# Predictive Modeling - XGBoost

DS Development Presentations

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#### Contents

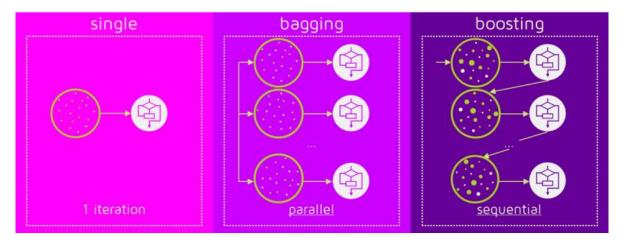
- Overview of XGBoost
- Some math behind XGBoost Gradient Boosting
- XGBoost in action Diabetic Retinopathy classification

Disclaimer: changed my topic

# 1. Overview of XGBoost What is it? What are its features?

## What is Boosting?

 Boosting = sequential building of a strong learner from weak learners



Commonly used weak learner = decision trees

#### What is XGBoost?

- Created in 2014 by Tianqi Chen
- eXtreme Gradient Boosting
  - "The name xgboost, though, actually refers to the engineering goal to push the limit of computations resources for boosted tree algorithms. Which is the reason why many people use xgboost."
- Speed & Performance
- Available in most popular platforms/interfaces (CLI, C++, Python, R, Julia, Scala, Hadoop)

#### **XGBoost Features**

- Model Features
  - Gradient Boosting
  - Stochastic Gradient Boosting
    - Sub-sampling at multiple levels
  - Regularized Gradient Boosting
    - L1 and L2 regularization
  - Classification and Regression

#### **XGBoost Features**

- System Features
  - Parallelization
    - Parallel node construction
  - Distributed Computing
  - Out-of-Core Computing
    - For large datasets > RAM
  - Cache Optimization

#### **XGBoost Features**

- Algorithm Features
  - Sparse Aware
    - Automatic handling of missing values
  - Block Structure
    - Supports parallelization
  - Continued Training
    - Save your current parameters

# 2. Math Behind XGBoost Gradient Boosting & the Objective Function

# The Objective Function

$$obj(\theta) = L(\theta) + \Omega(\theta)$$
 $\downarrow$ 
 $\downarrow$ 
Objective Loss Reg'zn function function

#### **Common Loss Functions**

- Regression and Classification use the same algorithms/formulas, just different loss functions
- Regression MSE

$$L(\theta) = \sum (y_i - \hat{y}_i)^2$$

Classification – log loss

$$L(\theta) = \sum [y_i \ln(1 + e^{-\hat{y}_i}) + (1 - y_i) \ln(1 + e^{\hat{y}_i})]$$

#### Decision Tree Ensemble = Adding up the trees

The prediction for individual i

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

K = # trees

f = function in F; a tree

F = set of all possible CARTs (class'fn and regression trees)

#### Updating the objective function

The loss function within obj can be expressed as:

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

- Optimize this!
- Find a way to express  $\hat{y}_i$ 
  - Calculating  $\hat{y}_i$ : iterative process

• The prediction value at step  $t(\hat{y}_i^{(t)})$ 

$$\hat{y}_{i}^{(0)} = 0.5 \text{ (default initial guess)}$$

$$\hat{y}_{i}^{(1)} = f_{1}(x_{i}) = \hat{y}_{i}^{(0)} + f_{1}(x_{i})$$

$$\hat{y}_{i}^{(2)} = f_{1}(x_{i}) + f_{2}(x_{i}) = \hat{y}_{i}^{(1)} + f_{2}(x_{i})$$
...

$$\hat{y}_i^{(t)} = \sum_{k=1}^t f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i)$$

• The prediction value at step  $t(\hat{y}_i^{(t)})$ 

$$\hat{y}_i^{(0)} = 0.5$$
 (default initial guess)

$$\hat{y}_i^{(1)} = f_1(x_i) = \hat{y}_i^{(0)} + f_1(x_i)$$

$$\hat{y}_i^{(2)} = f_1(x_i) + f_2(x_i) = \hat{y}_i^{(1)} + f_2(x_i)$$

...

What tree do we want at each step?

$$\hat{y}_i^{(t)} = \sum_{k=1}^t f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i)$$

The tree that optimizes our objective!

$$obj^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t)}\right) + \sum_{i=1}^{t} \Omega(f_i)$$

$$= \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + constants$$
We use the previous  $\hat{y}_i$ 

Let's rewrite this

 We take the second-order Taylor expansion of the loss function (for not-so-friendly loss functions)

$$f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2$$

$$l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) \approx l\left(y_i, \hat{y}_i^{(t-1)}\right) +$$

$$\left[\frac{\partial}{\partial \hat{y}_i^{(t-1)}} l\left(y_i, \hat{y}_i^{(t-1)}\right)\right] f_t(x_i) + \frac{1}{2} \left[\frac{\partial^2}{\partial \left(\hat{y}_i^{(t-1)}\right)^2} l\left(y_i, \hat{y}_i^{(t-1)}\right)\right] f_t(x_i)^2$$

gradient

hessian

 We take the second-order Taylor expansion of the loss function (for not-so-friendly loss functions)

$$f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2$$

$$l\left(y_{i}, \hat{y}_{i}^{(t-1)} + f_{t}(x_{i})\right) \approx l\left(y_{i}, \hat{y}_{i}^{(t-1)}\right) + g_{i}f_{t}(x_{i}) + \frac{1}{2}h_{i}f_{t}(x_{i})^{2}$$

The objective is then

$$obj^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + C$$

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

We can remove the constants

$$obj^{(t)} = \sum_{i=1}^{n} l\left(y_{i}, \hat{y}_{i}^{(t-1)} + f_{t}(x_{i})\right) + \Omega(f_{t}) + C$$

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$$= \sum_{i=1}^{n} \left[g_{i}f_{t}(x_{i}) + \frac{1}{2}h_{i}f_{t}(x_{i})^{2}\right] + \Omega(f_{t})$$

Our optimization goal

# Specifics of the regularization term

Redefine the definition of a tree f(x)

$$f_t(x) = w_{q(x)}, w \in \mathbb{R}^T, q: \mathbb{R}^d \to \{1, 2, ..., T\}$$

w = vector of scores on leaves

q = function assigning data points to leaves

T = number of leaves

 This is a more explicit version of our function f(x), in terms of leaf weights

#### Specifics of the regularization term

We then express the regularization term as

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

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

Rewriting our objective function:

$$obj^{(t)} \approx \sum_{i=1}^{n} \left[ g_i w_{q(x_i)} + \frac{1}{2} h_i w_{q(x_i)}^2 \right] + \gamma T + \frac{1}{2} \lambda \sum_{j=1}^{T} w_j^2$$

$$= \sum_{j=1}^{T} \left[ \left( \sum_{i \in I_j} g_i \right) w_j + \frac{1}{2} \left( \sum_{i \in I_j} h_i \right) w_j^2 \right] + \gamma T + \frac{1}{2} \lambda \sum_{j=1}^{T} w_j^2$$

Rewriting our objective function:

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Switching sums from by-individual to by-leaf

Rewriting our objective function:

$$obj^{(t)} \approx \sum_{i=1}^{n} \left[ g_i w_{q(x_i)} + \frac{1}{2} h_i w_{q(x_i)}^2 \right] + \gamma T + \frac{1}{2} \lambda \sum_{j=1}^{T} w_j^2$$

$$= \sum_{j=1}^{T} \left[ \left( \sum_{i \in I_j} g_i \right) w_j + \frac{1}{2} \left( \sum_{i \in I_j} h_i + \lambda \right) w_j^2 \right] + \gamma T$$

Make notation more compact

Rewriting our objective function:

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$$= \sum_{j=1}^{T} \left[ G_j w_j + \frac{1}{2} (H_j + \lambda) w_j^2 \right] + \gamma T$$

This is quadratic!

The optimum solution for the quadratic eq'n:

$$w_j^* = -\frac{G_j}{H_j + \lambda} \left( Recall: -\frac{b}{a} \right)$$

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The best objective:

$$obj^* = \sum_{j=1}^{T} \left[ G_j \left( -\frac{G_j}{H_j + \lambda} \right) + \frac{1}{2} \left( H_j + \lambda \right) \left( -\frac{G_j}{H_j + \lambda} \right)^2 \right] + \gamma T$$

The optimum solution for the quadratic eq'n:

$$w_j^* = -\frac{G_j}{H_j + \lambda} \left( Recall: -\frac{b}{a} \right)$$

The best objective:

$$obj^* = -\frac{1}{2} \sum_{j=1}^{I} \frac{G_j^2}{H_j + \lambda} + \gamma T$$

The optimum solution for the quadratic eq'n:

$$w_j^* = -\frac{G_j}{H_j + \lambda} \left( Recall: -\frac{b}{a} \right)$$

The best objective:

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

This can measure how good a tree structure is

#### **Building Trees**

We now have a measure for how good a tree is.

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

- Ideal: enumerate all possible trees and pick the best one
- Practical: <u>optimize one level of the tree at a time</u>
  - I.e. find the best split at each level of the tree
  - We now have a way to find the optimum tree!

#### **Building Trees**

We now have a measure for how good a tree is.

$$obj^* = -\frac{1}{2} \sum_{j=1}^{T} \frac{G_j^2}{H_j + \lambda} + \gamma T$$
 Removed in implementation Minimize -> Maximize

- Ideal: enumerate all possible trees and pick the best one
- Practical: <u>optimize one level of the tree at a time</u>
  - I.e. find the best split at each level of the tree
  - We now have a way to find the optimum tree!

#### Splitting Nodes – optimizing one level at a time

We try to split a node into two leaves; the gain is:

$$Gain = \frac{1}{2} \begin{bmatrix} G_L^2 \\ H_L + \lambda \end{bmatrix} + \begin{bmatrix} G_R^2 \\ H_R + \lambda \end{bmatrix} - \begin{bmatrix} (G_L + G_R)^2 \\ H_L + H_R + \lambda \end{bmatrix} - \begin{bmatrix} \gamma \\ H_L + H_R + \lambda \end{bmatrix}$$
Left Right Original/score score Unsplit

If the gain is negative, we prune

## Splitting Nodes – optimizing one level at a time

We try to split a node into two leaves; the gain is:

$$Gain = \boxed{\frac{1}{2} \left[ \frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} \right] - \gamma}$$

Removed in implementation to run faster. eXtreme!

- If the gain is negative, we prune
- We want gain to be high = large separation

Leaf weights:

$$w_j^* = -\frac{G_j}{H_j + \lambda}$$

Loss function:

$$y_i \ln \left(1 + e^{-\hat{y}_i}\right) + \left(1 - y_i\right) \ln \left(1 + e^{\hat{y}_i}\right)$$

$$g = \boxed{-(y_i - \hat{y}_i)} \text{ (-) Residuals}$$

$$h = \hat{y}_i \times (1 - \hat{y}_i)$$

We sequentially fit on residuals because of the gradient!

We try to split a node into two leaves; the gain is:

$$Gain = \left[ \frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} \right] - \gamma$$

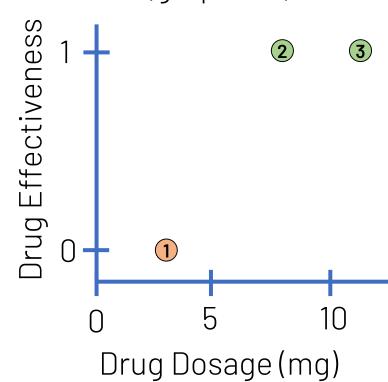
Score:

$$\frac{G^2}{H+\lambda} = \frac{(\sum g)^2}{\sum h+\lambda} = \frac{\left(\sum (residuals)\right)^2}{\sum \hat{y}_i \times (1-\hat{y}_i) + \lambda}$$

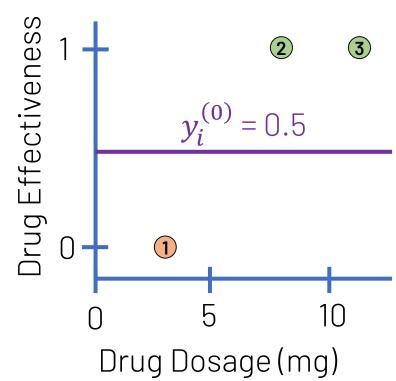
#### Data:

Index	Drug Dosage (mg)	Drug is Effective
1	3	0
2	8	1
3	11	1

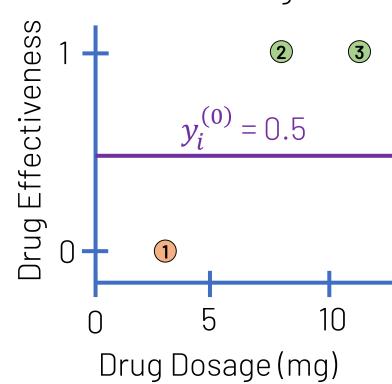
Data (graphical):



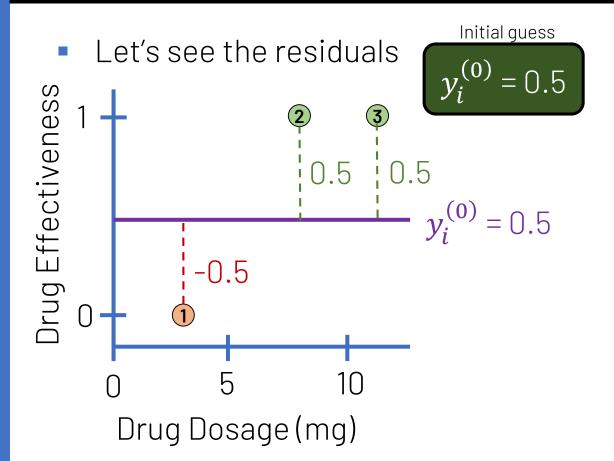
Base score (default initial guess) is 0.5



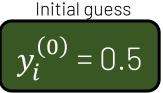
Build w/ initial guess



Initial guess  $y_i^{(0)} = 0.5$ 



Let's see the residuals



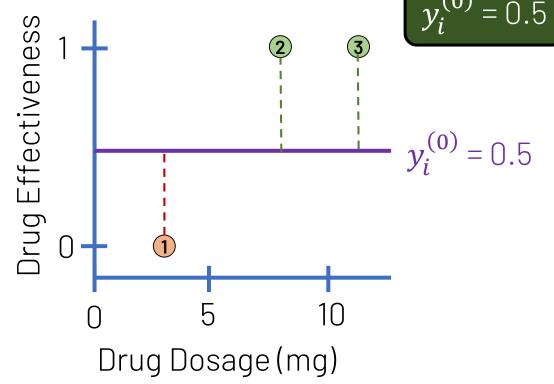




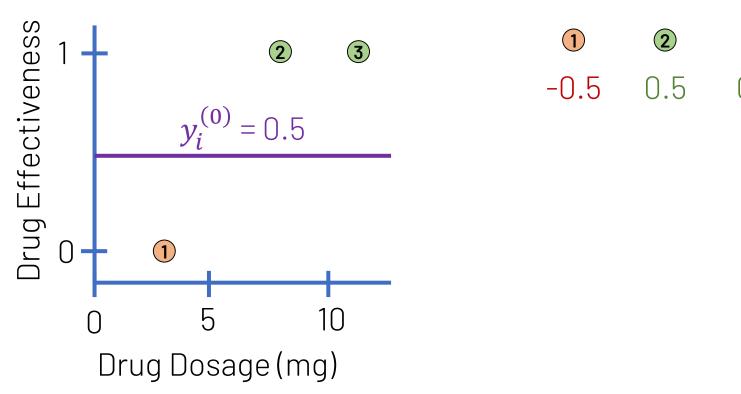


$$-0.5$$

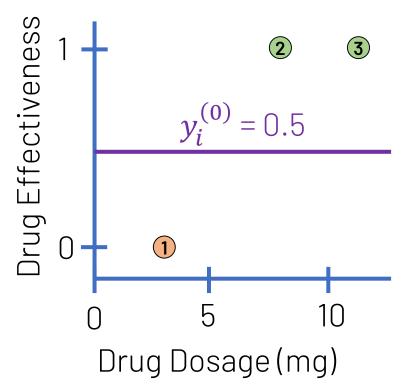


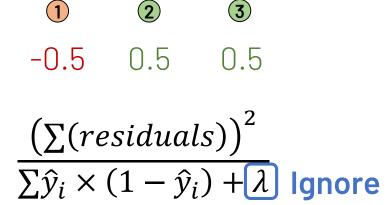


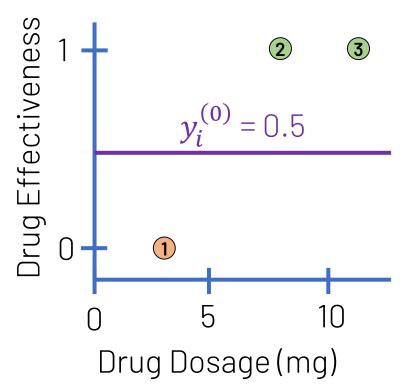
Let's make a new tree with these residuals



3

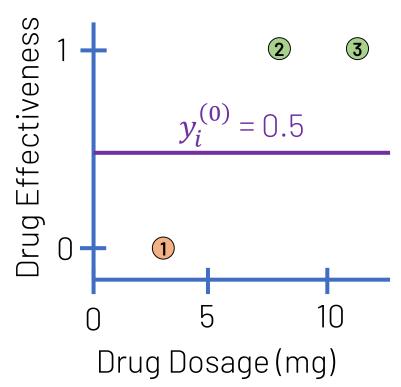






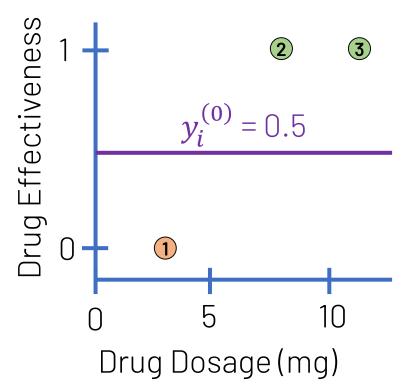


$$\frac{\left(\sum (residuals)\right)^2}{\sum \hat{y}_i \times (1 - \hat{y}_i)}$$



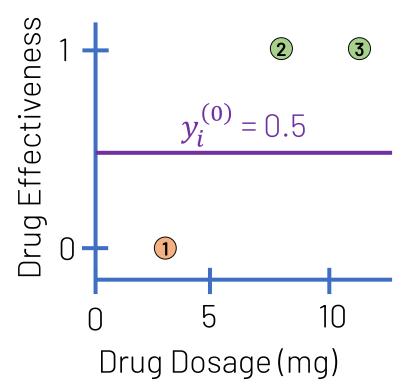


$$\frac{(-0.5 + 0.5 + 0.5)^2}{(0.5)(1 - 0.5) \times 3}$$



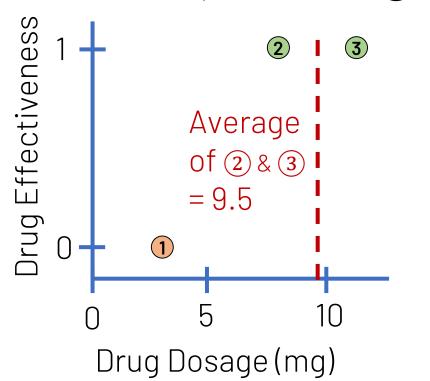


$$\frac{(0.5)^2}{0.75} = \frac{1}{3}$$



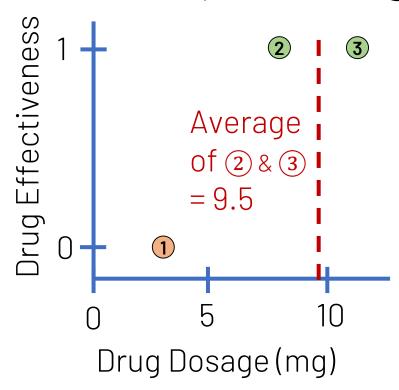


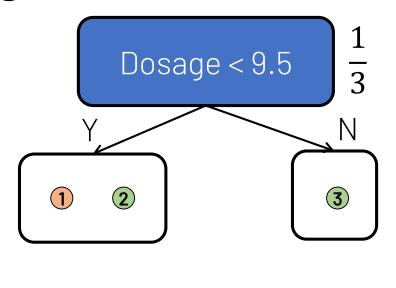
Use the split between (2) & (3)



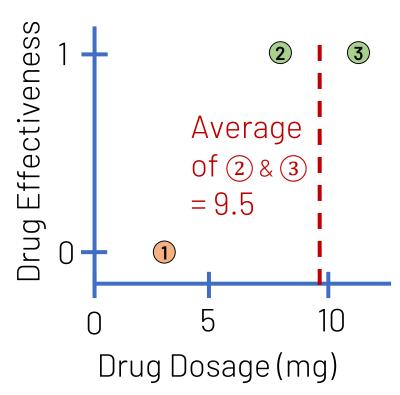
Dosage < 9.5

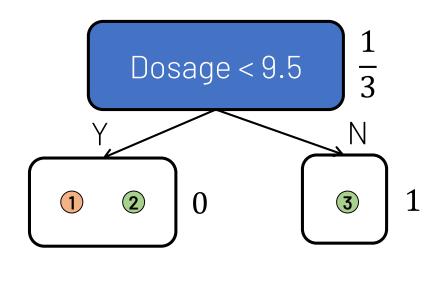
Use the split between (2) & (3)



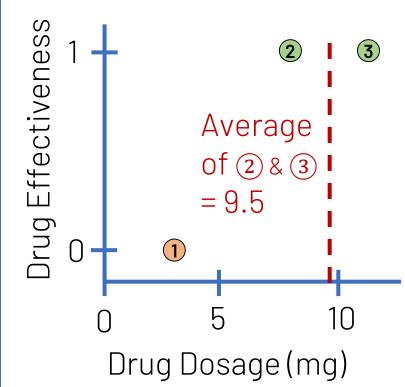


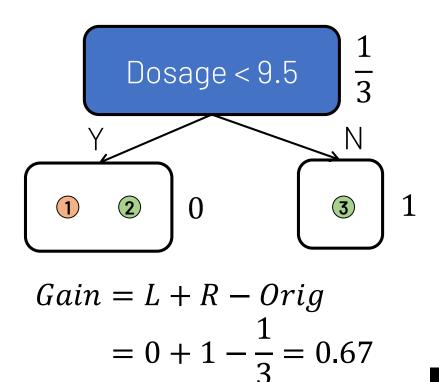
Calculate the scores of the L & R leaves

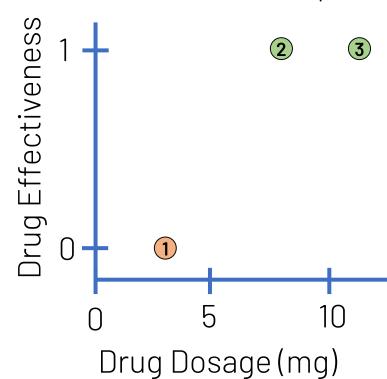


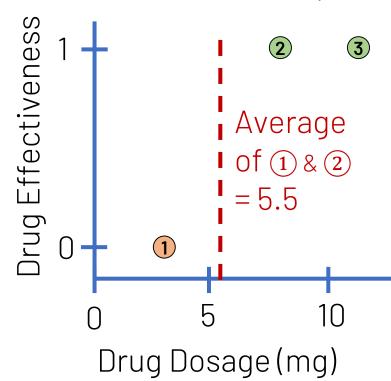


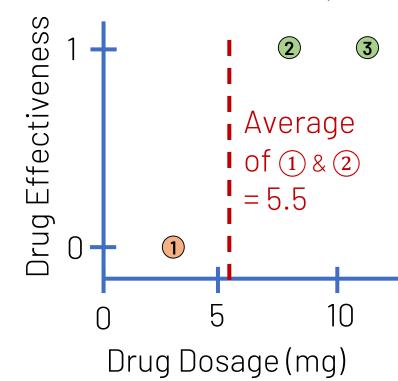
Calculate the Gain

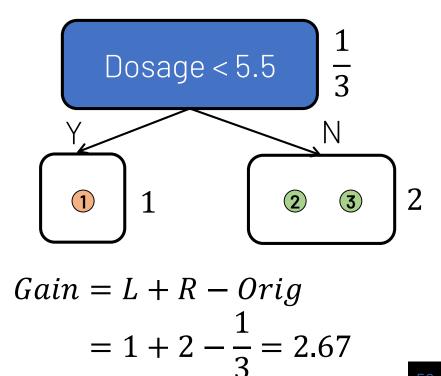


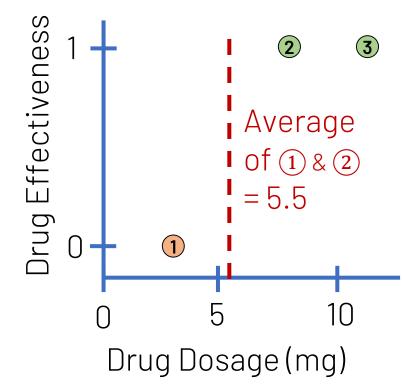


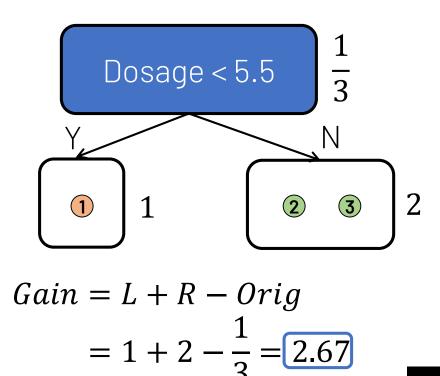




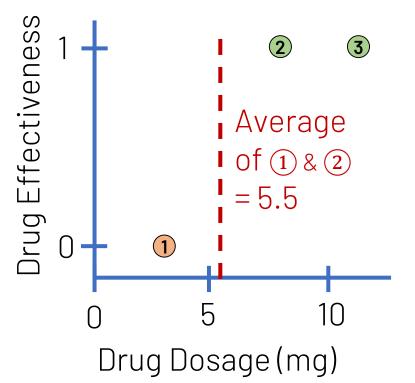


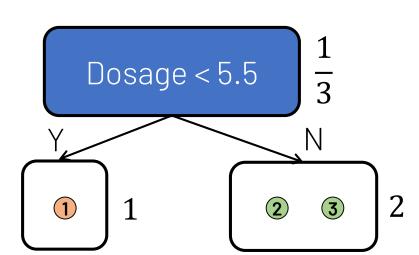






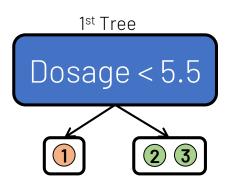
For now, let's stop splitting



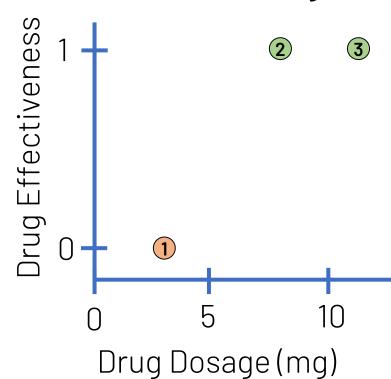


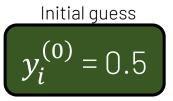
Initial guess We now have a tree **Drug Effectiveness** 3 Drug Dosage (mg)

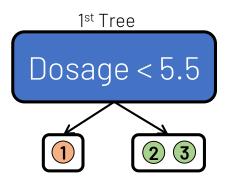
Initial guess We now have a tree **Drug Effectiveness** 3 Drug Dosage (mg)



We calc. leaf weights



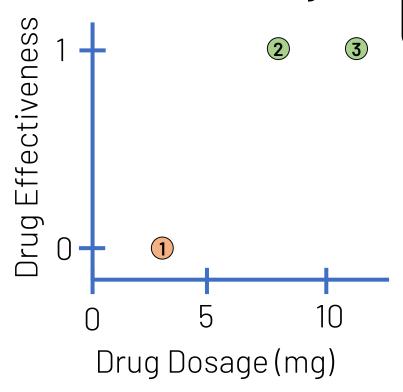


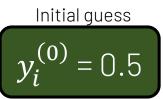


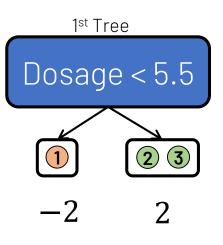
Recall: equation for leaf weights

$$w_{j}^{*} = -\frac{G_{j}}{H_{j} + \lambda}$$
$$= \frac{\sum (residuals)}{\sum \hat{y}_{i} \times (1 - \hat{y}_{i})}$$

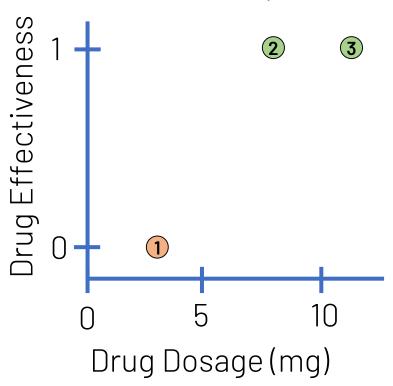
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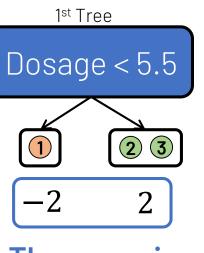


We make new preds.



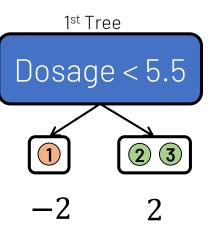
 $y_i^{(0)} = 0.5$ 

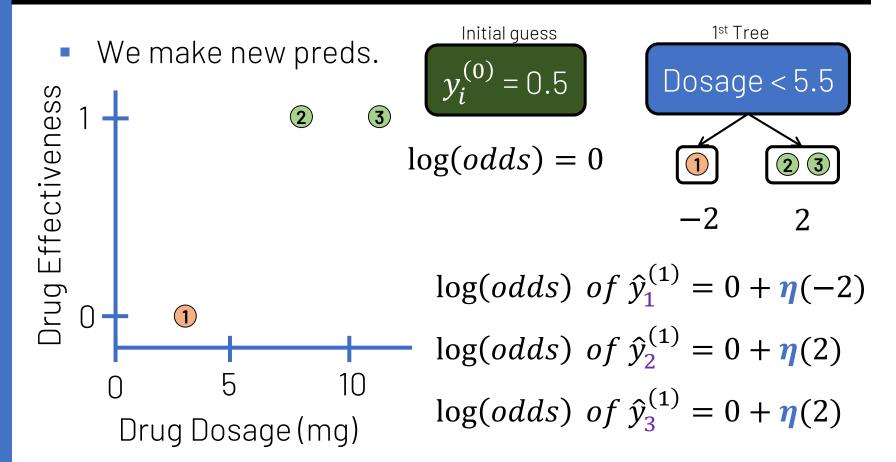
This is in probability

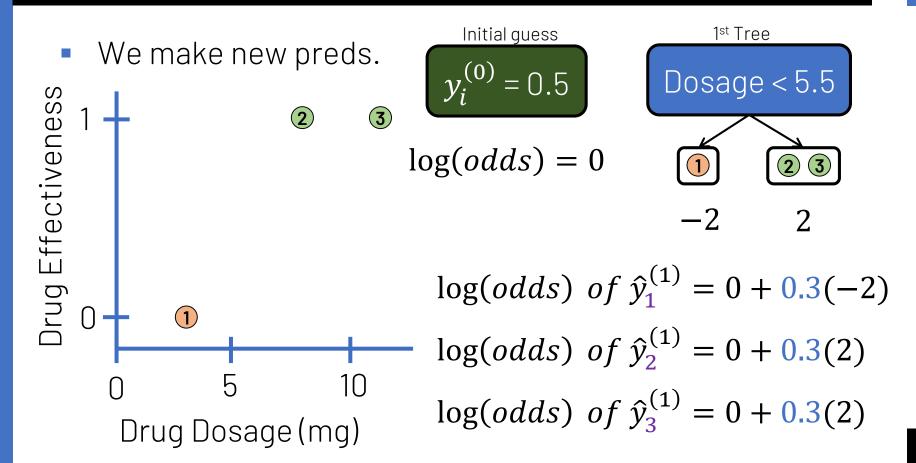


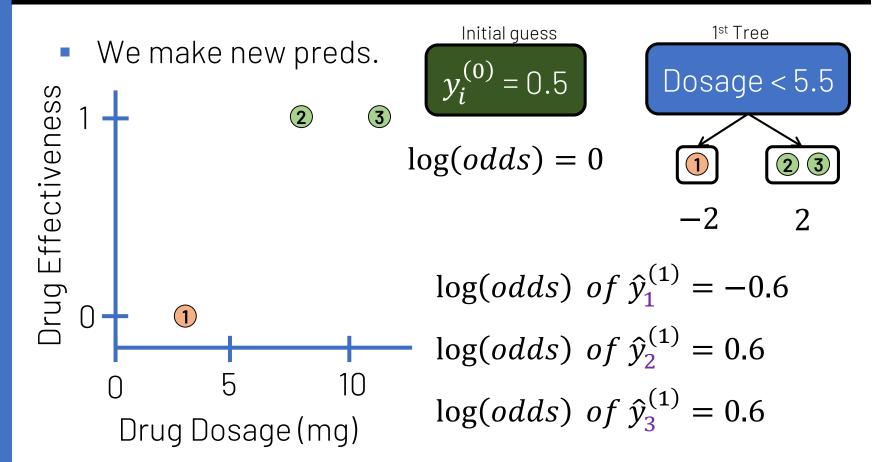
These are in log(odds)

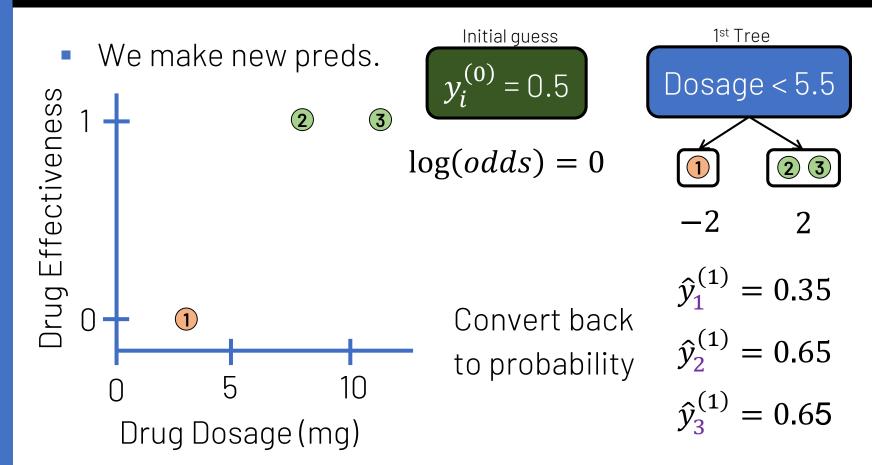
Initial guess We make new preds. **Drug Effectiveness** 3  $\log(odds) = 0$ 1 Drug Dosage (mg)

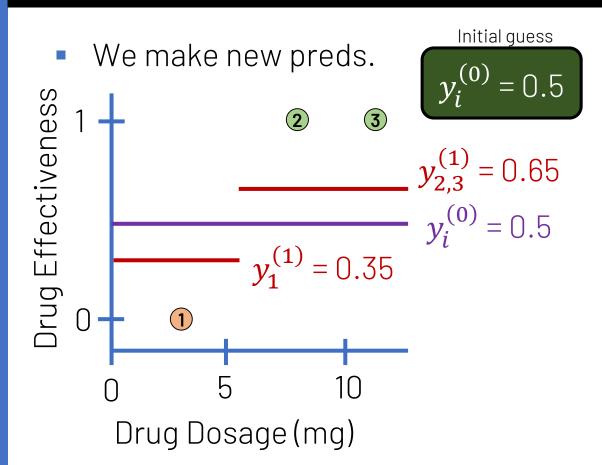


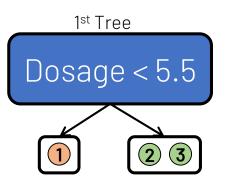




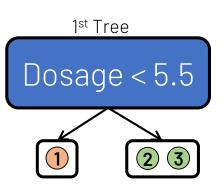






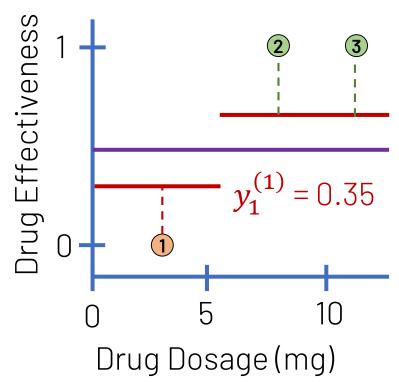


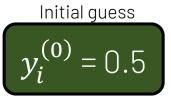
Initial guess We have new residuals **Drug Effectiveness** Drug Dosage (mg)



#### Simple Classification Example

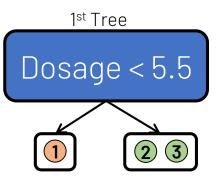
We have new residuals





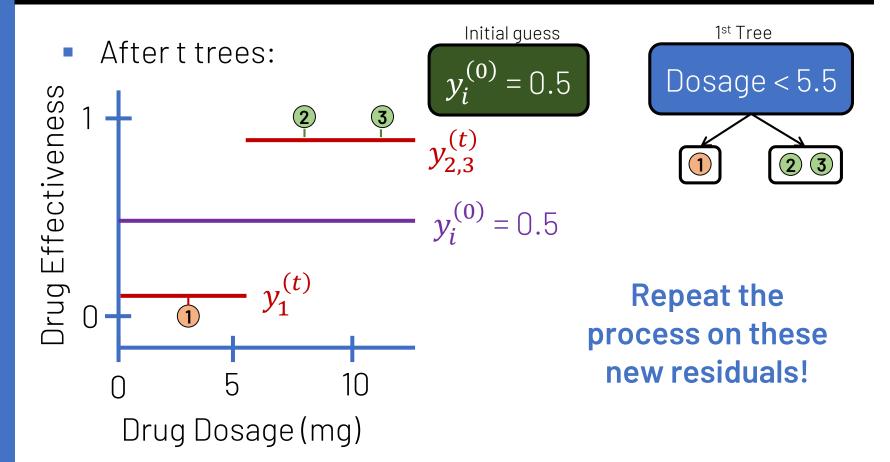
$$y_{2,3}^{(1)} = 0.65$$

$$y_i^{(0)} = 0.5$$



Repeat the process on these new residuals!

### Simple Classification Example



# **3. XGBoost in Action**Staging of Diabetic Retinopathy

## **Diabetic Retinopathy Data**

- Diabetic Retinopathy retinal disease caused by diabetes
- 3,662 retinal images labeled as:

0	No DR
1	Mild
2	Moderate
3	Severe
4	Proliferative







Images have been pre-processed

## Methodology

- 1. Perform PCA
  - a. Reduce ~150,000 cols to 2,500 cols (97% var exp.)
- 2. Train on 80% of the data
- 3. Test on the remaining 20% and analyze the results

#### Code Snippets - XGBoost

```
from xgboost import XGBClassifier, DMatrix Import
import xgboost as xgb
```

Split the data into train and test sets

### Code Snippets - XGBoost

Perform PCA on the training set

```
In [43]:
         pca = PCA(n components = 2500)
In [44]: | %%time
          PC train = pca.fit transform(X train) PCA on train
         Wall time: 1min 47s
In [45]: pca.explained_variance_ratio_.sum()
Out[45]: 0.9725809679667871
          Use the same PCA transformations on the test set
          %%time
In [46]:
          PC_test = pca.transform(X_test) Apply same transform on test
         Wall time: 4.78 s
```

#### **XGBoost Learning API**

#### **XGB Learning API, Default Parameters**

Convert the np arrays into xgb D-Matrices

```
Special matrix format
```

```
In [47]: D_train = DMatrix(PC_train, label = y_train)
In [48]: D_test = DMatrix(PC_test, label = y_test)
```

Train with default parameters

Wall time: 1min 12s

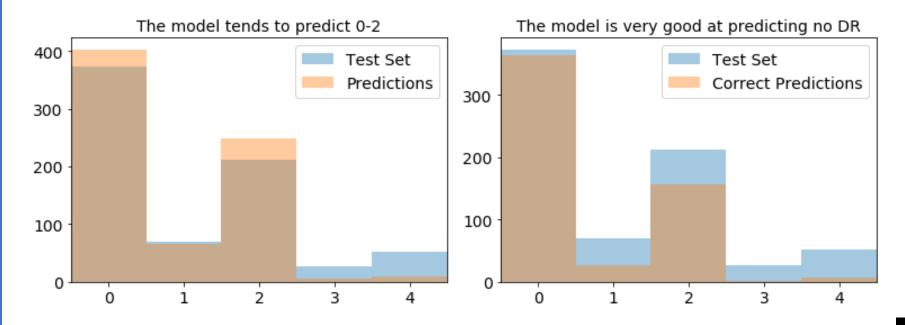
#### XGBoost SKLearn API

```
In [222]: xgb clf = XGBClassifier(objective = 'multi:softprob',
                                   num class = 5,
                    sklearn API
                                   random state = 2020)
In [224]: %%time
          xgb clf.fit(PC train,y train)
          Wall time: 1min 13s
Out[224]: XGBClassifier(base score=0.5, booster=None, colsample bylevel=1,
                        colsample bynode=1, colsample bytree=1, gamma=0, gpu id=-1,
                        importance type='gain', interaction constraints=None,
                        learning rate=0.300000012, max delta step=0, max depth=6,
                        min child weight=1, missing=nan, monotone constraints=None,
                        n estimators=100, n jobs=0, num class=5, num parallel tree=
          1,
                        objective='multi:softprob', random state=2020, reg_alpha=0,
                        reg lambda=1, scale pos weight=None, subsample=1,
                        tree method=None, validate parameters=False, verbosity=Non
          e)
```

#### Results

#### Same result w/ either API

```
Precision = 0.5877645479277815
Recall = 0.4579484696597348
Accuracy = 0.757162346521146
```



#### Using the raw data

Train the model

```
In [144]: %%time
    model_orig = xgb.train(param_orig, D_train_orig, steps)

Wall time: 20min 1s 20x slower
```

#### **Raw Data**

```
Precision = 0.631724365975003
Recall = 0.49475581427020543
Accuracy = 0.7612551159618008
```

#### **PCA**

```
Precision = 0.5877645479277815

Recall = 0.4579484696597348

Accuracy = 0.757162346521146
```

Results are slightly better w/ raw data, but it's slower

# Next Presentations

## Possible follow-up presentations:

- Hyperparameters & tuning
  - esp. for multilabel classification (not supported)
- LGBM & CatBoost

#### Main Sources

- A series of StatQuest XGBoost Videos
  - XGBoost Part 1: XGBoost Trees for Regression
  - XGBoost Part 2: XGBoost Trees For Classification
  - XGBoost Part 3: Mathematical Details
- A Gentle Introduction to XGBoost for Applied Machine Learning
- Introduction to Boosted Trees
- Original XGBoost Presentation
- Original XGBoost Manuscript
- XGBoost Docs (Parameters, Python package)

## Thank you!

Questions?

