XGboost: A Scalable Tree Boosting System

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Courtesy: slides are adopted partly from Tianqi Chen

Outline

- **Introduction**
- What does XGBoost learn
- What can XGBoost System do for you
- Impact of XGBoost

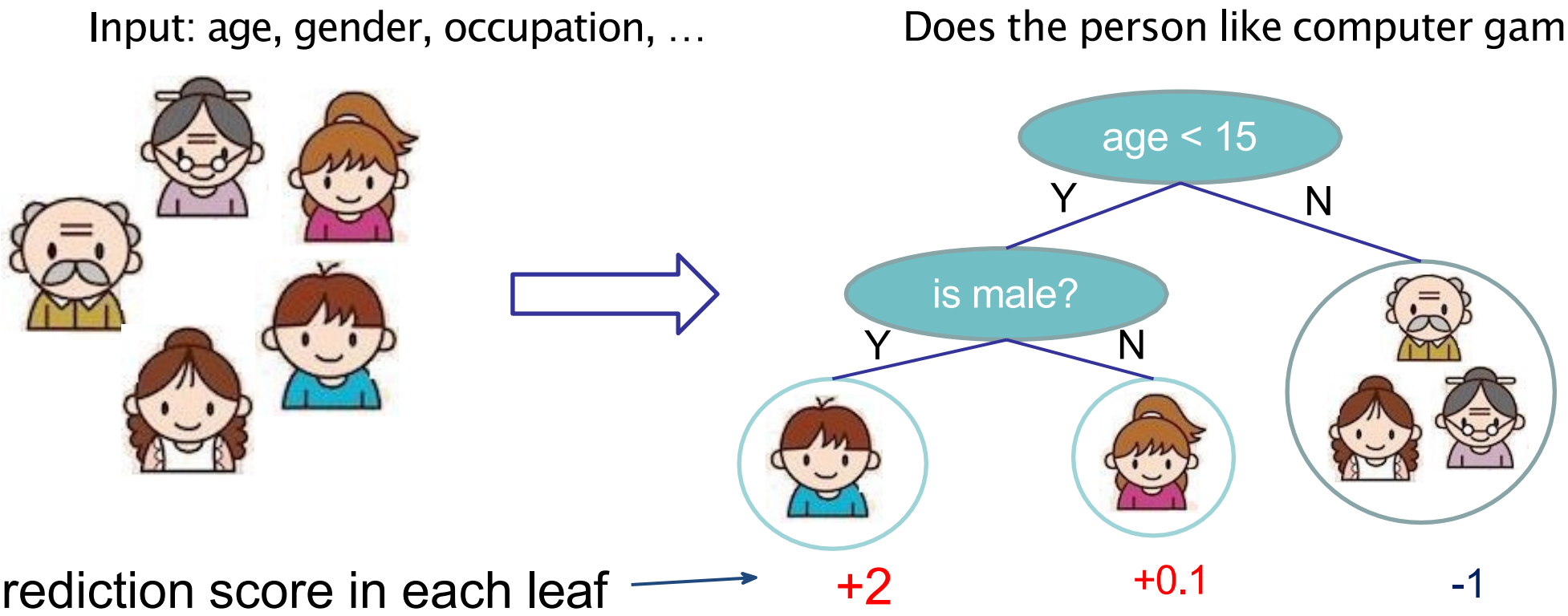
Machine Learning Algorithms and Common Use-cases

- Linear Models for Ads Clickthrough
- Factorization Models for Recommendation
- Deep Neural Nets for Images, Audios etc.

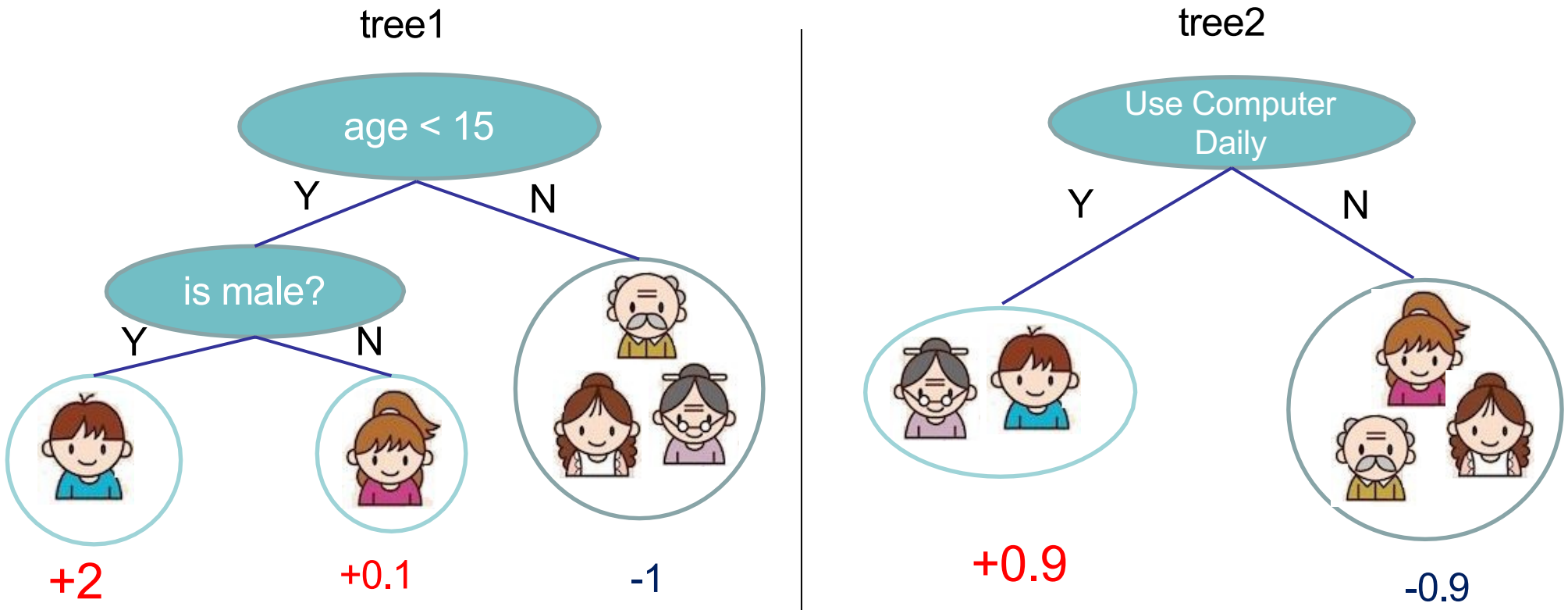
- **Trees** for tabular data: the *secret sauce* in machine learning
  - Anomaly detection
  - Ads clickthrough
  - Fraud detection
  - Insurance risk estimation
  - ...

Regression Tree

- Regression tree (also known as CART)
- This is what it would looks like for a commercial system



When Trees forms a Forest (Tree Ensembles)



f() = 2 + 0.9= 2.9

f()= -1 - 0.9= -1.9

Variant of algorithms to learn Tree Ensembles

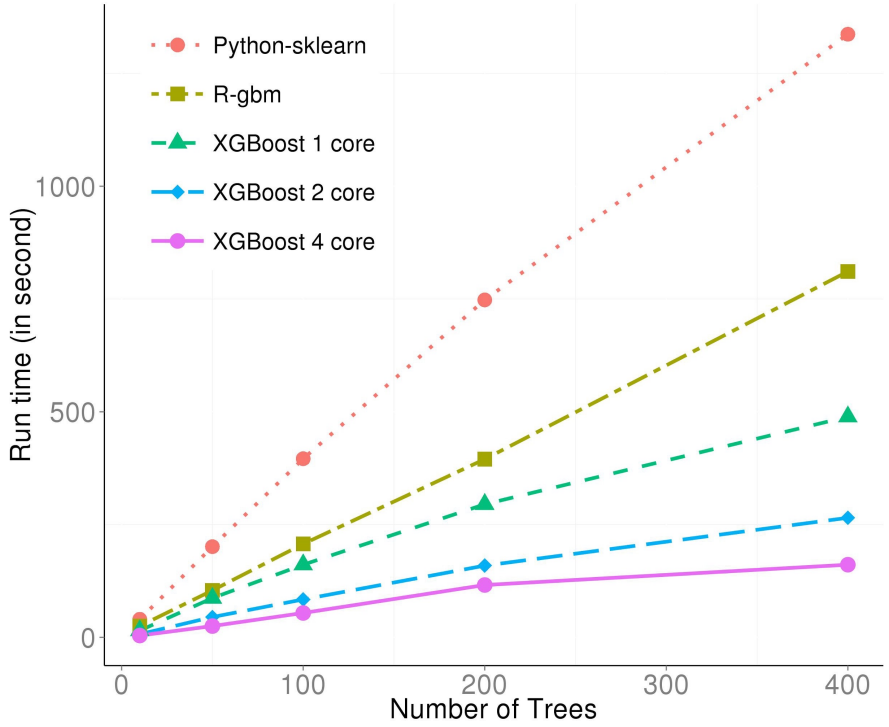
- Random Forest (*Breiman 1997)*
  - RandomForest packages in R and python
- Gradient Tree Boosting *(Friedman 1999)*
  - R GBM
  - sklearn.ensemble.GradientBoostingClassifier
- Gradient Tree Boosting with Regularization (variant of original GBM)
  - Regularized Greedy Forest (RGF)
  - XGBoost

Learning Trees : Advantage and Challenges

- Advantages of tree-based methods
  - Highly accurate: almost half of data science challenges are won by tree based methods.
  - Easy to use: invariant to input scale, get good performance with little tuning.
  - Easy to interpret and control
- Challenges on learning tree(ensembles)
  - Control over-fitting
  - Improve training speed and scale up to larger dataset

What is XGBoost

- A Scalable System for Learning Tree Ensembles
  - Model improvement
    - Regularized objective for better model
  - Systems optimizations
    - Out of core computing
    - Parallelization
    - Cache optimization
    - Distributed computing
  - Algorithm improvements
    - Sparse aware algorithm
    - Weighted approximate quantile sketch.



- *In short, faster tool for learning better models*

What does XGBoost learn

- A self-contained derivation of general gradient boosting algorithm
- Resembles the original GBM derivation by *Friedman*
- Only preliminary of calculus is needed

Elements of Supervised Learning

- **Model**: how to make prediction $\hat{y}_i = f(x_i)$
  - Linear model: $\hat{y}_i = \sum_j w_j x_{ij}$
- **Parameters**: the things we need to learn from data
  - Linear model: $\Theta = \{w_j | j = 1, \cdots, d\}$
- **Objective Function**: $Obj(\Theta) = L(\Theta) + \Omega(\Theta)$

Training Loss measures how well model fit on training data

Regularization, measures complexity of model

  - Linear model: $L(\Theta) = \sum_i (\hat{y}_i - y_i)^2$, $\Omega(\Theta) = \lambda \|w\|_2^2$

Elements of Tree Learning

- Model: assuming we have K trees

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

Space of Regression trees

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

Training Loss measures how well model fit on training data

Regularization, measures complexity of trees

Trade off in Learning

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

Training Loss measures how well model fit on training data

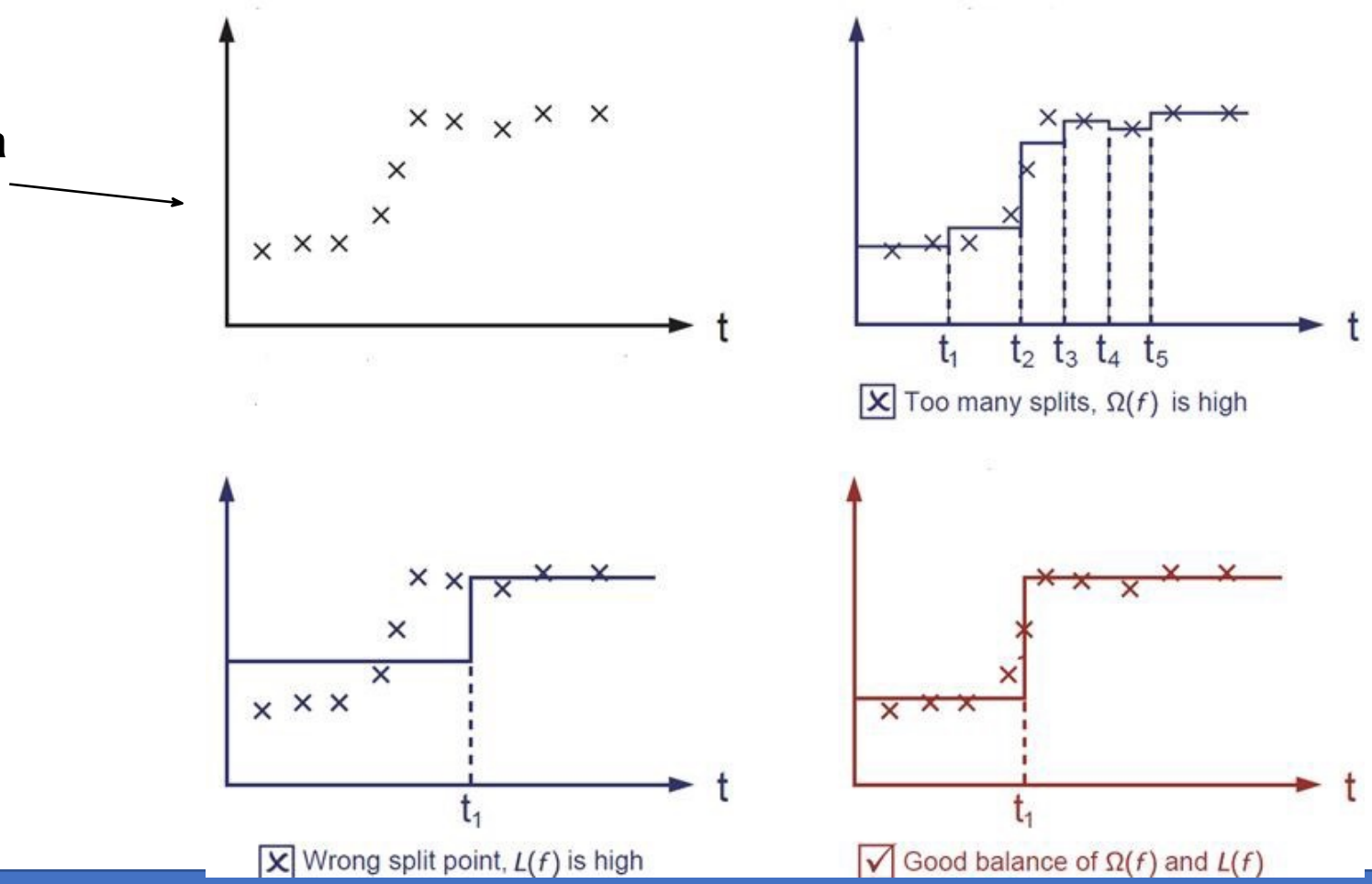
Regularization, measures complexity of trees

- Optimizing training loss encourages **predictive** models
  - Fitting well in training data at least get you close to training data which is hopefully close to the underlying distribution
- Optimizing regularization encourages **simple** models
  - Simpler models tends to have smaller variance in future predictions, making prediction **stable**

Why do we need regularization

Consider the example of learning tree on a single variable t

Raw Data

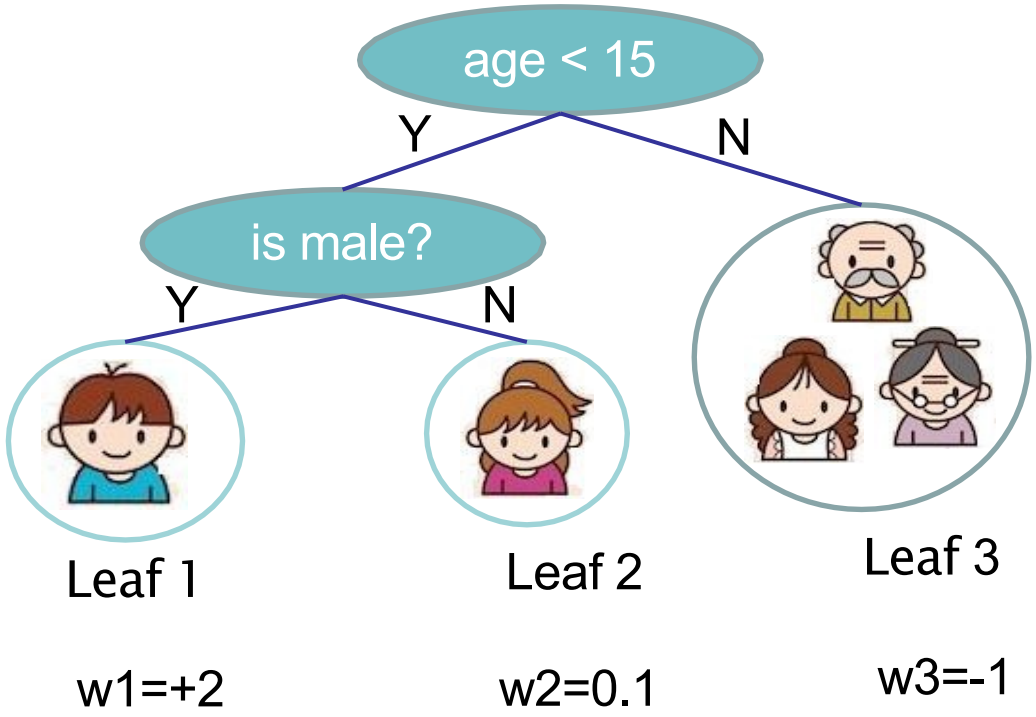


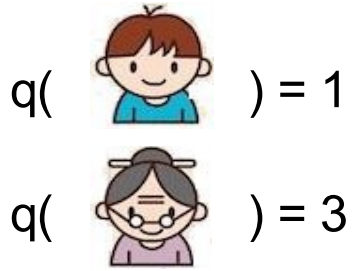
Define Complexity of a Tree

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

The leaf weight of the tree

The structure of the tree

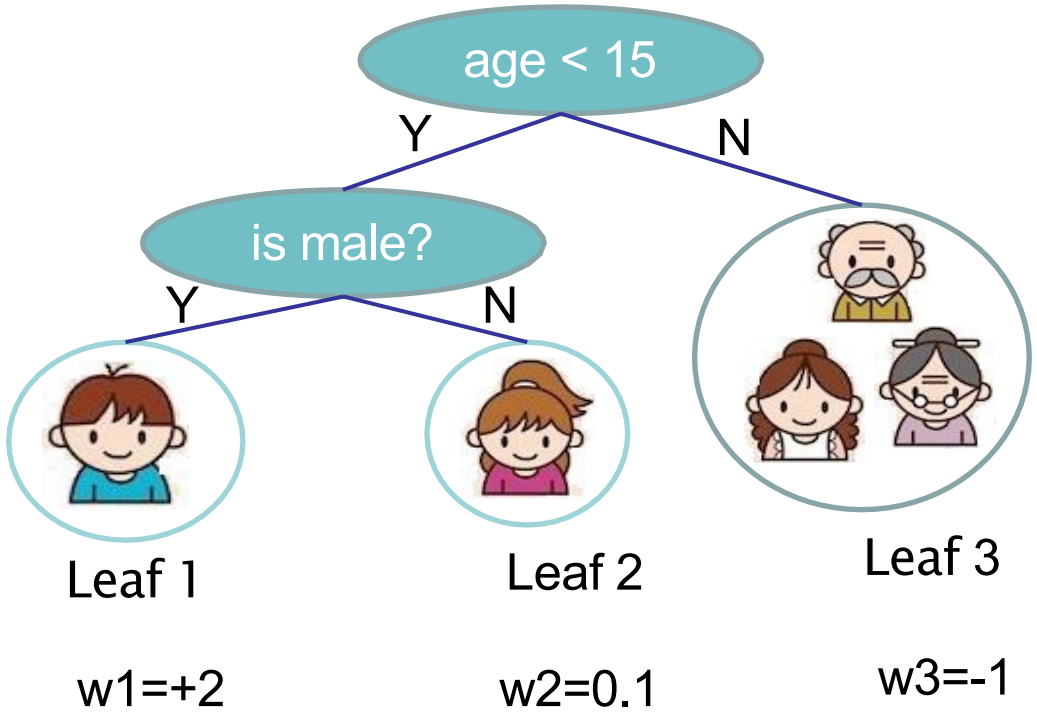




Define Complexity of a Tree (cont')

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

Number of leaves **L2 norm of leaf scores**



$$\Omega = \gamma 3 + \frac{1}{2}\lambda(4 + 0.01 + 1)$$

How can we learn tree ensembles

- Objective: $\sum_{i=1}^{n} l(y_i, \hat{y}_i) + \sum_k \Omega(f_k), f_k \in \mathcal{F}$
- We can not use methods such as SGD.
- Solution: **Additive Training (Boosting)**
  - Start from constant prediction, add a new function each time

$$
\begin{aligned}
\hat{y}_i^{(0)} &= 0 \\
\hat{y}_i^{(1)} &= f_1(x_i) = \hat{y}_i^{(0)} + f_1(x_i) \\
\hat{y}_i^{(2)} &= f_1(x_i) + f_2(x_i) = \hat{y}_i^{(1)} + f_2(x_i) \\
&\dots \\
\hat{y}_i^{(t)} &= \sum_{k=1}^{t} f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i)
\end{aligned}
$$

New function

Model at training round t

Keep functions added in previous round

Additive Training

- How do we decide which f to add: Optimize the objective!
- The prediction at round t is $\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + f_t(x_i)$

This is what we need to decide in round t

$$\begin{aligned} Obj^{(t)} &= \sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t)}) + \sum_{i=1}^{t} \Omega(f_i) \\ &= \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + constant \end{aligned}$$

Goal: find f_t to minimize this

- Consider square loss

$$\begin{aligned} Obj^{(t)} &= \sum_{i=1}^{n} \left(y_i - (\hat{y}_i^{(t-1)} + f_t(x_i))\right)^2 + \Omega(f_t) + const \\ &= \sum_{i=1}^{n} \left[2(\hat{y}_i^{(t-1)} - y_i) f_t(x_i) + f_t(x_i)^2\right] + \Omega(f_t) + const \end{aligned}$$

This is usually called residual from previous round

Taylor Expansion Approximation of Loss

- Goal $Obj^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + constant$
- 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 $g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial^2_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$

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

- *In terms of square loss*

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

Our New Goal

- Objective, with constants removed

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

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

- Define the instance set in leaf j as
  - Regroup the objective by leaf

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

  - This is sum of T independent quadratic function

The Structure Score

- Two facts about single variable quadratic function

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

- Let us define $G_j = \sum_{i \in I_j} g_i \quad H_j = \sum_{i \in I_j} h_i$

$$\begin{aligned} Obj^{(t)} &= \sum_{j=1}^{T} \left[(\sum_{i \in I_j} g_i) w_j + \frac{1}{2} (\sum_{i \in I_j} h_i + \lambda) w_j^2 \right] + \gamma T \\ &= \sum_{j=1}^{T} \left[G_j w_j + \frac{1}{2} (H_j + \lambda) w_j^2 \right] + \gamma T \end{aligned}$$

- Assume the structure of tree (q(x)) is fixed, the optimal weight in each leaf, and the resulting objective value are

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

This measures how good a tree structure is!

The Structure Score Calculation

Instance index gradient statistics

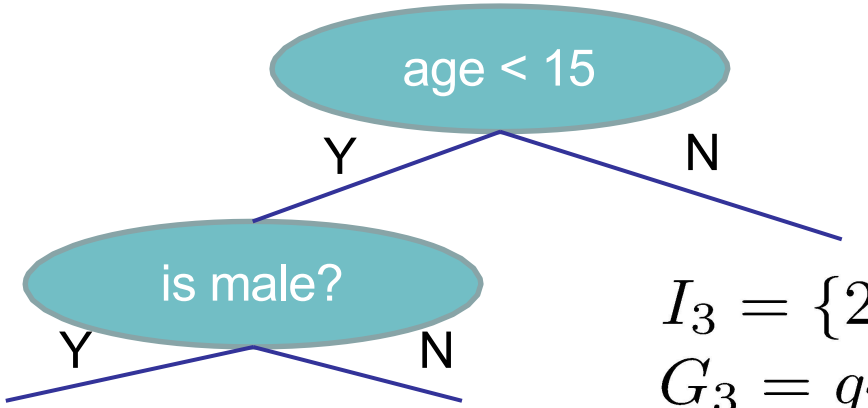
1  g1, h1

2  g2, h2

3  g3, h3

4  g4, h4

5  g5, h5



$$I_1 = \{1\}$$
$$G_1 = g_1$$
$$H_1 = h_1$$

$$I_2 = \{4\}$$
$$G_2 = g_4$$
$$H_4 = h_4$$

$$I_3 = \{2, 3, 5\}$$
$$G_3 = g_2 + g_3 + g_5$$
$$H_3 = h_2 + h_3 + h_5$$

$$Obj = -\sum_j \frac{G_j^2}{H_j + \lambda} + 3\gamma$$

The smaller the score is, the better the structure is

Searching Algorithm for Single Tree

- Enumerate the possible tree structures q
- Calculate the structure score for the q, using the scoring eq.

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

- Find the best tree structure, and use the optimal leaf weight

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

- But… there can be infinite possible tree structures..

Greedy Learning of the Tree

- In practice, we grow the tree greedily
  - Start from tree with depth 0
  - For each leaf node of the tree, try to add a split. The change of objective after adding the split is

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

The complexity cost by introducing additional leaf

the score of left child

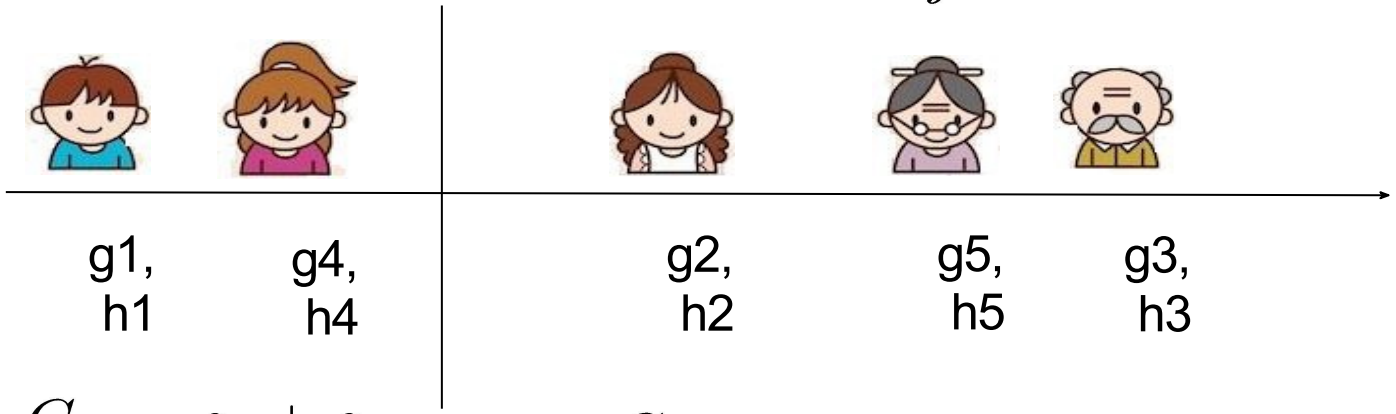
the score of right child

the score of if we do not split

  - Remaining question: how do we find the best split?

Efficient Finding of the Best Split

- What is the gain of a split rule $x_j < a$? Say x_j is age



$G_L = g_1 + g_4$ $\quad G_R = g_2 + g_3 + g_5$

- All we need is sum of g and h in each side, and calculate
- Left to right linear scan over sorted instance is enough to decide the best split along the feature

Pruning and Regularization

- Recall the gain of split, it can be negative!

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

  - When **the training loss reduction** is smaller than **regularization**
  - Trade-off between simplicity and predictiveness
- Pre-stopping
  - Stop split if the best split have negative gain
  - But maybe a split can benefit future splits..
- Post-Prunning
  - Grow a tree to maximum depth, recursively prune all the leaf splits with negative gain

What can XGBoost can do for you

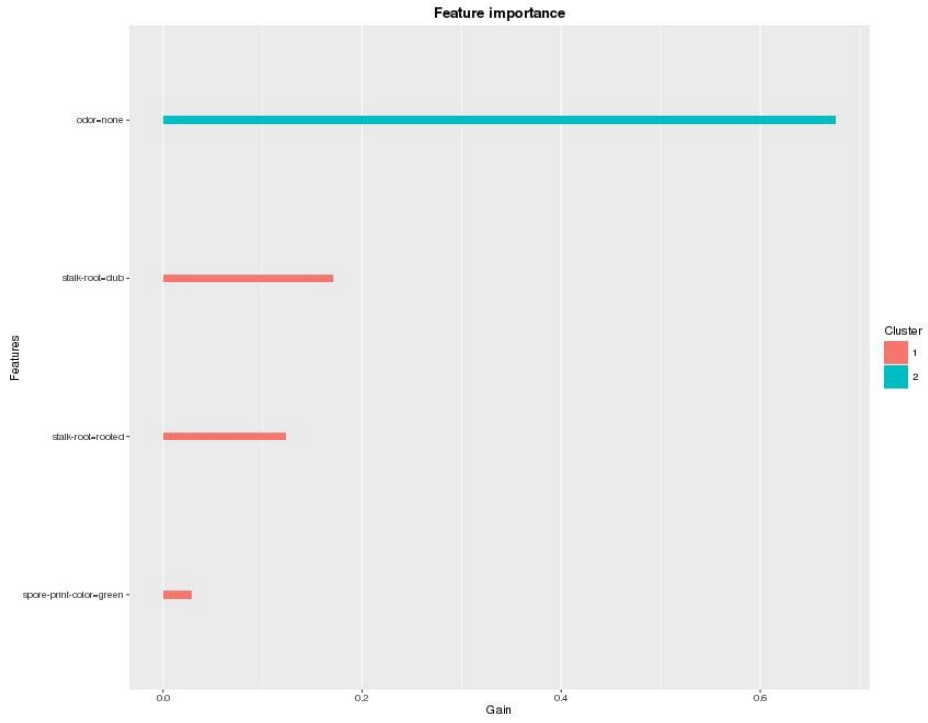
- Push the limit of computation resources to solve **one** problem
  - Gradient tree boosting
- Automatic handle missing value
- Interactive Feature analysis
- Extendible system for more functionalities
- Deployment on the Cloud

Getting Started (python)

```python
import xgboost as xgb

# read in data
dtrain = xgb.DMatrix('demo/data/agaricus.txt.train')
dtest = xgb.DMatrix('demo/data/agaricus.txt.test')

# specify parameters via map
param = {'max_depth':2, 'eta':1, 'silent':1, 'objective':'binary:logistic' }
num_round = 2
bst = xgb.train(param, dtrain, num_round)

# make prediction
preds = bst.predict(dtest)
```

Feature Importance Analysis

```
bst <- xgboost(data = train$data, label = train$label, max.depth = 2,
                        eta = 1, nthread = 2, nround = 2,objective = "binary:logistic")
importance_matrix <- xgb.importance(agaricus.train$data@Dimnames[[2]], model = bst)
xgb.plot.importance(importance_matrix)
```



Extendibility: Modular Library

- Plugin system
  - Enable you to plugin customized data loader, metrics, learners
  - Optionally build with some of the plugins
  - https://github.com/dmlc/xgboost/tree/master/plugin

- Modular library to for even more extensions
  - Recent pull request of supporting DART (dropout in tree boosting)
    - Reuse of all data loading and tree learning modules
    - Around 300 lines of additional code

Extendibility on Language API: Early Stopping

```
bst <- xgb.cv(data = train$data, label = train$label, nfold = 5,
                    nrounds = 20, objective = "binary:logistic",
                    early.stop.round = 3, maximize = FALSE)
```

```
##  [0]  train-error:0.000921+0.000343   test-error:0.001228+0.000686
##  [1]  train-error:0.001228+0.000172   test-error:0.001228+0.000686
##  [2]  train-error:0.000653+0.000442   test-error:0.001075+0.000875
##  [3]  train-error:0.000422+0.000416   test-error:0.000767+0.000940
##  [4]  train-error:0.000192+0.000429   test-error:0.000460+0.001029
##  [5]  train-error:0.000192+0.000429   test-error:0.000460+0.001029
##  [6]  train-error:0.000000+0.000000   test-error:0.000000+0.000000
##  [7]  train-error:0.000000+0.000000   test-error:0.000000+0.000000
##  [8]  train-error:0.000000+0.000000   test-error:0.000000+0.000000
##  [9]  train-error:0.000000+0.000000   test-error:0.000000+0.000000
## Stopping. Best iteration: 7
```

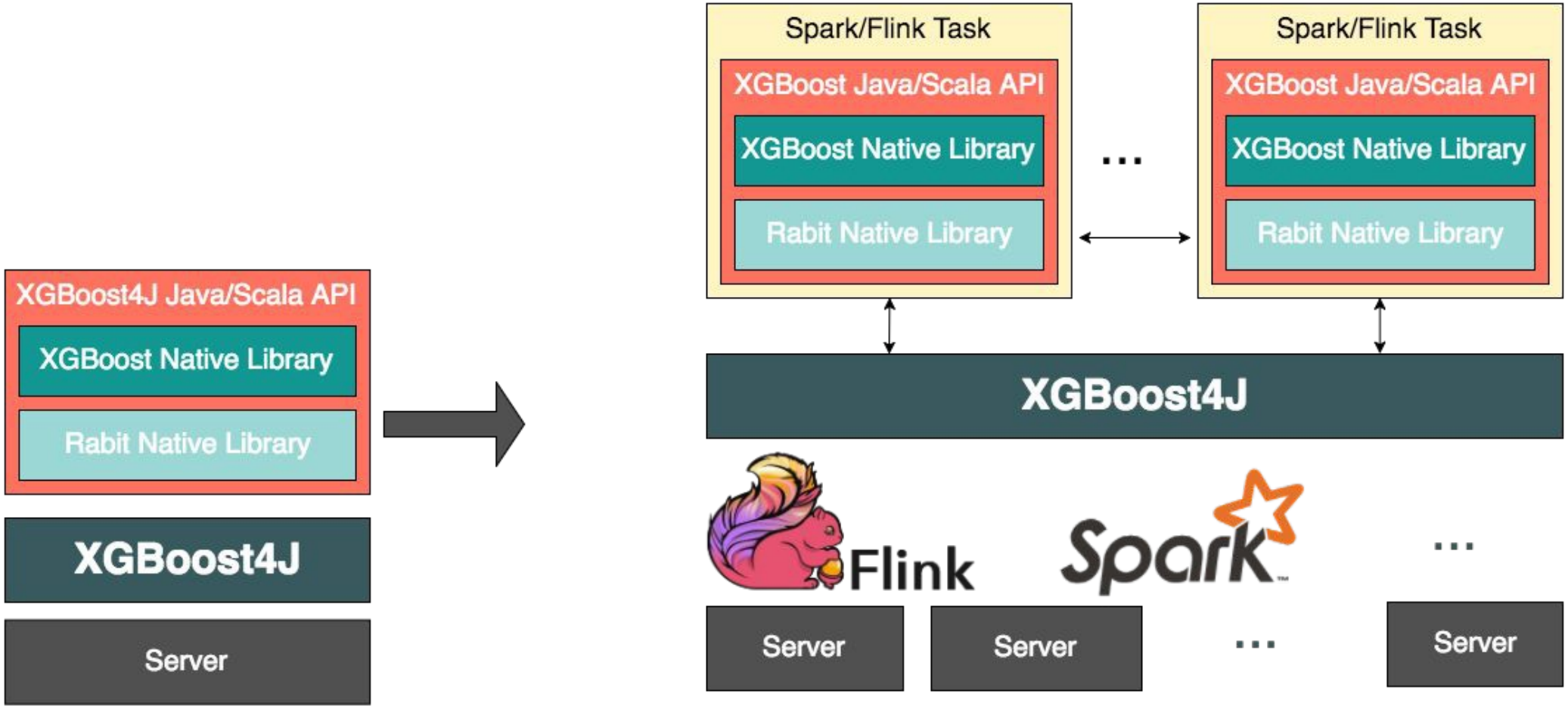
This feature is contributed by users, because they can directly hack the R/python API easily:)

Many more similar examples

What can XGBoost **cannot** do for you

- Feature engineering
- Hyper parameter tuning
- A lot more cases ...

XGBoost on DataFlow (cont')



Thank You