

Introduction to Big Data Analysis Ensemble Methods

Zhen Zhang

Southern University of Science and Technology

Outlines

Introduction

Bagging and Random Forest

Boosting and AdaBoost

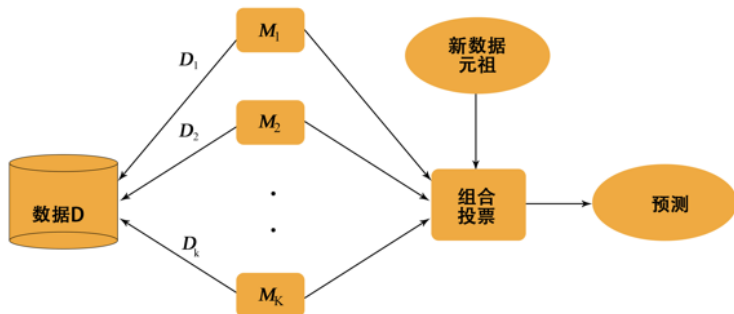
Gradient Boosting Decision Tree

XGBoost

Conclusion and Python Examples

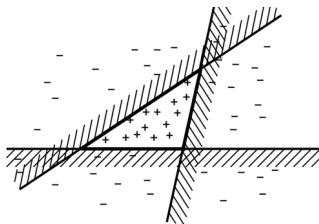
Ensemble Methods

- 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 misclassification rate
 - Misclassification 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

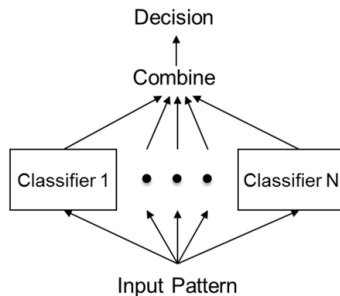
Two commonly used ensemble methods

- 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



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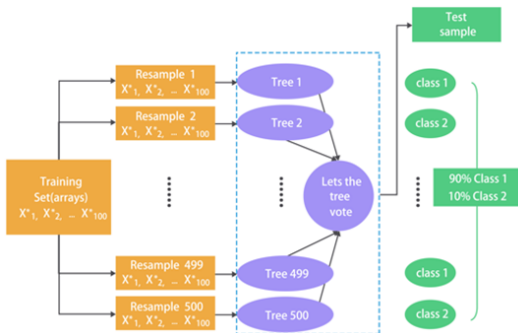
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Conclusion and Python Examples

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 $m = 1, \dots, M$, 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 $\lim_{n \rightarrow \infty} (1 - \frac{1}{n})^n = 0.368$.

Algorithm

- Input : training set $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$
 - 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

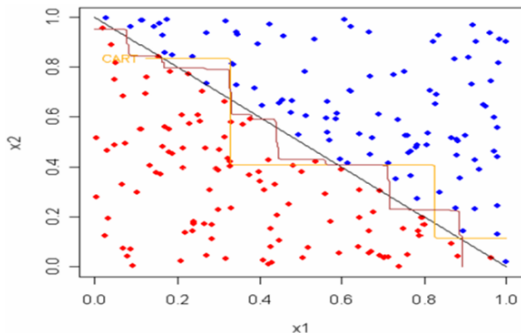
- In bagging, we use the same model to train different sample set in each iteration ; assume the models $\{\hat{f}_m(x)\}_{m=1}^M$ have the same variance $\sigma^2(x)$, while the correlation of each pair is $\rho(x)$
- Then the variance of the final model is :

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

- As $M \rightarrow \infty$, $\text{Var}(\hat{f}_{bag}(x)) \rightarrow \rho(x) \sigma^2(x)$. 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 $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$
- 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,

$$\hat{f}_{rf}(x) = \frac{1}{M} \sum_{m=1}^M T_m(x) : \text{for classification, make majority vote}$$

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

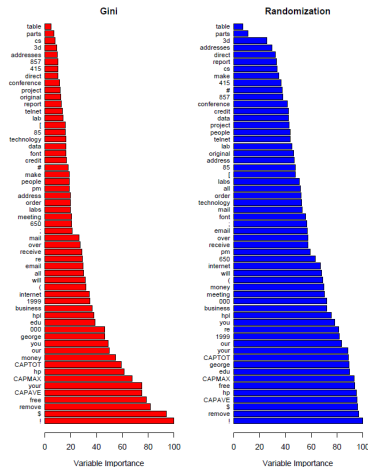
Model Evaluation

- 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) errors : 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 (\mathbf{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 :

$$\hat{f}_{oob}(\mathbf{x}_i) = \arg \max_{y \in \mathcal{Y}} \sum_{m=1}^M \mathbb{I}(\hat{f}_m(\mathbf{x}_i) = y) \mathbb{I}(\mathbf{x}_i \notin D_m)$$
 3. Compute the number of misclassified samples, and take the ratio of this number to the total number of samples as OOB error : $Err_{oob} = \frac{1}{N} \sum_{i=1}^N \mathbb{I}(\hat{f}_{oob}(\mathbf{x}_i) \neq y_i)$

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

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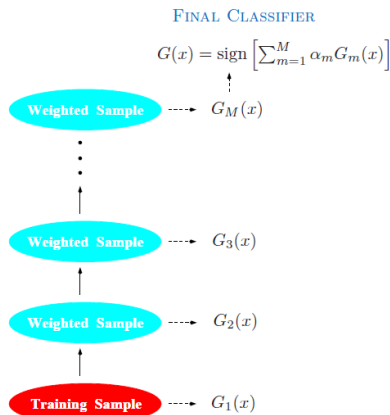
Gradient Boosting Decision Tree

XGBoost

Conclusion and Python Examples

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 $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$
- 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 $f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$

- 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 :

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

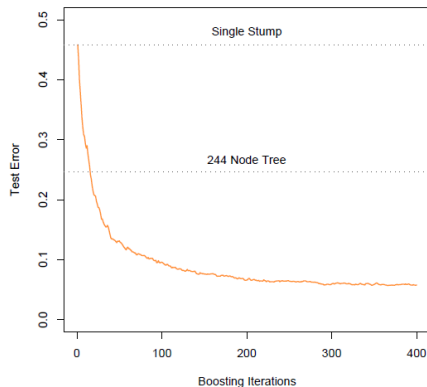
- $G_m = \arg \min_G \sum_{i=1}^n w_i^{(m)} I(y_i \neq G(x_i))$.
- $\beta_m = \arg \min_{\beta} \left[\epsilon_m (e^\beta - e^{-\beta}) + e^{-\beta} \right] = \frac{1}{2} \log \frac{1-\epsilon_m}{\epsilon_m}$ where
 $\epsilon_m = (\sum_{i=1}^n w_i^{(m)} I(y_i \neq G(x_i))) / \sum_{i=1}^n w_i^{(m)}$ is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

AdaBoost Algorithm

- Input : training set $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$, loss function $L(y, f(x))$
 - Output : Weighted classifier $G(x)$
1. Initialize $w_i = 1/N$, $i = 1, \dots, N$
 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 $\epsilon_m = (\sum_{i=1}^n w_i^{(m)} I(y_i \neq G_m(x_i))) / \sum_{i=1}^n w_i^{(m)}$
 - 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 $i = 1, \dots, N$
 3. Output $G(x) = \text{sign} \left[\sum_{m=1}^M \alpha_m G_m(x) \right]$

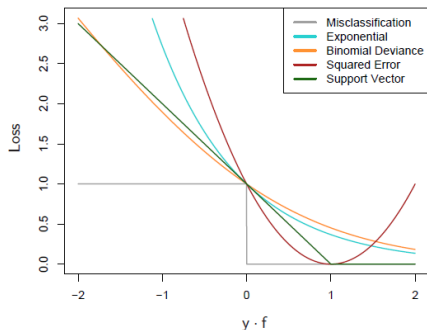
Illustration

- 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

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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

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

- Approximate suboptimal solutions :
 1. Finding γ_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
 $\gamma_j = \text{modal class in } R_j$ for misclassification loss
 2. Finding R_j given γ_j : Difficult, need to estimate γ_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

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

- Numerical optimization : $\hat{\mathbf{f}} = \arg \min_{\mathbf{f}} L(\mathbf{f})$ where $\mathbf{f} = \{f(x_1), f(x_2), \dots, f(x_N)\}$,
- 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 $\mathbf{g}_{im} = \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)} \right]_{f(x_i)=f_{m-1}(x_i)}$, 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	$ y_i - f(x_i) $	$\text{sign}[y_i - f(x_i)]$
Regression	Huber	$y_i - f(x_i)$ for $ y_i - f(x_i) \leq \delta_m$ $\delta_m \text{sign}[y_i - f(x_i)]$ for $ y_i - f(x_i) > \delta_m$ where $\delta_m = \alpha \text{th-quantile}\{ y_i - f(x_i) \}$
Classification	Deviance	k th component: $I(y_i = \mathcal{G}_k) - p_k(x_i)$

GBDT Algorithm

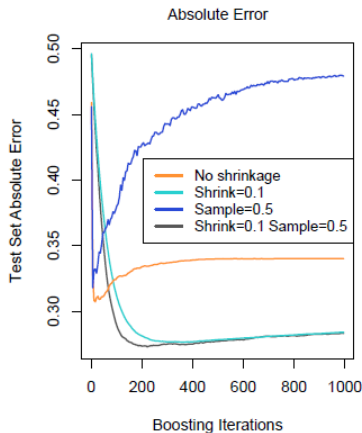
- Input : training set $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$, loss function $L(y, f(x))$
- Output : boosting tree $\hat{f}(x)$

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 $i = 1, 2, \dots, N$ 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 $R_{jm}, j = 1, \dots, J_m$
 - 2.3 For $j = 1, \dots, J_m$, 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 η 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 : $f_S(X_S) = E_{X_C} f(X_S, X_C)$
 - 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

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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 :

$$F(\Theta_m) = \sum_{i=1}^N L(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m)) + R(\Theta_m), \text{ where}$$

$R(\Theta)$ is regularization term (L^0 , L^1 or L^2 penalties)

- Taylor expansion up to second order :

$$F(\Theta_m) \approx \sum_{i=1}^N \left[L(y_i, f_{m-1}(x_i)) + g_i^{(m)} T(x_i; \Theta_m) + \frac{1}{2} h_{ii}^{(m)} T(x_i; \Theta_m)^2 \right] + R(\Theta_m), \text{ where}$$

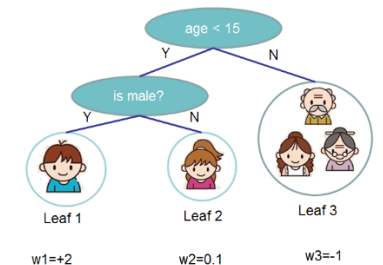
$$g_i^{(m)} = \left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)} \right]_{f(x_i)=f_{m-1}(x_i)}$$

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), γ_{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 :

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

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

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

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

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

- Simplified cost function :






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

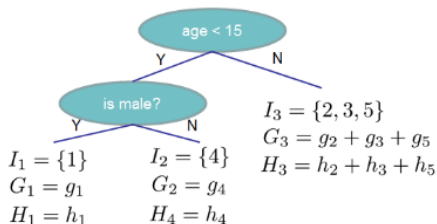
Structure Score

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

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

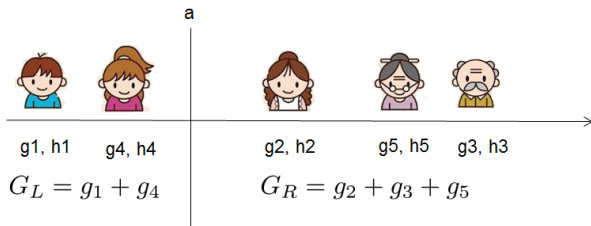
- It is similar to information gain : minimizing the structure score leads to the best tree

样本号	梯度数据
1 	g_1, h_1
2 	g_2, h_2
3 	g_3, h_3
4 	g_4, h_4
5 	g_5, h_5



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 $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$, 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 $gain = 0$, $G = \sum_{i \in I} g_i$, $H = \sum_{i \in I} h_{ij}$
 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 $L(y, f) = (y - f)^2$:
 $g_i^{(m)} = 2(f_i - y_i) = 2 \times \text{residue}$, $h_{ii}^{(m)} = 2$
- Logistic loss $L(y, f) = y \ln(1 + e^{-f}) + (1 - y) \ln(1 + e^f)$:
 $g_i^{(m)} = -y_i \left(1 - \frac{1}{1 + e^{-f_{m-1}(x_i)}} + (1 - y_i) \frac{1}{1 + e^{-f_{m-1}(x_i)}} \right) =$
 $\text{Pred} - \text{Label}$, $h_{ii}^{(m)} = \frac{e^{-f_{m-1}(x_i)}}{(1 + e^{-f_{m-1}(x_i)})^2} = \text{Pred} \times (1 - \text{Pred})$

Outlines

Introduction

Bagging and Random Forest

Boosting and AdaBoost

Gradient Boosting Decision Tree

XGBoost

Conclusion and Python Examples

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

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- 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