# Introduction to Big Data Analysis
# Ensemble Methods

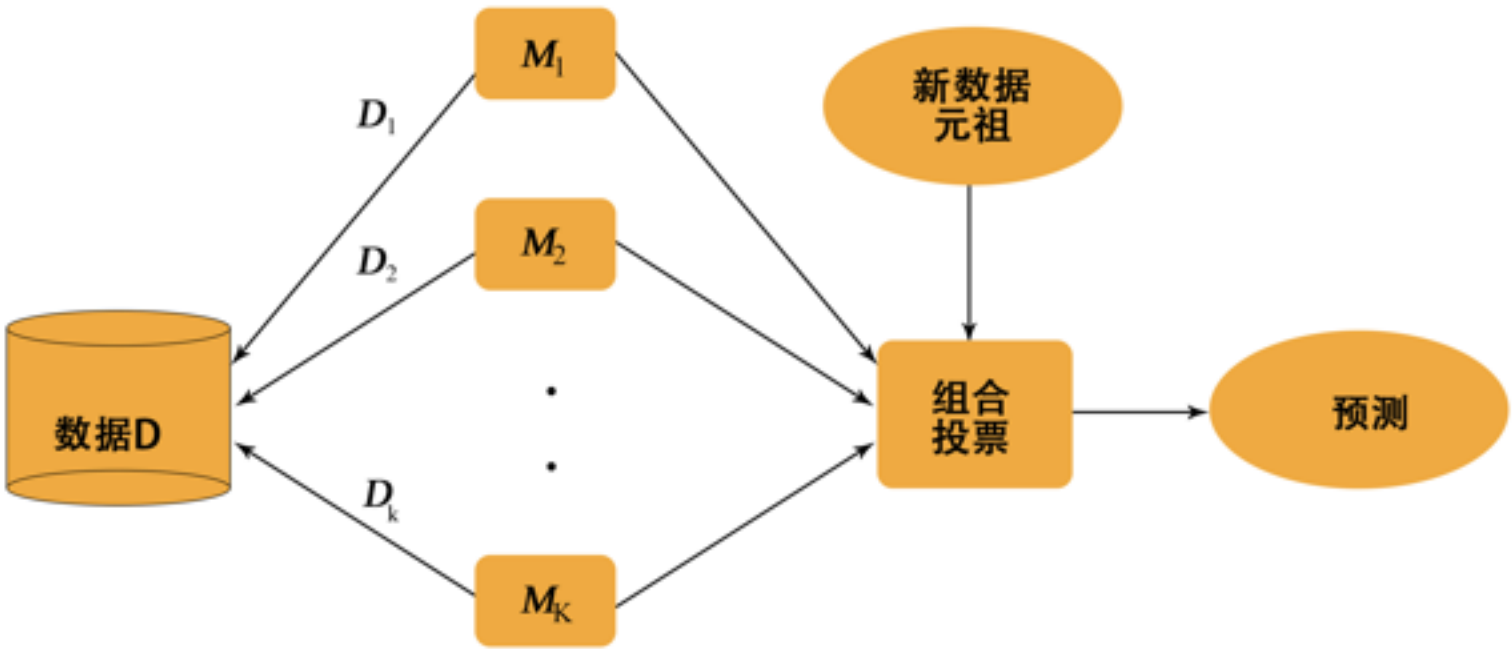
Zhen Zhang

Southern University of Science and Technology

# Outlines

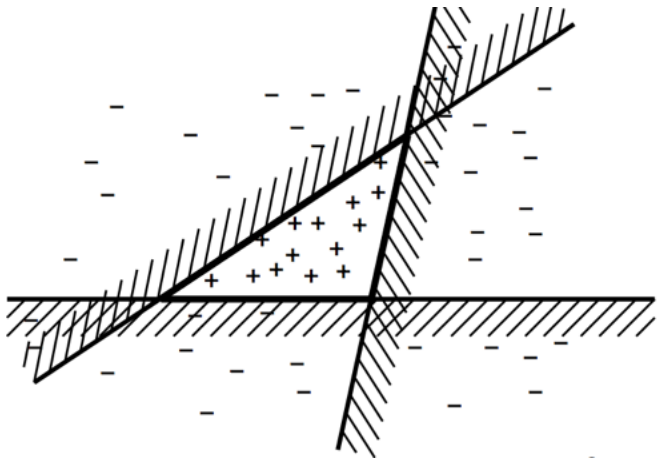
# Ensemble Methods

- Wisdom of Crowds ("三个臭皮匠，顶个诸葛亮")
- Multiple weak learners (base learners, may be heterogenous) can improve learning performance



# Why it can improve the performance

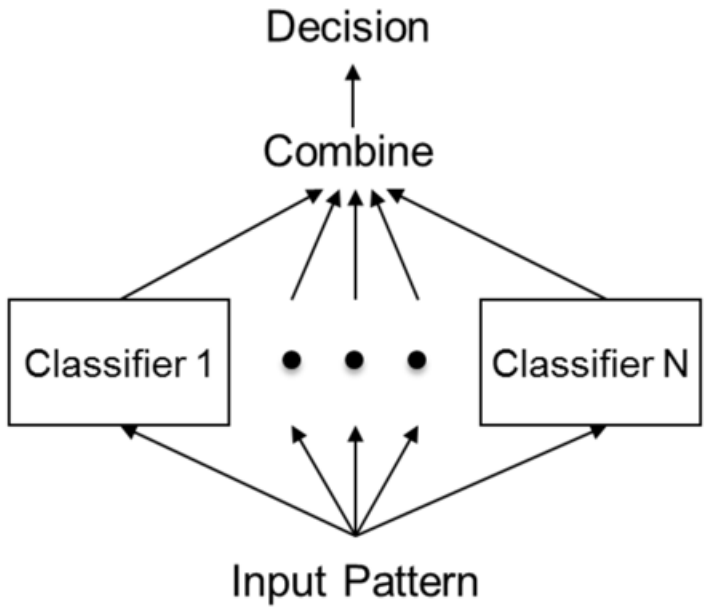
- More expressive, can approximate larger functional space
  - Single linear classifier (perceptron) does not work
  - Try multiple classifiers



- Reduce misclassfication rate
  - Misclassfication rate of single classifier is p
  - Choose $N$ classifiers, same but independent, voting
  - Error rate of majority vote $= \sum_{k>N/2} \binom{N}{k} p^k (1-p)^{N-k}$
  - When $N = 5, p = 0.1$, Error rate $< 0.01$

# Two commonly used ensemble methods

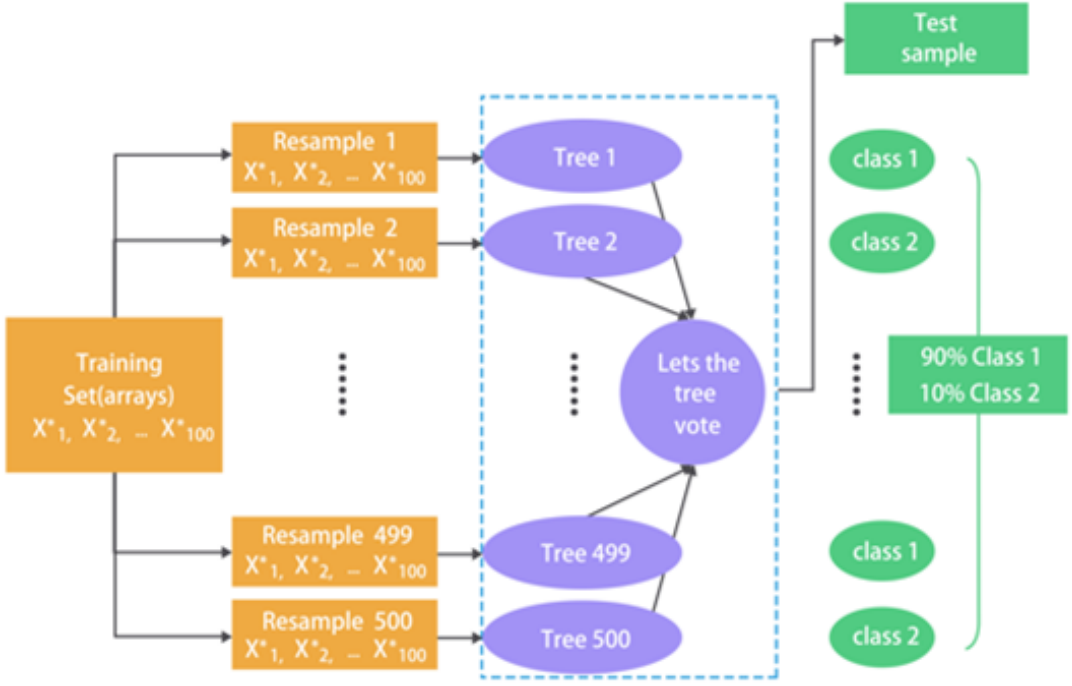
- Bagging
  - Random sampling : generating independent models, and averaging for regressions (making majority vote for classifications)
  - Reducing variances
  - Example : Random forests
- Boosting
  - Sequential training : training the subsequent models based on the errors of previous models
  - Reducing bias
  - Examples : AdaBoost and GBDT



# Outlines

# Bagging

- Bagging is short for bootstrap aggregation
- Bagging generates a committee of predictors and combine them in a certain manner to the final model
- Single predictor suffers from instability, while bagging could improve the stability by majority vote (classification) or averaging (regression) over all single predictors



# Sampling

- Given a dataset $D$ of $n$ samples, at the iteration $m = 1, \ldots, M$, the training set $D_m$ is obtained by sampling from $D$ with replacement. Then $D_m$ is used to construct classifier $\hat{f}_m(x)$.
- Sampling with replacement : some samples in $D$ may be missing in $D_m$, while some other samples may occur more than once
- On average, 63.2% of the samples in $D$ could be selected into $D_m$. In fact, for each sample, the probability that it is not selected in one round is $1 - \frac{1}{n}$. Then it is not selected in all $n$ rounds with probability $\lim_{n\to\infty}(1 - \frac{1}{n})^n = 0.368$.

# Algorithm

- Input : training set $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$
- Output : additive model $\hat{f}_{bag}(x)$

1. For $m = 1$ to $M$ :
   - 1.1 Sample from $D$ with replacement to obtain $D_m$
   - 1.2 Train a model $\hat{f}_m(x)$ from the dataset $D_m$ : for classification, $\hat{f}_m(x)$ returns a K-class 0-1 vector $e_k$ ; for regression, it is just a value
2. Compute bagging estimate $\hat{f}_{bag}(x) = \frac{1}{M} \sum_{m=1}^{M} \hat{f}_m(x)$ : for classification, make majority vote $\hat{G}_{bag}(x) = \arg\max_k \hat{f}_k(x)$ ; for regression, just return the average value

# Variance Reduction

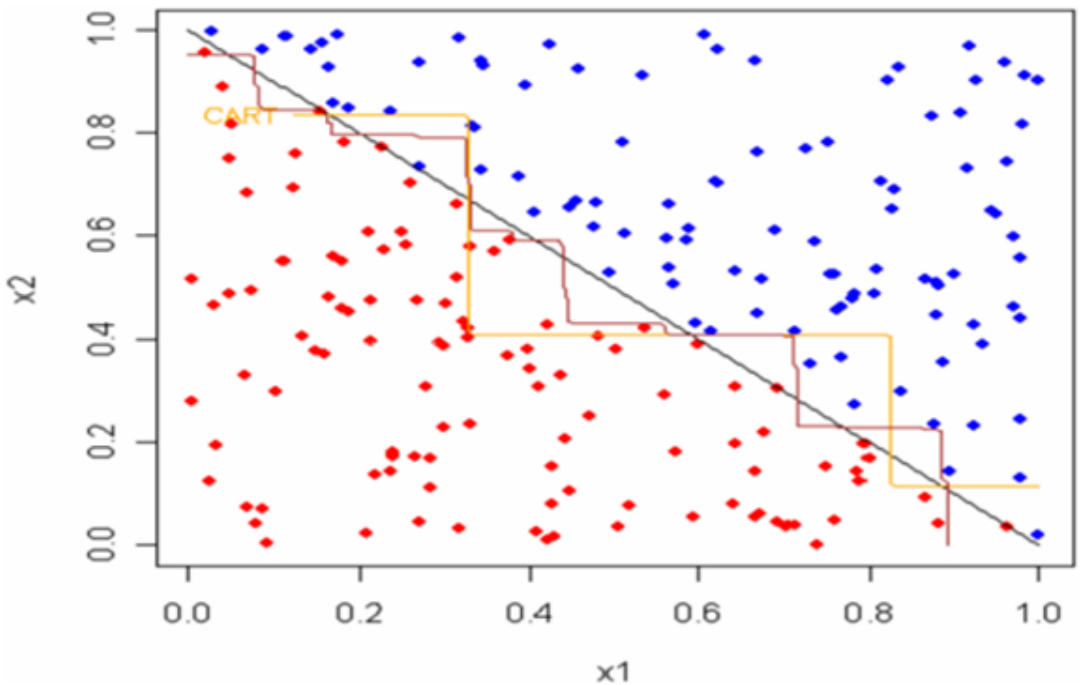
- In bagging, we use the same model to train different sample set in each iteration ; assume the models $\{\hat{f}_m(x)\}_{m=1}^{M}$ have the same variance $\sigma^2(x)$, while the correlation of each pair is $\rho(x)$
- Then the variance of the final model is :

$$\begin{aligned}\mathrm{Var}(\hat{f}_{bag}(x)) &= \frac{1}{M^2}\Big(\sum_{m=1}^{M}\mathrm{Var}(\hat{f}_m(x)) + \sum_{t\neq m}\mathrm{Cov}(\hat{f}_t(x)\hat{f}_m(x))\Big) \\ &= \rho(x)\sigma^2(x) + \frac{1-\rho(x)}{M}\sigma^2(x)\end{aligned}$$

- As $M \to \infty$, $\mathrm{Var}(\hat{f}_{bag}(x)) \to \rho(x)\sigma^2(x)$. This usually reduces the variance.
- If $\rho(x) = 0$, the variance could approach zero
- The random sampling in bagging is to reduce the correlation $\rho(x)$, i.e., make the sub-predictors as independent as possible

# Limitations of Decision Tree

- Stuck at local optimum : The greedy algorithm makes it stop at the local optimum, as it seeks the maximal information gain in each tree split
- Decision boundary : Use one feature in each split, the decision boundary is parallel to the coordinate axes
- Bad representability and instability



# Random Forest

- Random Forest further reduces the variance by adding independency to the committee of decision trees
- This is achieved by introducing more randomness.
- More randomness :
  - Sampling on the training data with replacement
  - Select features at random
- No pruning is needed.
- Example : RF consisting of 3 independent trees, each with an error rate of 40%. Then the probability that more than one tree misclassify the samples is
  $0.4^3 + 3 * 0.4^2 * (1 - 0.4) = 0.352$

# Random Forest Algorithm

- Input : training set $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$
- Output : additive model $\hat{f}_{rf}(x)$

1. For $m = 1$ to $M$ :
   - 1.1 Sample from $D$ with replacement to obtain $D_m$
   - 1.2 Grow a random-forest tree $T_m$ to the dataset $D_m$ : by recursively repeating the following steps for each terminal node of the tree, until the minimum node size $n_{min}$ is reached
     - 1.2.1 Select $q$ features at random from the $p$ features
     - 1.2.2 Pick the best feature/split-point among the $q$
     - 1.2.3 Split the node into two daughter nodes
2. Output the ensemble of trees $\{T_m\}_{m=1}^{M}$ : for regression, $\hat{f}_{rf}(x) = \frac{1}{M} \sum_{m=1}^{M} T_m(x)$ : for classification, make majority vote

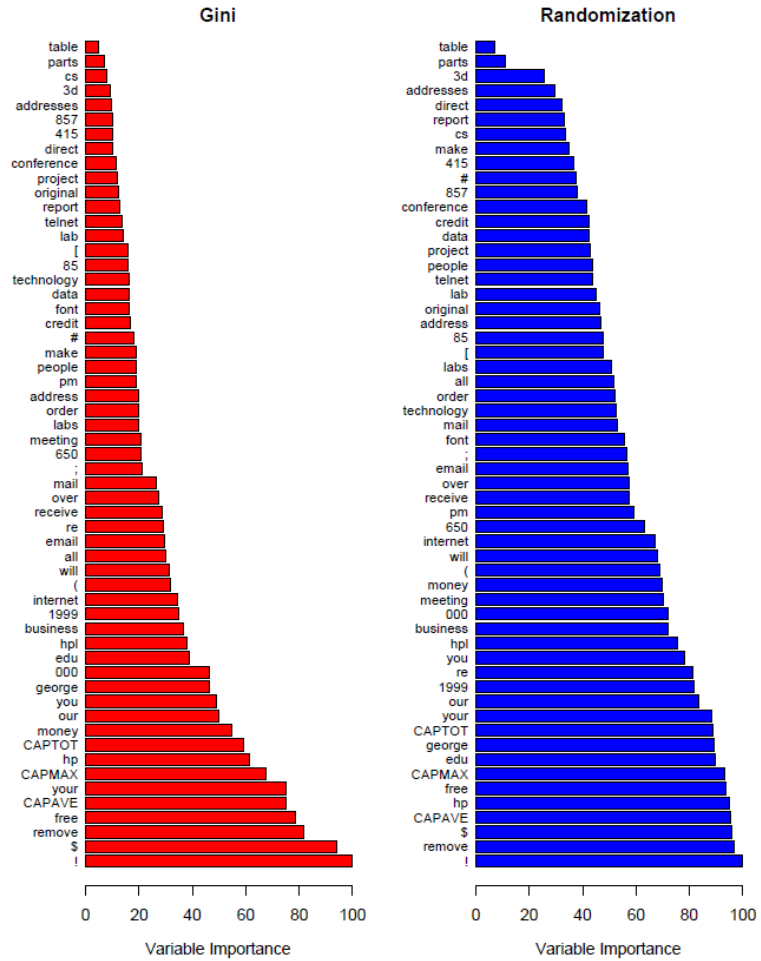
- Small value of $q$ increases the independency of trees ; empirically, $q = \log_2 p + 1$

# Model Evaluation

- Margins : The difference between the percentage of decision trees that correctly classify the samples and the percentage of trees misclassifying the samples
- Out-of-bag (OOB) erros : The observation is called out-of-bag sample to some trees if it is not sampled for those trees. Denote the training set in the $m$-th sampling by $D_m$. OOB error is computed as :
  1. For each observation $(x_i, y_i)$, find the trees which treat it as OOB sample : $\{\hat{T}_m(\mathbf{x}) : (\mathbf{x}_i, y_i) \notin D_m\}$
  2. Use those trees to classify this observation and make majority vote as the label of this observation :
     $\hat{f}_{oob}(\mathbf{x}_i) = \arg\max_{y \in \mathcal{Y}} \sum_{m=1}^{M} \mathrm{I}(\hat{f}_m(\mathbf{x}_i) = y)\mathrm{I}(\mathbf{x}_i \notin D_m)$
  3. Compute the number of misclassified samples, and take the ratio of this number to the total number of samples as OOB error : $Err_{oob} = \frac{1}{N}\sum_{i=1}^{N} \mathrm{I}(\hat{f}_{oob}(\mathbf{x}_i) \neq y_i)$

# Feature Importance

- Using split criteria
  - The improvement in the split-criterion as feature importance
  - It is accumulated over all the trees for each variable
- Using OOB randomization
  - Randomly permute the values of each feature in the OOB samples, and compute the prediction accuracy
  - The decrease in accuracy as a result of this permutation is averaged over all trees as feature importance



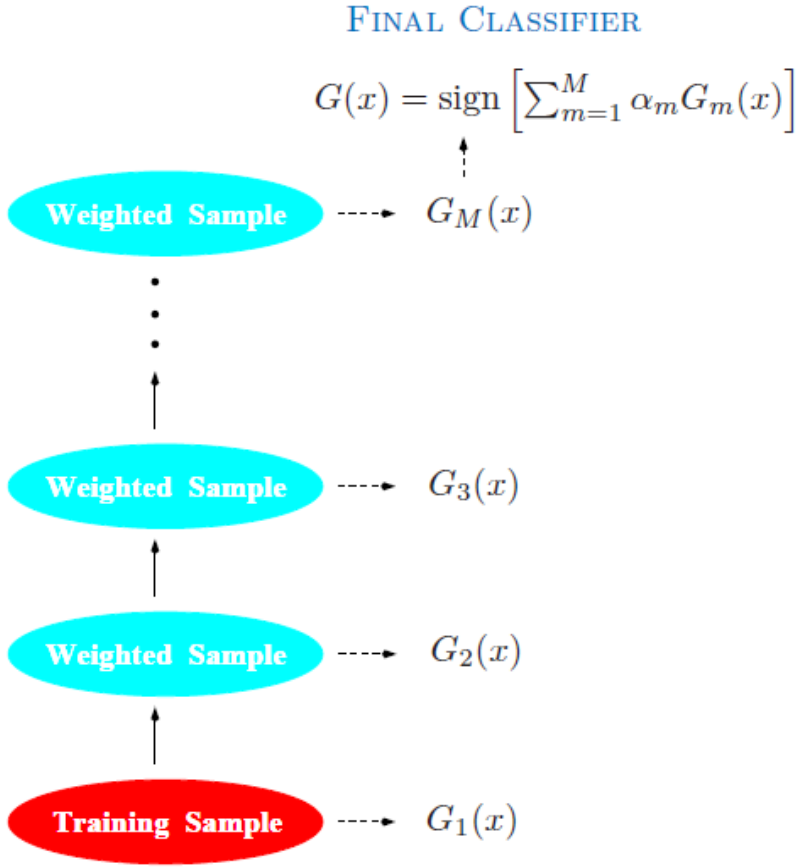
# Pros and Cons

- Where it is good
  - Bagging or random forest (RF) work for models with high variance but low bias
  - Better for nonlinear estimators
  - RF works for very high-dimensional data, and no need to do feature selection as RF gives the feature importance
  - Easy to do parallel computing
- Disadvantage
  - Overfitting when the samples are large-sized with great noise, or when the dimension of data is low
  - Slow computing performance comparing to single tree
  - Hard to interpret

# Outlines

# Boosting

- Boosting : combines the outputs of many "weak" classifiers to produce a powerful "committee"
- Weak classifier : error rate $< 0.5$ (random guessing)
- Sequentially apply the weak classifiers to the repeatedly modified data, emphasizing the misclassified samples
- Combine weak classifiers through a weighted majority vote or averaging to produce the final prediction



# Boosting Fits an Additive Model

- Additive model : $f(x) = \sum_{m=1}^{M} \beta_m b(x; \gamma_m)$
- Possible choices for basis function $b(x; \gamma)$ :
  - Neural networks : $\sigma(\gamma_0 + \gamma_1^T x)$, where $\sigma(t) = 1/(1 + e^{-t})$
  - Wavelets
  - Cubic spline basis
  - Trees
  - Eigenfunctions in reproducing kernel Hilbert space (RKHS)
- Parameter fitting : $\min_{\{\beta_m, \gamma_m\}} \sum_{i=1}^{N} L(y_i, \sum_{m=1}^{M} \beta_m b(x_i; \gamma_m))$
- Loss function : squared error $L(y, f(x)) = (y - f(x))^2$ or likelihood-based loss

# Forward Stagewise Additive Modeling

- Input : training set $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$
- Output : additive model $f_M(x)$

1. Initialize $f_0(x) = 0$
2. For $m = 1$ to $M$ :
   - 2.1 Compute $(\beta_m, \gamma_m) = \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma))$
   - 2.2 Update $f_m(x) = f_{m-1}(x) + \beta_m b(x_i; \gamma_m)$

- Squared error loss : in step 2.1,
  $L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma)) = (\underbrace{y_i - f_{m-1}(x_i)}_{\text{residual}} - \beta b(x_i; \gamma)^2$

# Exponential Loss and AdaBoost

- Exponential loss : $L(y, f(x)) = \exp(-yf(x))$
- Classifier as basis function : $b(x; \gamma) = G(x) \in \{-1, 1\}$
- Let $w_i^{(m)} = \exp(-y_i f_{m-1}(x_i))$, then step 2.1 turns to be :

$$(\beta_m, G_m) = \arg\min_{\beta, G} \sum_{i=1}^{n} w_i^{(m)} \exp(-\beta y_i G(x_i))$$

$$= \arg\min_{\beta, G} \left[ \sum_{y_i \neq G(x_i)} w_i^{(m)} (e^{\beta} - e^{-\beta}) + e^{-\beta} \sum_{i=1}^{n} w_i^{(m)} \right]$$

- $G_m = \arg\min_{G} \sum_{i=1}^{n} w_i^{(m)} I(y_i \neq G(x_i))$.
- $\beta_m = \arg\min_{\beta} \left[ \epsilon_m (e^{\beta} - e^{-\beta}) + e^{-\beta} \right] = \frac{1}{2} \log \frac{1-\epsilon_m}{\epsilon_m}$ where

  $\epsilon_m = (\sum_{i=1}^{n} w_i^{(m)} I(y_i \neq G(x_i))) / \sum_{i=1}^{n} w_i^{(m)}$ is weighted error rate

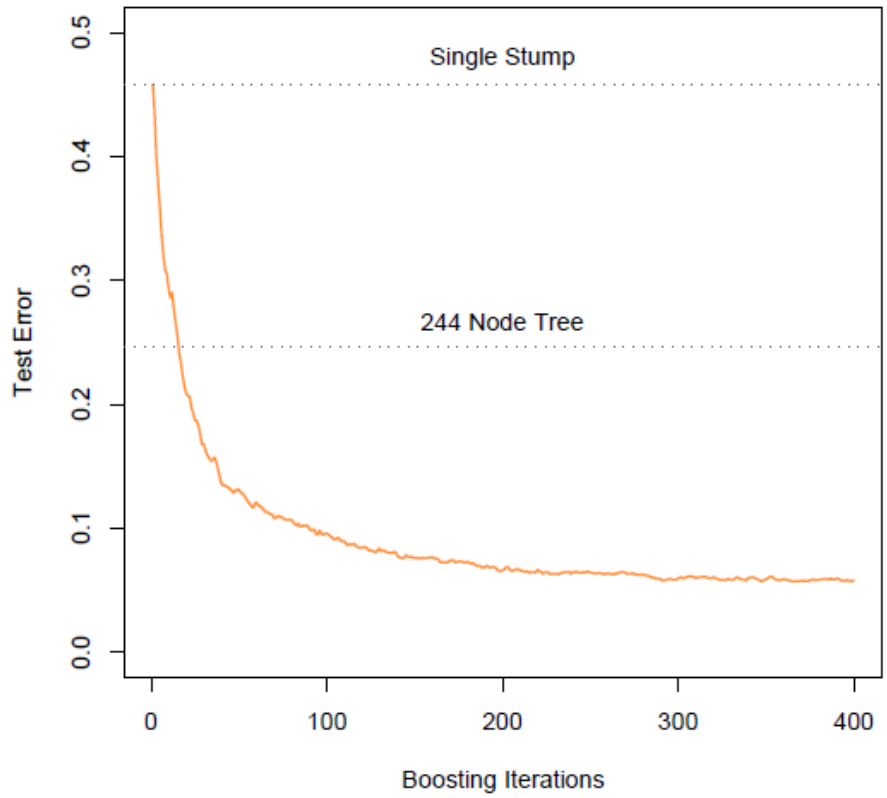
# AdaBoost Algorithm

- Input : training set $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$, loss function $L(y, f(x))$
- Output : Weighted classifier $G(x)$

1. Initialize $w_i = 1/N$, $i = 1, \ldots, N$
2. For $m = 1$ to $M$ :
   - 2.1 Fit a classifier $G_m(x)$ to the training data $D$ with weight $\{w_i\}$
   - 2.2 Compute the error $\epsilon_m = (\sum_{i=1}^{n} w_i^{(m)} I(y_i \neq G(x_i)))/\sum_{i=1}^{n} w_i^{(m)}$
   - 2.3 Compute $\alpha_m = \log \frac{1-\epsilon_m}{\epsilon_m}$ $(\alpha_m = 2\beta_m > 1)$
   - 2.4 Update the weight $w_i^{(m+1)} = w_i^{(m)} \exp(\alpha_m I(y_i \neq G_m(x_i))$, for $i = 1, \ldots, N$
3. Output $G(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m G_m p(x)\right]$

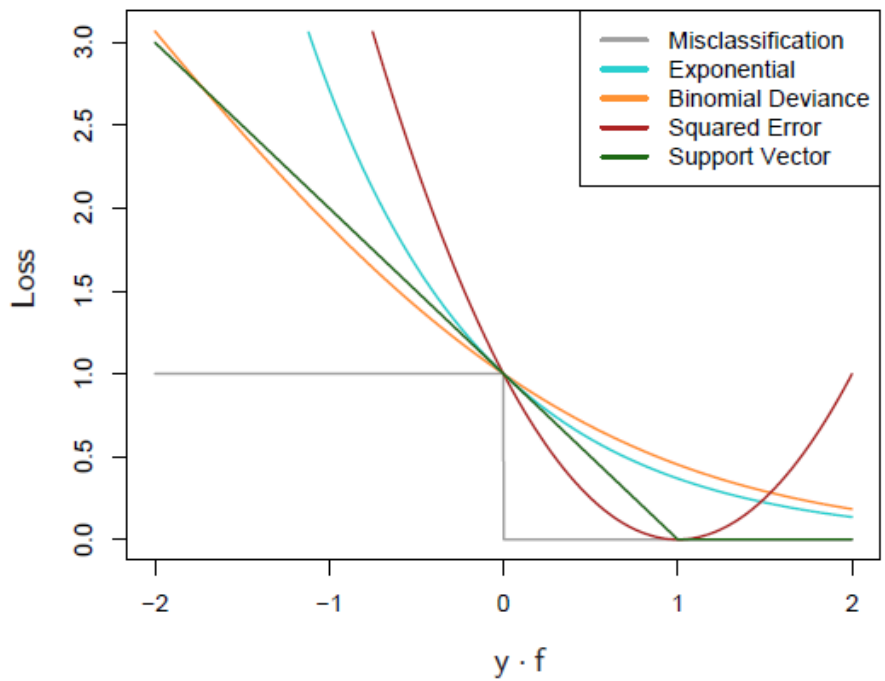
# Illustration

- Weights of weak classifiers : the better the classifier is, the larger its weight is
- Weights of samples : Re-weighting after each step, increase the weights for misclassified samples
- Simulation : 2-class classification, 1000 training samples from each class, 10,000 test samples ; two-leaf classification tree (stump) as base learner



# Loss Functions

- For classification, exponential loss and binomial negative log-likelihood (deviance) loss $\log(1+\exp(-2yf))$ share the same population minimizer ; thus it is equivalent to MLE rule
- For classification, squared error loss is not good (not monotonically decreasing) ; the exponential loss is good and binomial deviance is better (less penalty for large $-yf$)



# Pros and Cons

- Where it is good
  - AdaBoost improve the classification performance comparing to weak classifiers
  - Many choices for weak classifiers : trees, SVMs, kNNs, etc.
  - Only one tuning parameter $M$ : # of weak classifiers
  - prevent overfitting suffered by single weak classifiers (e.g. complex decision tree)
- Disadvantage
  - Weak interpretability
  - Overfitting when using very bad weak classifiers
  - Sensitive to outliers
  - Not easy for parallel computing

# Outlines

# Boosting Tree

- Using classification trees or regression trees as base learners
- $f_M(x) = \sum_{m=1}^{M} T(x; \Theta_m)$ where $T(x; \Theta) = \sum_{j=1}^{J} \gamma_j I(x \in R_j)$
- Parameter set $\Theta = \{R_j, \gamma_j\}_{j=1}^{J}$
- Parameter finding : minimizing the empirical risk

$$\hat{\Theta} = \arg\min_{\Theta} \sum_{j=1}^{J} \sum_{x_i \in R_j} L(y_i, \gamma_j) \qquad \text{(Combinatorial optimizationp)}$$

- Approximate suboptimal solutions :
  1. Finding $\gamma_j$ given $R_j$ : $\gamma_j = \bar{y}_j = \frac{1}{|R_j|} \sum_{y_i \in R_j} y_i$ for $L^2$ loss ; and
     $\gamma_j$ = modal class in $R_j$ for misclassification loss
  2. Finding $R_j$ given $\gamma_j$ : Difficult, need to estimate $\gamma_j$ as well ; greedy, top-down recursive partitioning algorithm

# Boosting Tree as Forward Stagewise Algorithm

- $\hat{\Theta}_m = \arg\min_{\Theta_m} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m))$
  1. $\hat{\gamma}_{jm} = \arg\min_{\gamma_{jm}} \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \gamma_{jm})$
  2. Finding $R_{jm}$ is more difficult than for a single tree in general.
- Squared-error loss : fit a tree to the residual
  $L(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m)) = (\underbrace{y_i - f_{m-1}(x_i)}_{\text{residual}} - T(x_i; \Theta_m))^2$
- Two-class classification and exponential loss : AdaBoost for trees, $\hat{\Theta}_m = \arg\min_{\Theta_m} \sum_{i=1}^{N} w_i^{(m)} \exp[-y_i T(x_i; \Theta_m)]$
  1. $\hat{\gamma}_{jm} = \log \frac{\sum_{x_i \in R_{jm}} w_i^{(m)} I(y_i = 1)}{\sum_{x_i \in R_{jm}} w_i^{(m)} I(y_i = -1)}$
- Absolute error or the Huber loss : robust but slow

# Gradient Descent for General Loss

- Supervised learning is equivalent to the optimization problem

$$\min_f L(f) = \min_f \sum_{i=1}^{N} L(y_i, f(x_i))$$

- Numerical optimization : $\hat{\mathbf{f}} = \arg\min_{\mathbf{f}} L(\mathbf{f})$ where $\mathbf{f} = \{f(x_1), f(x_2), \ldots, f(x_N)\}$,
- Approximate $\hat{\mathbf{f}}$ by $\mathbf{f}_M = \sum_{m=0}^{M} \mathbf{h}_m$, where $\mathbf{f}_0 = \mathbf{h}_0$ is initial guess
- Gradient descent method : $\mathbf{f}_m = \mathbf{f}_{m-1} - \rho_m \mathbf{g}_m$, where $g_{im} = \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x_i)=f_{m-1}(x_i)}$, and $\mathbf{h}_m = -\rho_m \mathbf{g}_m$

# Gradient Boosting Decision Tree (GBDT)

- Find a tree $T(x; \Theta_m)$ by minimization problem

$$\tilde{\Theta}_m = \arg\min_{\Theta_m} \sum_{i=1}^{N} (-g_{im} - T(x_i; \Theta_m))^2$$

In general $\tilde{R}_{jm} \neq R_{jm}$

| Setting | Loss Function | $-\partial L(y_i, f(x_i))/\partial f(x_i)$ |
|---|---|---|
| Regression | $\frac{1}{2}[y_i - f(x_i)]^2$ | $y_i - f(x_i)$ |
| Regression | $\lvert y_i - f(x_i)\rvert$ | $\text{sign}[y_i - f(x_i)]$ |
| Regression | Huber | $y_i - f(x_i)$ for $\lvert y_i - f(x_i)\rvert \leq \delta_m$<br>$\delta_m \text{sign}[y_i - f(x_i)]$ for $\lvert y_i - f(x_i)\rvert > \delta_m$<br>where $\delta_m = \alpha$th-quantile$\{\lvert y_i - f(x_i)\rvert\}$ |
| Classification | Deviance | $k$th component: $I(y_i = \mathcal{G}_k) - p_k(x_i)$ |

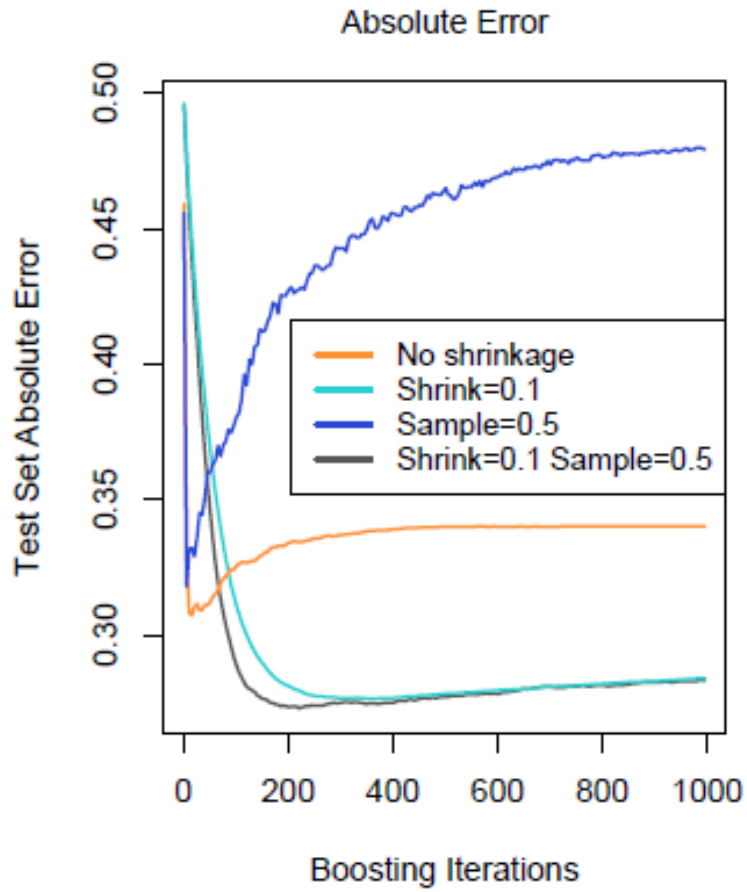
# GBDT Algorithm

- Input : training set $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$, loss function $L(y, f(x))$
- Output : boosting tree $\hat{f}(x)$

1. Initialize $f_0(x) = \arg\min_{\gamma} \sum_{i=1}^{N} L(y_i, \gamma)$
2. For $m = 1$ to $M$ :
   - 2.1 For $i = 1, 2, \ldots, N$ compute $r_{im} = \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}$
   - 2.2 Fit a regression tree to the target (residual) $r_{im}$, giving terminal regions $R_{jm}$, $j = 1, \ldots, J_m$
   - 2.3 For $j = 1, \ldots, J_m$, compute $\gamma_{jm} = \arg\min_{\gamma} \sum_{x_i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \gamma)$
   - 2.4 Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x_i \in R_{jm})$
3. $\hat{f}(x) = f_M(x)$

# Regularization Techniques

- Shrinkage : the step 2.4 is modified as
  $f_m(x) = f_{m-1}(x) +$
  $\nu \sum_{j=1}^{J_m} \gamma_{jm} I(x_i \in R_{jm})$
- Subsampling : at each iteration, sample a fraction $\eta$ of the training set and grow the next tree using the subsample
- Shrinkage + subsampling : best performance



# Feature importance and Partial Dependence Plots

- Feature importance
  - When fitting a single tree $T$, at each node $t$, one feature $X_{v(t)}$ and one separate value $X_{v(t)} = c_{v(t)}$ are chosen to improve a certain quantity of criterion (e.g. GINI, entropy, squared error, etc.)
  - Sum all these improvements $i_t$ brought by each feature $X_k$ over all internal nodes : $I_k(T) = \sum_{t=1}^{J-1} i_t I(v(t) = k)$
  - Average the improvements of all trees $\Rightarrow$ importance of that feature : $I_k = \frac{1}{M} \sum_{m=1}^{M} I_k(T_m)$
- Partial Dependence Plots
  - Partial dependence of $f(X)$ on $X_S$ : $f_S(X_S) = \mathrm{E}_{X_C} f(X_S, X_C)$
  - Estimate by empirical mean : $\bar{f}_S(X_S) = \frac{1}{N} \sum_{i=1}^{N} f(X_S, x_{iC})$

# Pros and Cons

- Where it is good
  - For all regression problems
  - Better for two-class classification, possible for multi-class problems (not suggested)
  - Various nonlinearity, strong representability
- Disadvantage
  - Sequential process, inconvenient for parallel computing
  - High computational complexity, not suitable for high-dimensional problems with sparse features

# Outlines

# Introduction

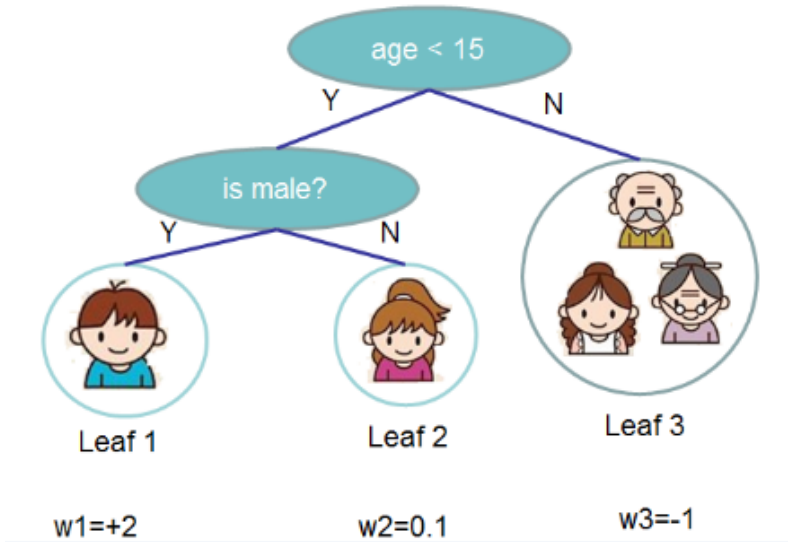
- Developed by Tianqi Chen (http ://homes.cs.washington.edu/∼tqchen/)
- Distributed gradient boosting : can be parallelized
- Highly efficient
- Good performance
- Out-of-Core Computing for big dataset
- Cache Optimization of data structures and algorithms

# Cost Functions

- Cost function :
  $F(\Theta_m) = \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m)) + R(\Theta_m)$, where
  $R(\Theta)$ is regularization term ($L^0$, $L^1$ or $L^2$ penalties)
- Taylor expansion up to second order :
  $F(\Theta_m) \approx \sum_{i=1}^{N} \left[ L(y_i, f_{m-1}(x_i)) + g_i^{(m)} T(x_i; \Theta_m) + \frac{1}{2} h_{ii}^{(m)} T(x_i; \Theta_m)^2 \right] + R(\Theta_m)$, where
  $g_i^{(m)} = \left[ \frac{\partial L(y_i, f(x_i))}{\partial f(x_i)} \right]_{f(x_i)=f_{m-1}(x_i)}$ is the gradient of loss function, and $h_{ii}^{(m)} = \left[ \frac{\partial^2 L(y_i, f(x_i))}{\partial f(x_i)^2} \right]_{f(x_i)=f_{m-1}(x_i)}$ is the diagonal of the Hessian of loss function (off-diagonals are zeros).

# Penalties

- Take regression trees as examples : Let $J_m$ be the number of leaf nodes (number of rectangles in the partition), $\gamma_{jm}$ is the approximate constant (weight $w$) in the leaf node (region) $R_{jm}$
- The complexity of tree is the sum of $L^0$ and $L^2$ norm of $\{\gamma_{jm}\}$ : $R(\Theta_m) = \frac{1}{2}\lambda \sum_{j=1}^{J_m} \gamma_{jm}^2 + \mu J_m$




$$R = \frac{1}{2}\lambda(4 + 0.01 + 1) + 3\mu$$

# Optimal solutions

- Reformulation of approximated cost function :

$$F(\Theta_m) \approx \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i)) + \sum_{j=1}^{J_m} \left[ \left( \sum_{x_i \in R_{jm}} g_i^{(m)} \right) \gamma_{jm} + \frac{1}{2} \left( \sum_{x_i \in R_{jm}} h_{ii}^{(m)} + \lambda \right) \gamma_{jm}^2 \right] + \mu J_m =$$

$$\sum_{j=1}^{J_m} \left[ G_j^{(m)} \gamma_{jm} + \frac{1}{2} (H_j^{(m)} + \lambda) \gamma_{jm}^2 \right] + \mu J_m + constant, \text{ where}$$

$$G_j^{(m)} = \sum_{x_i \in R_{jm}} g_i^{(m)} \text{ and } H_j^{(m)} = \sum_{x_i \in R_{jm}} h_{ii}^{(m)}$$

- By differentiation w.r.t. $\gamma_{jm}$, we have the optimal solution :

$$\hat{\gamma}_{jm} = -\frac{G_j^{(m)}}{H_j^{(m)} + \lambda}$$

- Simplified cost function :

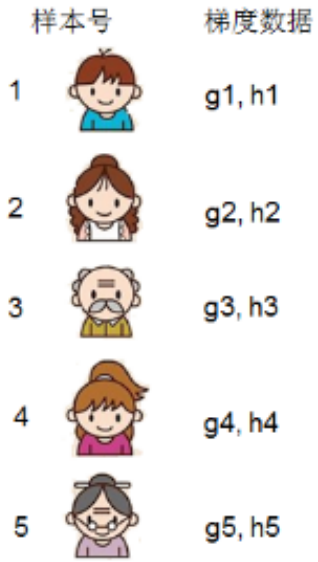
$$F(\Theta_m) = -\frac{1}{2} \sum_{j=1}^{J_m} \frac{(G_j^{(m)})^2}{H_j^{(m)} + \lambda} + \mu J_m + constant$$

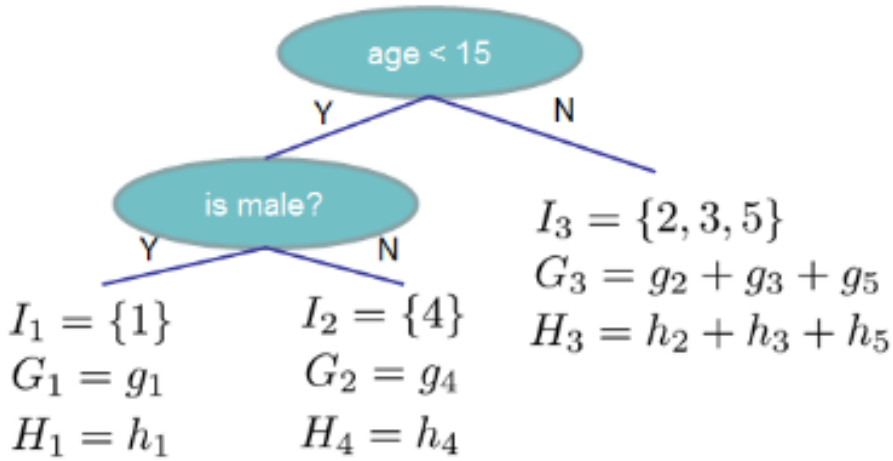
# Structure Score

- Neglecting the constant term, we obtain the structure score :

$$SS = -\frac{1}{2}\sum_{j=1}^{J_m}\frac{(G_j^{(m)})^2}{H_j^{(m)}+\lambda} + \mu J_m$$

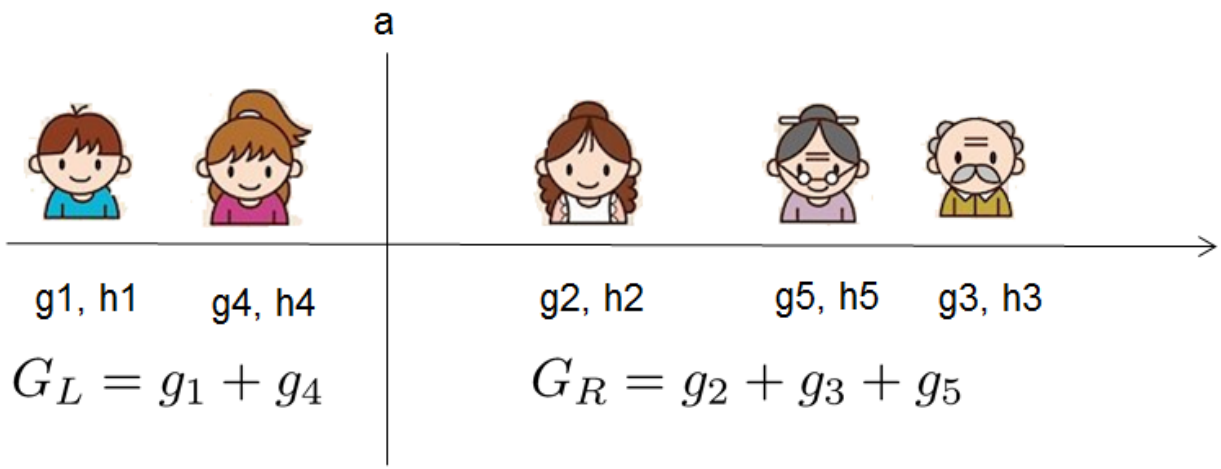
- It is similar to information gain : minimizing the structure score leads to the best tree



# Node Splitting - Greedy Algorithm

- When splitting a node into left (L) and right (R) child nodes, we are maximizing $Gain = \frac{1}{2}\left[\frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{(G_L+G_R)^2}{H_L+H_R+\lambda}\right] - \gamma$
- Enumerate all possible splits at $x < a$ (e.g., age$<$ 15) from left to right



# Greedy Algorithm for split finding

- Input : training set $D = \{(x_1, y_1), \ldots, (x_N, y_N)\}$, loss function $L(y, f(x))$, the index set $I = \{i | x_i \in R_{jm}\}$ of current node $R_{jm}$, feature dimension $d$
- Output : best split

1. Initialize $gain = 0$, $G = \sum_{i \in I} g_i$, $H = \sum_{i \in I} h_{ii}$
2. For $k = 1$ to $K$ :
   - 2.1 $G_L = 0$, $H_L = 0$
   - 2.2 For $j$ in sorted($I$, by $x_{jk}$), do
     - 2.2.1 $G_L = G_L + g_j$, $H_L = H_L + h_{jj}$, $G_R = G - G_L$, $H_R = H - H_L$
     - 2.2.2 $score = \max(score, \frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{G^2}{H + \lambda})$
3. Output split with max score

# Loss Functions

- Square loss $L(y, f) = (y - f)^2$ :
  $g_i^{(m)} = 2(f_i - y_i) = 2 \times \mathit{residue}$, $h_{ii}^{(m)} = 2$
- Logistic loss $L(y, f) = y \ln(1 + e^{-f}) + (1 - y) \ln(1 + e^{f})$ :
  $g_i^{(m)} = -y_i \left(1 - \frac{1}{1+e^{-f_{m-1}(x_i)}} + (1 - y_i) \frac{1}{1+e^{-f_{m-1}(x_i)}}\right) =$
  $\mathit{Pred} - \mathit{Label}$, $h_{ii}^{(m)} = \frac{e^{-f_{m-1}(x_i)}}{(1+e^{-f_{m-1}(x_i)})^2} = \mathit{Pred} \times (1 - \mathit{Pred})$

# Outlines

# Conclusions

- Ensemble methods have integrable abilities of single models, achieving better performance
- Easy to generalize to new data
- When there are strong noises, easy to overfit
- Computationally intensive

# Python Examples

- Random forest :

```
from sklearn.ensemble import RandomForestClassifier
rf = RandomForestClassifier(n_estimators=100)
# RandomForestClassifier(bootstrap=True, class_weight=None,
    pcriterion='gini', max_depth=None, max_features='auto',
    max_leaf_nodes=None, min_impurity_split=1e-07,
    min_samples_leaf=1, min_samples_split=2,
    min_weight_fraction_leaf=0.0, n_estimators=100,
    n_jobs=1, oob_score=False, random_state=None,
    verbose=0, warm_start=False)
# Feature importance in random forest
feature_imp = pd.Series(rf.feature_importances_)
rf.fit(X_train,Y_train)
Y_predict_rf = rf.predict(X_test)
oob_error = 1 - rf2.oob_score_
```

- AdaBoost :

```
from sklearn.ensemble import AdaBoostClassifier
adaboost = AdaBoostClassifier(n_estimators = 50)
adaboost.fit(X_train,Y_train)
adaboost.staged_predict(X_train)
Y_predict_ada = adaboost.predict(X_test)
```

# References


- 数据分析导论，博雅大数据学院
- 周志华，机器学习，2016
- T. Hastie, R. Tibshirani, and J. Friedman, The Elements of Statistical Learning : Data mining, Inference, and Prediction, 2nd Edition, 2009