XGBoost: Gradient Boosted Trees

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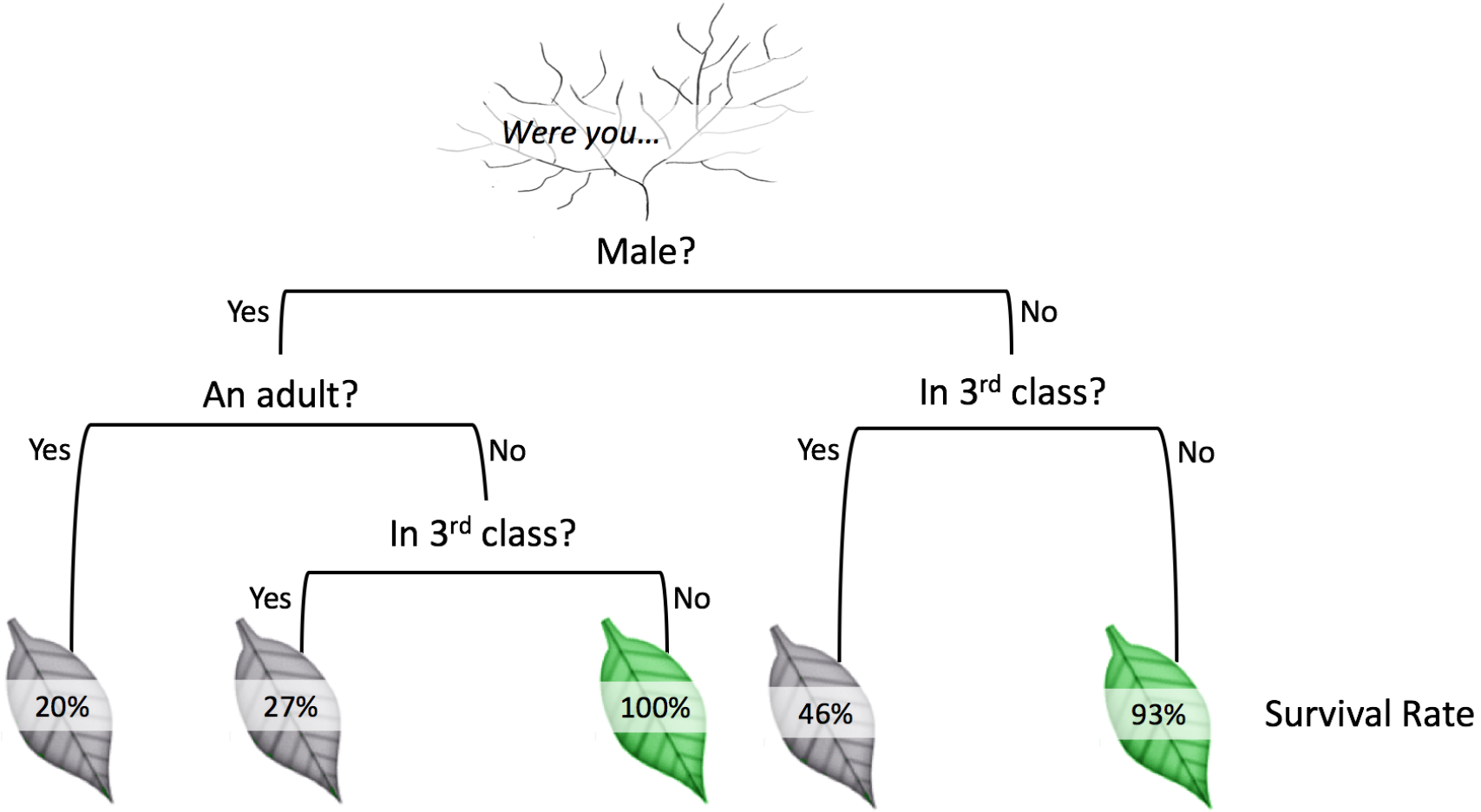
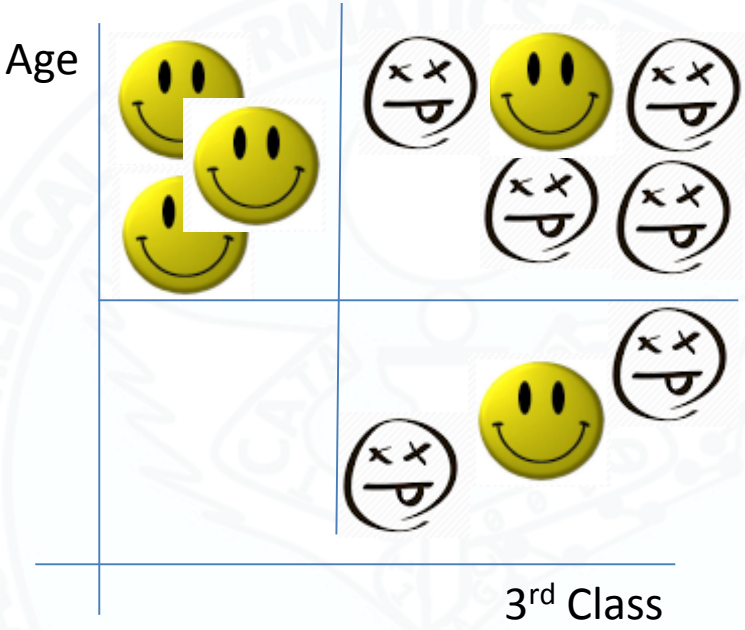
Decision Trees



- A tree predicting survival rate for titanic passengers
- A decision tree, in essence, "explains" a dataset by partitioning the space with respect to a single feature at a time

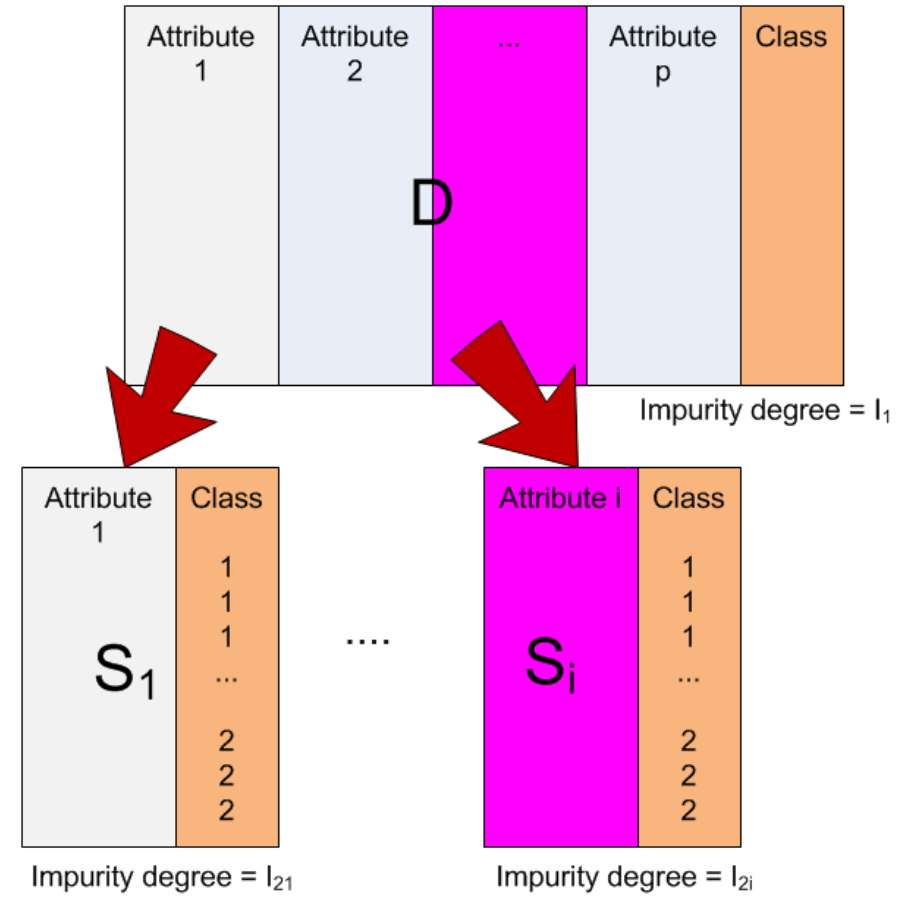
Decision Tree Learning



- Decision tree learning is the construction of a decision tree from class-labeled training tuples. A decision tree is a flow-chart-like structure, where each internal (non-leaf) node denotes a test on an attribute, each branch represents the outcome of a test, and each leaf (or terminal) node holds a class label. The topmost node in a tree is the root node.
- Algorithms for constructing decision trees usually work top-down, by choosing a variable at each step that best splits the set of items.

Top-down induction of decision trees (TDIDT)

- A tree can be “learned” by splitting the source set into subsets based on an attribute value test
- Pick the attribute that creates “purer” subsets (greedy approach!)
- This process is repeated on each derived subset in a recursive manner called recursive partitioning.
- The recursion is completed when the subset at a node has all the same value of the target variable, or when splitting no longer adds value to the predictions



Teknomo Kardi (2009): http://people.revoledu.com/kardi/tutorial/DecisionTree/

Measures of Impurity

- Gini impurity (CART)

To compute Gini impurity for a set of items with J classes, suppose $i \in \{1, 2, \ldots, J\}$, and let p_i be the fraction of items labeled with class i in the set.

$$I_G(p) = \sum_{i=1}^{J} p_i \sum_{k \neq i} p_k = \sum_{i=1}^{J} p_i(1 - p_i) = \sum_{i=1}^{J} (p_i - {p_i}^2) = \sum_{i=1}^{J} p_i - \sum_{i=1}^{J} {p_i}^2 = 1 - \sum_{i=1}^{J} {p_i}^2$$

- $GI(T, a) = I(T) - \sum_{k=1}^{|a|} \frac{|a_k|}{N} I(a_k)$
- Entropy-Based Information Gain (ID, C4.5, C5.0)

$$H(T) = I_E(p_1, p_2, \ldots, p_J) = -\sum_{i=1}^{J} p_i \log_2 p_i$$

$$\overbrace{IG(T,a)}^{\text{Information Gain}} = \overbrace{H(T)}^{\text{Entropy(parent)}} - \overbrace{H(T|a)}^{\text{Weighted Sum of Entropy(Children)}}$$

- $IG(T, a) = H(T) - \sum_{k=1}^{|a|} \frac{|a_k|}{N} H(a_k)$ a_k is the k[th] subset partition

Measuring Impurity

- Variance Reduction (Regression)

The variance reduction of a node N is defined as the total reduction of the variance of the target variable x due to the split at this node:

$$I_V(N) = \frac{1}{|S|^2} \sum_{i \in S} \sum_{j \in S} \frac{1}{2}(x_i - x_j)^2 - \left(\frac{1}{|S_t|^2} \sum_{i \in S_t} \sum_{j \in S_t} \frac{1}{2}(x_i - x_j)^2 + \frac{o1}{|S_f|^2} \sum_{i \in S_f} \sum_{j \in S_f} \frac{1}{2}(x_i - x_j)^2 \right)$$

where S, S_t, and S_f are the set of presplit sample indices, set of sample indices for which the split test is true, and set of sample indices for which the split test is false, respectively.

Data

Attributes				Classes
Gender	Car ownership	Travel Cost ($)/km	Income Level	Transportation mode
Male	0	Cheap	Low	Bus
Male	1	Cheap	Medium	Bus
Female	1	Cheap	Medium	Train
Female	0	Cheap	Low	Bus
Male	1	Cheap	Medium	Bus
Male	0	Standard	Medium	Train
Female	1	Standard	Medium	Train
Female	1	Expensive	High	Car
Male	2	Expensive	Medium	Car
Female	2	Expensive	High	Car

Travel Cost ($)/km	Transportation mode
Cheap	Bus
Cheap	Bus
Cheap	Bus
Cheap	Bus
Cheap	Train
Expensive	Car
Expensive	Car
Expensive	Car
Standard	Train
Standard	Train

4B, 3C, 3T

Entropy	1.571
Gini index	0.660
Classification error	0.600

Travel Cost ($)/km	Classes
Cheap	Bus
Cheap	Bus
Cheap	Bus
Cheap	Bus
Cheap	Train

4B, 1T

Entropy	0.722
Gini index	0.320
classification error	0.200

Travel Cost ($)/km	Classes
Expensive	Car
Expensive	Car
Expensive	Car

3C

Entropy	0.000
Gini index	0.000
classification error	0.000

Travel Cost ($)/km	Classes
Standard	Train
Standard	Train

2T

Entropy	0.000
Gini index	0.000
classification error	0.000

IG = 1.571- {(5/10)0.722+(2/10)0+(3/10)0 = 1.210

Teknomo Kardi (2009): http://people.revoledu.com/kardi/tutorial/DecisionTree/

Choosing the feature

Results of first Iteration

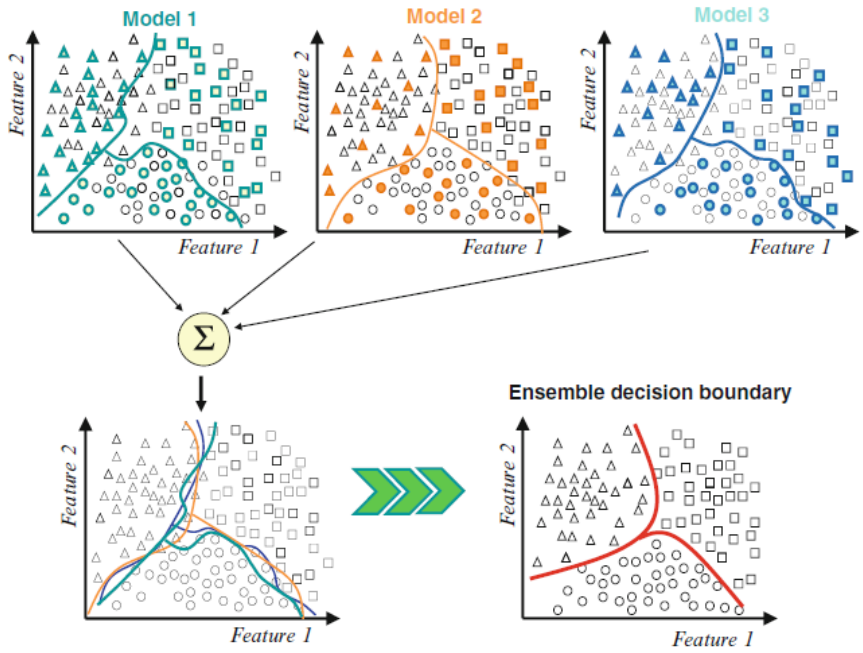
Gain	Gender	Car ownership	Travel Cost/KM	Income Level
Entropy	0.125	0.534	**1.210**	0.695
Gini index	0.060	0.207	**0.500**	0.293
Classification error	0.100	0.200	**0.500**	0.300

- Advantages and Disadvantages

Advantages	Disadvantages
Simple to understand and interpret	Less Accurate
Able to handle both numerical and categorical data	Optimal Decision Tree learning is NP-complete
Requires little data preparation	Sensitive to data changes
Uses a white box model	Can create overly complex boundaries
Possible to validate a model using statistical tests	Impurity metrics can bias results to more levels
Non-statistical approach that makes no assumptions of the training data or prediction residuals	Complexity control through tree depth parameter
Built-in feature selection and interpretation	Practical imlementation needs some “tricks”

Ensemble Methods

- Combine the predictions from multiple “weak” learners
  - Uncorrelated errors in predictions
    - Each learner makes errors on different examples
  - If errors are correlated, little advantage in combining the classifiers
- How to make different classifiers
  - Different Data set partitioning
  - Different Features
  - Different parameters
  - Learning errors from previously trained methods



Polikar 2006: http://users.rowan.edu/~polikar/RESEARCH/PUBLICATIONS/csm06.pdf
Ensemble Machine Learning Methods and Applications (chapter 1), 2012
https://doc.lagout.org/science/Artificial%20Intelligence/Machine%20learning/Ensemble%20Machine%20Learning_%20Methods%20and%20Applications%20%5BZhang%20%26%20Ma%202012-02-17%5D.pdf

Ensemble methods

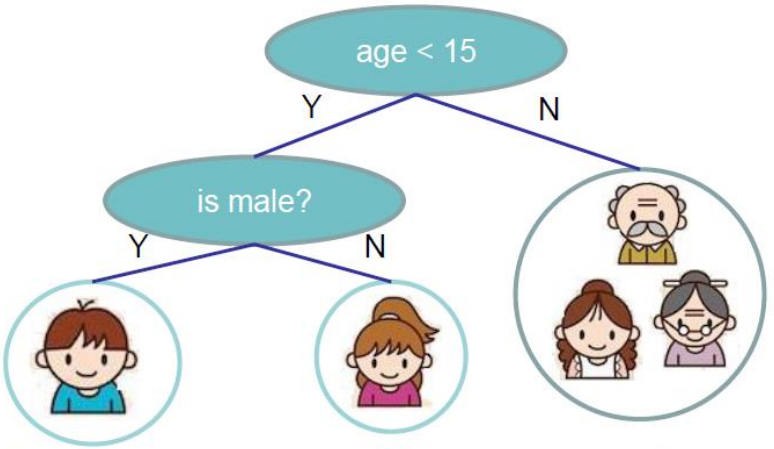
- Bootstrap Aggregation (Bagging)
  - Involves having each model in the ensemble vote with equal weight.
  - Trains each model in the ensemble using a randomly drawn subset of the training set.
  - Random Forest algorithm
- Boosting
  - Boosting involves incrementally building an ensemble by training each new model instance to emphasize the training instances that previous models mis-classified.
  - Adaboost
  - Gradient Boosted Trees
- Stacking (Stacked Generalization)
  - Build models and then build a model that predicts the output based on the prediction of individual models
- Bayesian Parameter Modeling, Bayesian Model Combination

https://en.wikipedia.org/wiki/Ensemble_learning

Tree Regression

Input: age, gender, occupation, …

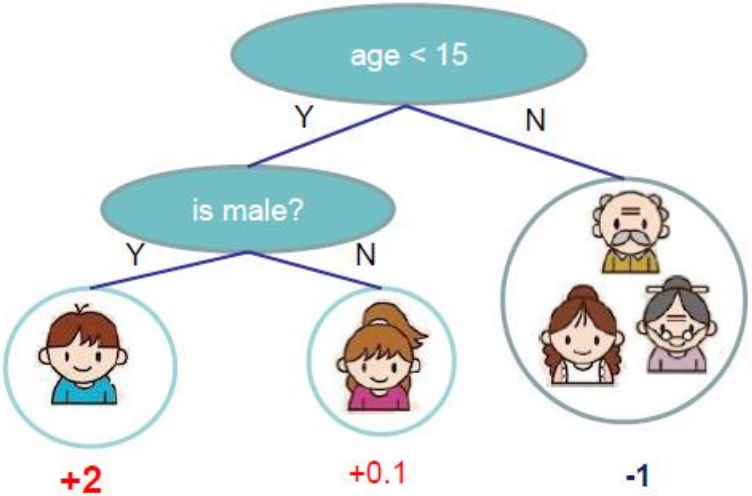
Does the person like computer games



prediction score in each leaf → **+2** +0.1 **-1**

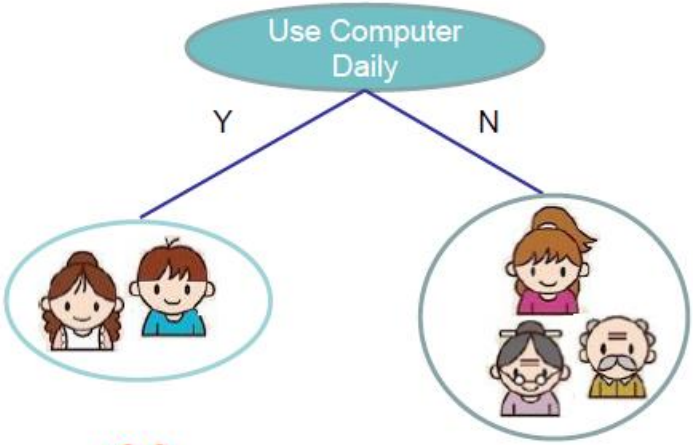
Regression Ensemble

tree1



+2 +0.1 **-1**

tree2



+0.9 **-0.9**

f() = 2 + 0.9= 2.9 f()= -1 - 0.9= -1.9

Prediction of is sum of scores predicted by each of the tree

XGBoost: A Scalable Tree Boosting System

- An implementation of gradient-boosted trees
- Uses structural risk minimization
- Incrementally builds a machine learning model by combining simple trees
- Very successful in different Kaggle Competitions
- Easy to use

SRM

$$f^* = argmin_f \{L(X, Y; f) + \lambda g(\|f\|)\}$$

X, Y is the training data
f is the learning function

Regularization
Classifier Complexity
(smoothing) term

Empirical Loss (or risk) term

Structural Risk

- Representation: Output score for a given example is the sum of K tree scores

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

- Loss: Sum of losses over individual examples (regression loss, classification loss, etc.)
- Model Complexity: Number of trees, norm of leaf weights, etc.

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

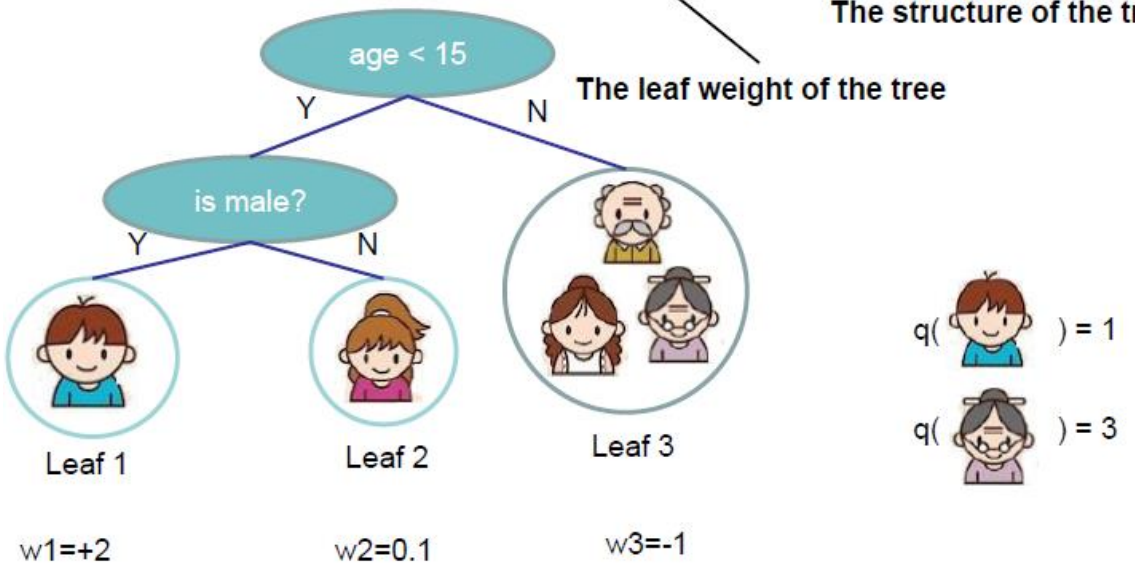
Structural Risk in Trees: Model Complexity

- Assume a regression tree with T leaves
- We define tree by a vector of scores in leafs, and a leaf index mapping function that maps an instance to a leaf

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

The structure of the tree

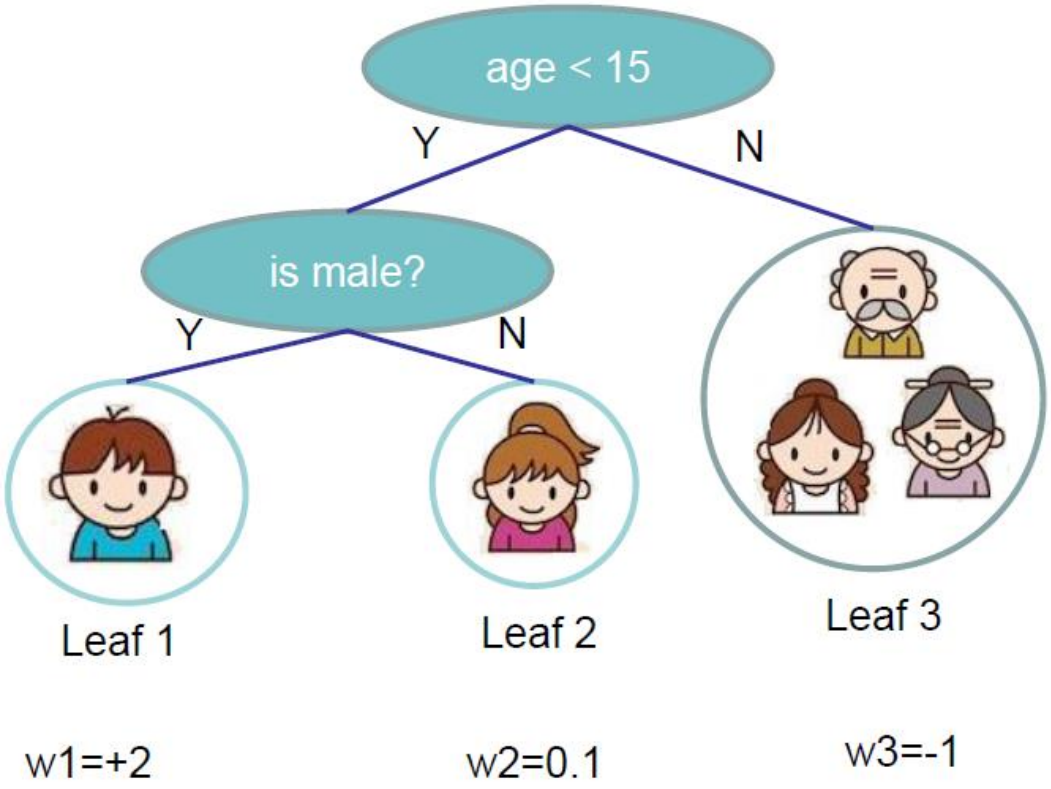
The leaf weight of the tree



Structural Risk in Trees : Model Complexity

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

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



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

Representation: Using Additive Boosting

- Start off with a simple predictor
- The next step predictor tries to reduce the error between the prediction of the previous stage and the target by addition

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

Evaluation: 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

Optimization: Taylor Expansion

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

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

- *If you are not comfortable with this, think of square loss*

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

- Compare what we get to previous slide

Optimization

- This gives (notice, g_i, h_i depend only on loss)

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

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

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

Regroup the objective by each leaf

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

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

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

Optimization

- We know

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

- Therefore, for our objective function

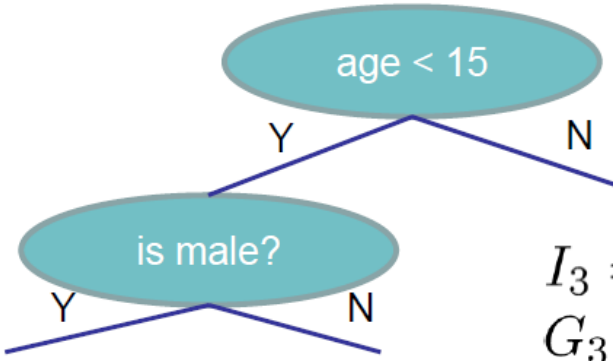
$$\begin{aligned} Obj^{(t)} &= \sum_{j=1}^{T} \left[(\sum_{i \in I_j} g_i) w_j + \tfrac{1}{2} (\sum_{i \in I_j} h_i + \lambda) w_j^2 \right] + \gamma T \\ &= \sum_{j=1}^{T} \left[G_j w_j + \tfrac{1}{2} (H_j + \lambda) w_j^2 \right] + \gamma T \end{aligned}$$

- We get

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

Structural Risk of Trees

Instance index		gradient statistics
1		g1, h1
2		g2, h2
3		g3, h3
4		g4, h4
5		g5, h5



$$I_1 = \{1\} \quad I_2 = \{4\} \quad I_3 = \{2, 3, 5\}$$
$$G_1 = g_1 \quad G_2 = g_4 \quad G_3 = g_2 + g_3 + g_5$$
$$H_1 = h_1 \quad H_4 = h_4 \quad H_3 = h_2 + h_3 + h_5$$

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

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 Split: Information Gain

- 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

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

The complexity cost by introducing additional leaf

the score of left child

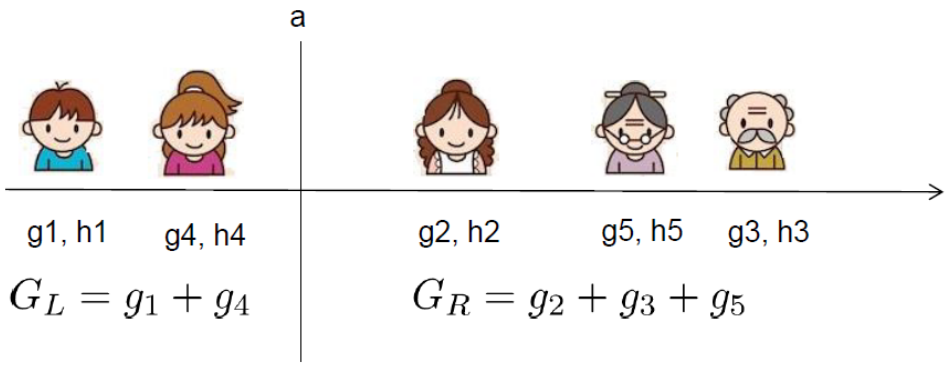
the score of right child

the score of if we do not split

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

Greedy Splitting

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



- All we need is sum of g and h in each side, and calculate

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

- Left to right linear scan over sorted instance is enough to decide the best split along the feature

- **Algorithm**
- For each node, enumerate over all features
  - For each feature, sorted the instances by feature value
    - Use a linear scan to decide the best split along that feature
  - Take the best split solution along all the features

Boosted Tree Algorithm

- Add a new tree in each iteration
- Beginning of each iteration, calculate

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

- Use the statistics to greedily grow a tree $f_t(x)$

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

- Add $f_t(x)$ to the model $\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + f_t(x_i)$
  - Usually, instead we do $y^{(t)} = y^{(t-1)} + \epsilon f_t(x_i)$
  - ϵ is called step-size or shrinkage, usually set around 0.1
  - This means we do not do full optimization in each step and reserve chance for future rounds, it helps prevent overfitting

Code

```
import pandas as pd
import numpy as np
import xgboost as xgb

train = pd.read_csv("../input/train.csv")
test = pd.read_csv("../input/test.csv")
submission = pd.read_csv("../input/sampleSubmission.csv")
#target is class_1, ..., class_9 - needs to be converted to 0, ..., 8
train['target'] = train['target'].apply(lambda val: np.int64(val[-1:]))-1

Xy_train = train.as_matrix()
X_train = Xy_train[:,1:-1]
y_train = Xy_train[:,-1:].ravel()

X_test = test.as_matrix()[:,1:]

dtrain = xgb.DMatrix(X_train, y_train, missing=np.NaN)
dtest = xgb.DMatrix(X_test, missing=np.NaN)

params = {"objective": "multi:softprob", "eval_metric": "mlogloss", "booster" : "gbtree",
          "eta": 0.05, "max_depth": 3, "subsample": 0.6, "colsample_bytree": 0.7, "num_class": 9}

num_boost_round = 100

gbm = xgb.train(params, dtrain, num_boost_round)
pred = gbm.predict(dtest)

print(gbm.eval(dtrain))
```

to account for examples importance we can assign weights to them in DMatrix (not done here)

Feature Importance

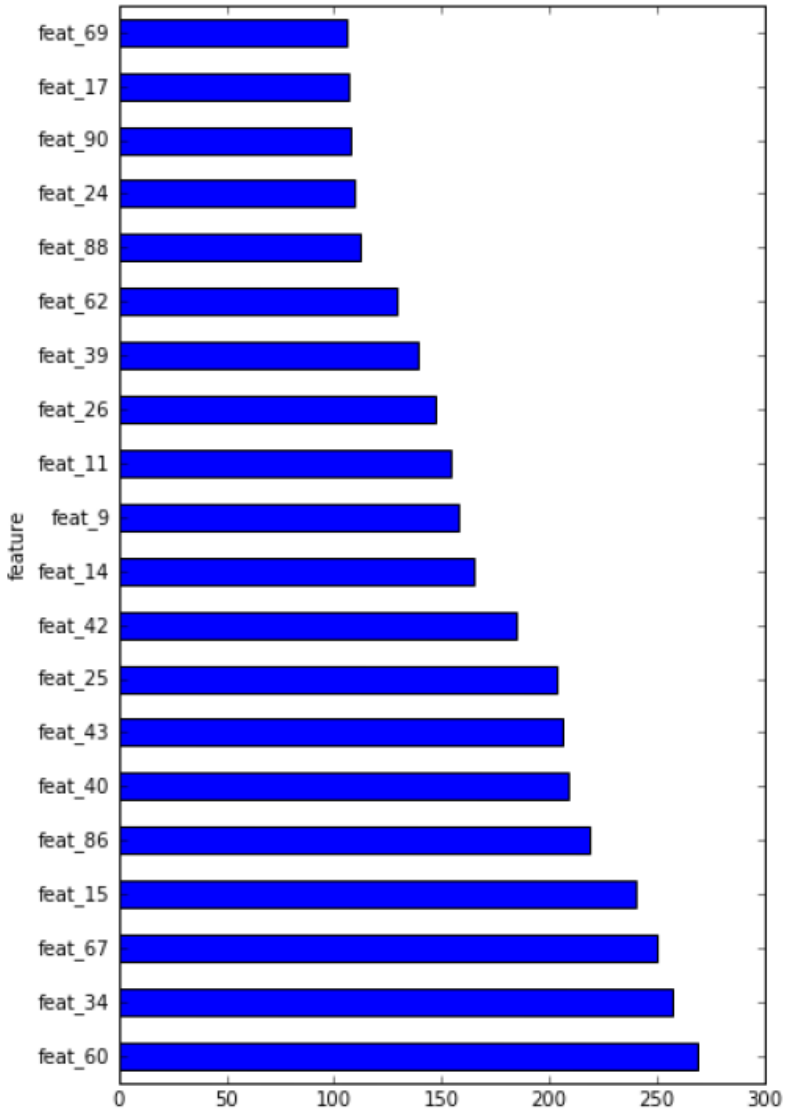
```
importance = gbm.get_fscore()

fdict = {}
for key, name in enumerate(train.columns[1:-1]):
    fdict['f{0}'.format(key)] = name

importance_with_names = []

for key, value in importance.items():
    importance_with_names.append((fdict[key], value))

pd.DataFrame(importance_with_names, columns=['feature',
'fscore']).\
set_index('feature').sort_values(['fscore'],
ascending=[0])[:20].\
plot(kind="barh", legend=False, figsize=(6, 10))
```



XGBoost via Scikit

```
import pandas as pd
import numpy as np
import xgboost as xgb
from sklearn.metrics import log_loss

train = pd.read_csv("../input/train.csv")
test = pd.read_csv("../input/test.csv")
submission = pd.read_csv("../input/sampleSubmission.csv")
#target is class_1, ..., class_9 - needs to be converted to 0, ..., 8
train['target'] = train['target'].apply(lambda val: np.int64(val[-1:]))-1

Xy_train = train.as_matrix()
X_train = Xy_train[:,1:-1]
y_train = Xy_train[:,-1:].ravel()

X_test = test.as_matrix()[:,1:]

num_boost_round = 100

gbm = xgb.XGBClassifier(max_depth=3, learning_rate=0.05, objective="multi:softprob", subsample=0.6,
                  colsample_bytree=0.7, n_estimators=num_boost_round)

gbm = gbm.fit(X_train, y_train)

pred = gbm.predict_proba(X_test)

y_hat_train = gbm.predict_proba(X_train)
print(log_loss(y_train, y_hat_train))
```

XGBoost Parameters

subsample

- ratio of instances to take
- example values: 0.6, 0.9

colsample_by_tree

- ratio of columns used for whole tree creation
- example values: 0.1, …, 0.9

colsample_by_level

- ratio of columns sampled for each split
- example values: 0.1, …, 0.9

eta

- how fast algorithm will learn (shrinkage)
- example values: 0.01, 0.05, 0.1

max_depth

- maximum numer of consecutive splits
- example values: 1, …, 15 (for dozen or so or more, needs to be set with regularization parametrs)

min_child_weight

- minimum weight of children in leaf, needs to be adopted for each measure
- example values: 1 (for linear regression it would be one example, for classification it is gradient of pseudo-residual)

alpha

- L1 norm (simple average) of weights for whole objective function

lambda

- L2 norm (root from average of squares) of weights, added as penalty to objective function

gamma

- L0 norm, multiplied by numer of leafs in a tree is used to decide whether to make a split

References

- **XGBoost: A Scalable Tree Boosting System**
- https://www.slideshare.net/JaroslawSzymczak1/xgboost-the-algorithm-that-wins-every-competition
  - Especially the feature importance
- https://homes.cs.washington.edu/~tqchen/pdf/BoostedTree.pdf

End of Lecture

We want to make a machine that will be proud of us.

- Danny Hillis