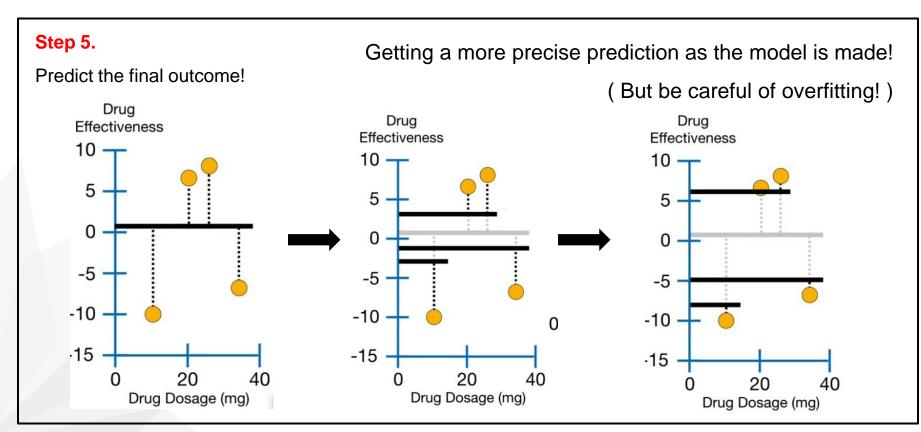




2. XGBoost Regression



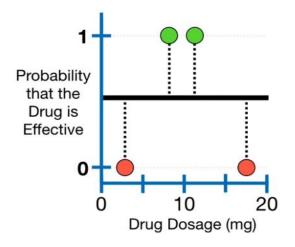
2. XGBoost Regression



3. XGBoost Classification

3. XGBoost Classification

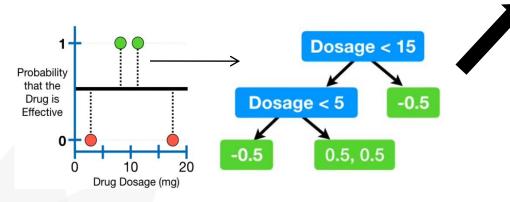
Example with simple data) X : drug dosage Y: Effective / Not Effective Drug Dosage (mg) Probability that the Drug is Effective 10 Drug Dosage (mg)



1

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

3. XGBoost Classification



(same as non-extreme GB)

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"

$$(\sum Residual_i)^2$$

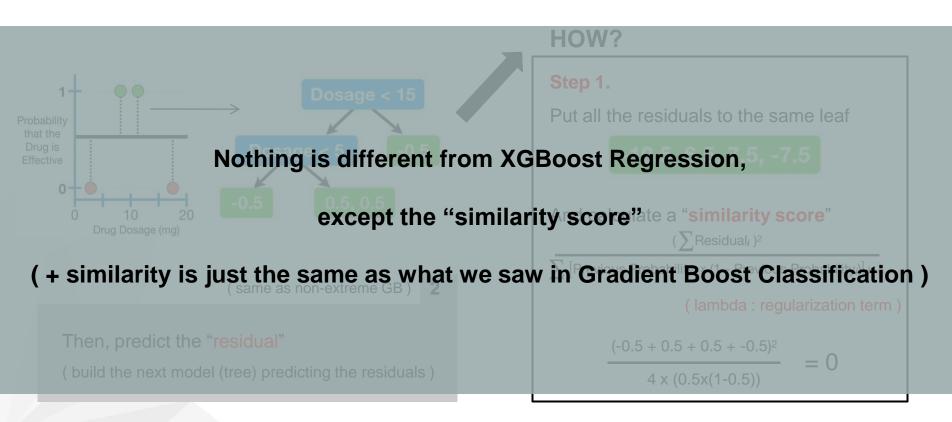
$$\sum$$
 [Previous Probability_i × (1 - Previous Probability_i)]+ λ

(lambda: regularization term)

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

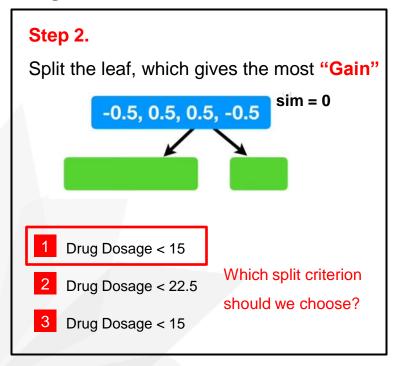


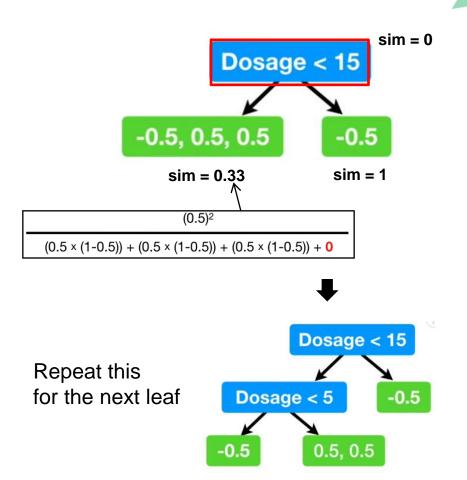
3. XGBoost Classification



2. XGBoost Regression

HOW?





3. XGBoost Classification

Step 3.

Pruning the tree

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

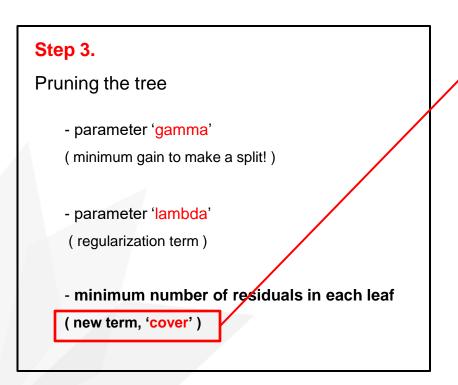
3. XGBoost Classification

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



```
(∑Residual<sub>i</sub>)²
[Previous Probability<sub>i</sub> × (1 - Previous Probability<sub>i</sub>)]+ λ
```

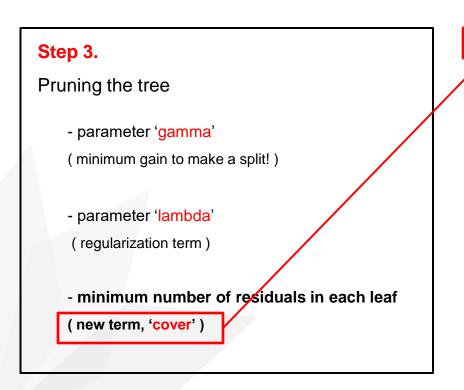
1

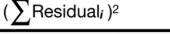
(in regression)

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

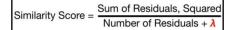
3. XGBoost Classification





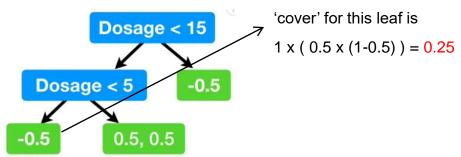
 \sum [Previous Probability_i × (1 - Previous Probability_i)]+ λ

(in regression)

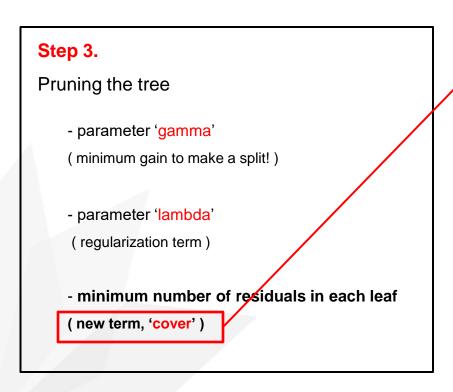


- cover can be defined as 'number of residuals'
- default value : 1 -> means that it has no affect on the growth of tree

Example)



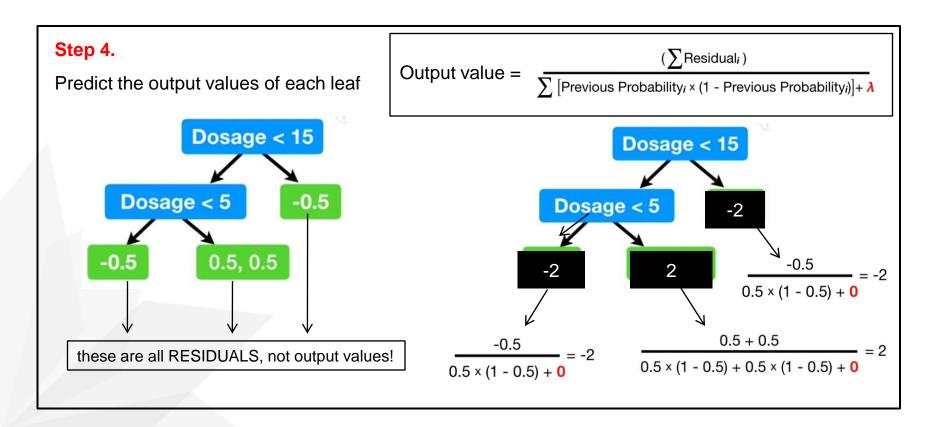
3. XGBoost Classification

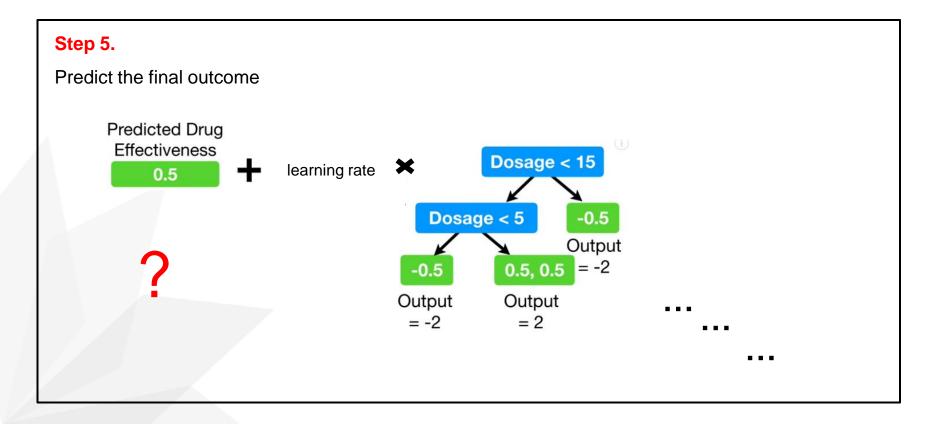


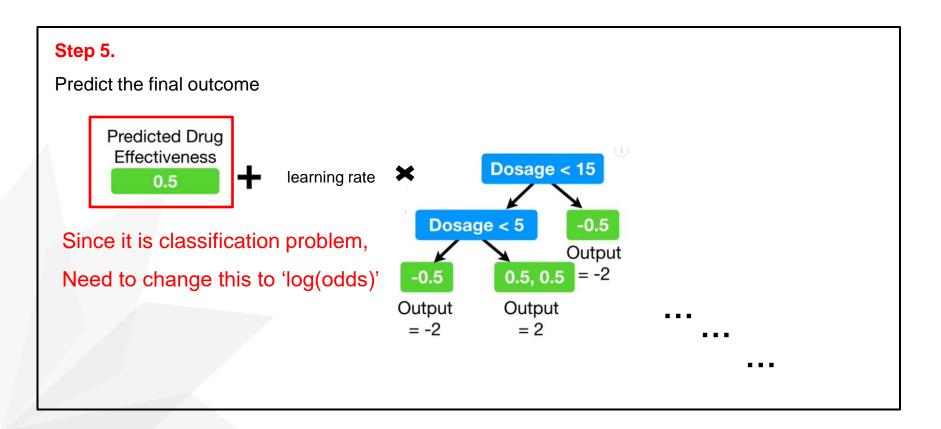
 $(\sum Residual_i)^2$ Previous Probability_i × (1 - Previous Probability_i) + λ Sum of Residuals, Squared Similarity Score = (in regression) - cover can be defined as 'number of residuals' - default value : 1 -> means that it has no affect on the growth of tree Example) 'cover' for this leaf is Dosage < 15 $1 \times (0.5 \times (1-0.5)) = 0.25$ Dosage < 5 -0.5 Default value for cover: 1 0.5, 0.5

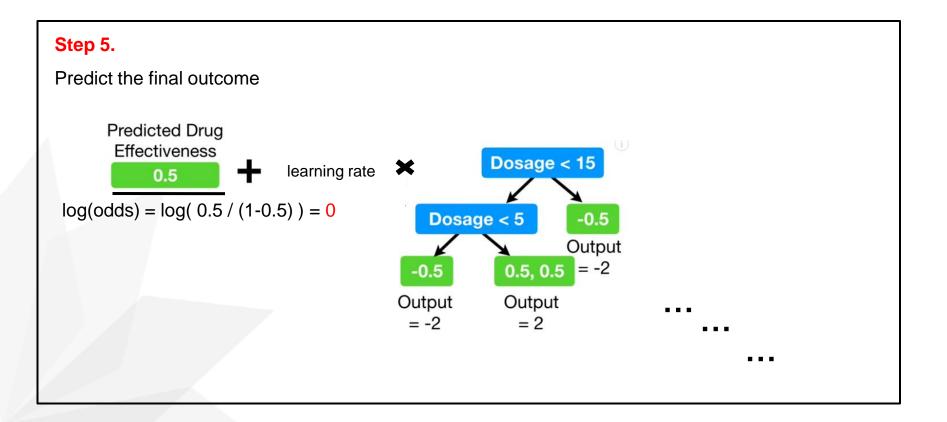
0.25 < 1) -> get pruned!

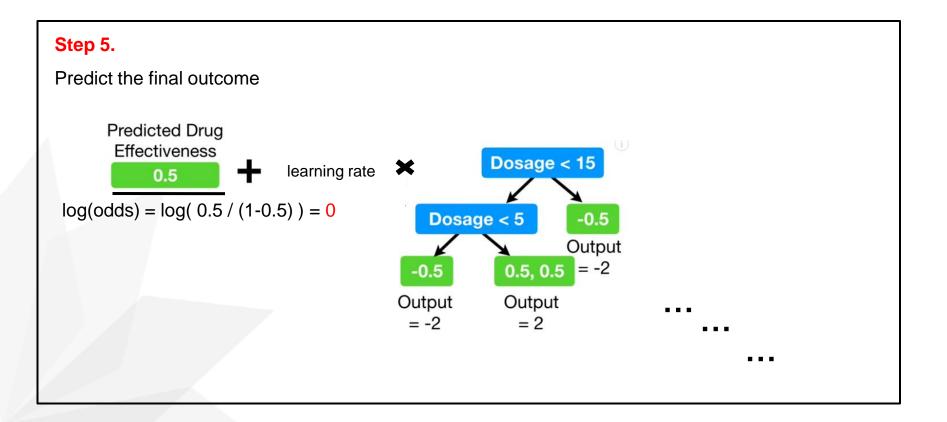
we call this parametr 'cover', "min_child_weight"





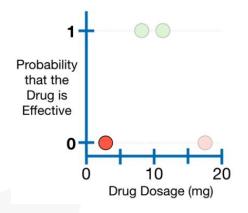


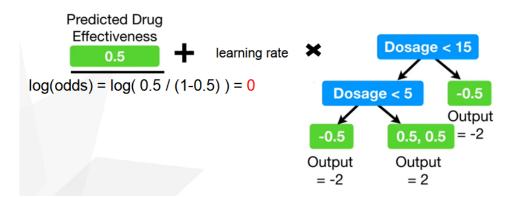




3. XGBoost Classification

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





Answer:

1)
$$0 + (0.3 \times (-2)) = -0.6$$

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

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

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. Boosting with Python

- 1) Adaboost
- 2) Gradient Boosting
- 3) XGBoost

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

