XGBoost: an extremely boosting method

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1. Introduction

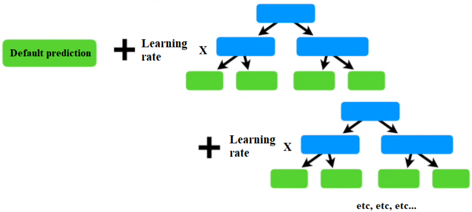
- Some **selling points** of XGBoost before we start:
  - XGboost is like generalized boosting - but EXTREME!!
  - XGboost is widely used in the winning solutions of Kaggle and KGG Cup

Original paper: Chen, T., Guestrin, C. (2016). XGBoost: A Scalable Tree Boosting System. arXiv:1603.02754.

2. XGBoost Regression: Intuition

Let's follow the algorithm:

1. Calculate the residuals
2. Make the first split of residuals and calculate *Similarity score* $= \frac{(\sum \text{Residuals})^2}{\text{Number of Residuals} + \lambda}$
3. Find $Gain = Left_{Similarity} + Right_{Similarity} - Root_{Similarity}$. Leave the first split in a form which maximizes gain
4. Continue splitting. Default depth is 6 levels
5. Prune the trees: if *Gain* - γ (3 by default) < 0, we prune
6. Calculate $Output = \frac{\sum \text{Residuals}}{\text{Number of Residuals} + \lambda}$
7. Find *Predicted values* = Default (0.5 by default) + Learning rate × Output
8. Go to step 1: calculate new residuals from the new predicted values



2. XGBoost Regression: Maths behind

Loss function $L(y, p) = \frac{1}{2}(y - p)^2$
Expression to be minimized $[\sum_{i=1}^{n} L(y_i, p_i)] + \gamma T + \frac{1}{2}\lambda O^2$

In other words, $min[[\sum_{i=1}^{n} L(y_i, p^0 + O)] + \frac{1}{2}\lambda O^2]$

Using Taylor second order approx, we find that $O = \frac{-(g_1+g_2+\cdots+g_n)}{(h_1+h_2+\cdots+h_n+\lambda)}$,

where *g* is the first order deriv.: -(*y*-*p*) — residuals
and *h* is the second order deriv.: 1 x n — number of residuals

Now look at the formulas from the previous 'intuition' slide

3. XGBoost Classification: Intuition (1)

- **Let's follow the algorithm:**

1. Calculate the residuals based on initial guess of 0.5
2. Make the first split (average of last two observations) and calculate $Similarityscore = \frac{(\sum \text{Residuals})^2}{\sum[\text{Previous probability x (1-Previous probability)}]+\lambda}$ of each leaf
3. Calculate $Gain = Left_{Similarity} + Right_{Similarity} - Root_{Similarity}$
4. Continue splitting with highest gain split. Default depth is 6 levels
5. Prune the trees by calculating Gain - γ (3 by default). If negative we prune the branch
6. Calculate $Output = \frac{\sum \text{Residuals}}{\sum[\text{Previous probability x (1-Previous probability)}]+\lambda}$
7. Find *Predicted values* = log odds of default + Learning rate (0.3 by default) × Output
8. Go to step 1: calculate new residuals from the new predicted values

Different Loss function $L(y,p) = -[y\log(p) + (1-y)\log(1-p)]$

3. XGBoost Classification: Intuition (2)

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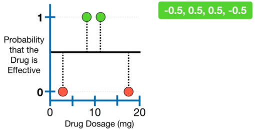
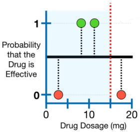
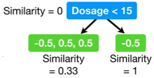
1. Calcualte residuals



2. Split

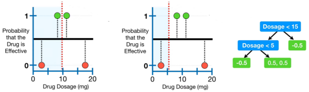


3. Calculate similarities and gain



Gain = 0.33 + 1 - 0 = 1.33

4. Repeat for other splits



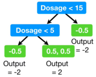
5. Pruning

Gain - γ

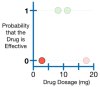
$\begin{cases} \text{If positive, then do not prune.} \\ \text{If negative, then prune.} \end{cases}$

6. Calculating output

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



7. Predicting values



log(odds) Prediction = 0 + (0.3 x -2) = -0.6

$$\text{Probability} = \frac{e^{\text{log(odds)}}}{1 + e^{\text{log(odds)}}}$$

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4. Implementation of XGBoost in R

Training of the model

NOTE: XGBoost works only with numeric values

```
data = load(file = "german.rda")
dummy = dummyVars("~.", data = german[,-c(2, 5, 13, 21)])
newdata = data.frame(predict(dummy, german[,-c(2, 5, 13, 21)]))
data = cbind(newdata, german[,c(2, 5, 13, 21)])
y = recode(data$Class,'good'=1, 'bad'=0)

xgb = xgboost(data = data.matrix(data[,-c(length(data))]),
              label = y, eta = 0.3,
              max_depth = 15,
              nround=25, objective = "binary:logistic" ,
              lambda = 1,
)
```

Making predictions

```r
predict(xgb, data.matrix(data[4,-c(length(data))]))
```

```
## [1] 0.8940502
```

5. Comparison of performance

Three algorithms:

- XGBoost
- LightGBM
- CatBoost

Defining functions(1/3) – Xgboost

```
give_xgboost_AUC <- function(X_train,X_test,y_train, y_test){
xgb = xgboost(data = data.matrix(X_train[,-c(length(X_train))]),
              objective = "binary:logistic" ,
              label = y_train,nrounds=25)
vec.prob=predict(xgb, data.matrix(X_test[,-c(length(X_test))]))

pred <- prediction(vec.prob, y_test)
auc = performance(pred, measure = "auc")
return(as.numeric(auc@y.values)  )
}
```

Defining functions(2/3) – Lightgbm

```
give_lightgbm_AUC <- function(X_train,X_test,y_train, y_test){

fit <- lightgbm(data = data.matrix(X_train[,-c(length(X_train))]),
                label = y_train,
                objective = "binary",nrounds=25)

vec.prob=predict(fit, data.matrix(X_test[,-c(length(X_test))]))
pred <- prediction(vec.prob, y_test)
auc = performance(pred, measure = "auc")
return(as.numeric(auc@y.values)  )
}
```

Defining functions (3/3) – CatBoost

```r
give_catboost_AUC <- function(X_train,X_test,y_train, y_test){
train_pool <- catboost.load_pool(
  data = X_train[,-c(length(X_train))], label = y_train)
test_pool <- catboost.load_pool(
  data = X_test[,-c(length(X_test))], label = y_test)

params <- list(iterations=25, loss_function='CrossEntropy',
               eval_metric='CrossEntropy',
               use_best_model=TRUE)
fit <- catboost.train(train_pool,test_pool, params)

vec.prob= catboost.predict(fit, test_pool)
pred <- prediction(vec.prob, y_test)
auc = performance(pred, measure = "auc")
return(as.numeric(auc@y.values))
}
```

Loop for comparing the performance

```r
xgboost_AUC<-lightgbm_AUC<-catboost_AUC<-NULL
for (i in (1:1000)){
vec <- sample(dim(data)[1],700)

X_train <- data[vec,]
X_test <- data[-vec,]
y_train <- y[vec]
y_test <- y[-vec]

xgboost_AUC=c(xgboost_AUC,
              give_xgboost_AUC(X_train,X_test,y_train, y_test))
lightgbm_AUC=c(lightgbm_AUC,
               give_lightgbm_AUC(X_train,X_test,y_train, y_test))
catboost_AUC=c(catboost_AUC,
               give_catboost_AUC(X_train,X_test,y_train, y_test))}
```

Results of the comparison

```r
print(c(mean (xgboost_AUC),mean (lightgbm_AUC),mean (catboost_AUC) ))
## [1] 0.7726709 0.7728125 0.7663909
print(sum(xgboost_AUC>lightgbm_AUC))
## [1] 500
print(sum(xgboost_AUC>catboost_AUC))
## [1] 600
```

6. Distinctive features of XGBoost

When the dataset gets large, XGBoost becomes handy

- Approximate Greedy Algorithm
- Parallel Learning
- Weighted Quantile Sketch
- Sparsity-Aware Split Finding
- Cache-Aware Access
- Blocks for Out-of-Core Computation

Grand finale

Thank you for attention!

(Invite us for a coffee afterwards if you want to speak about shap values)