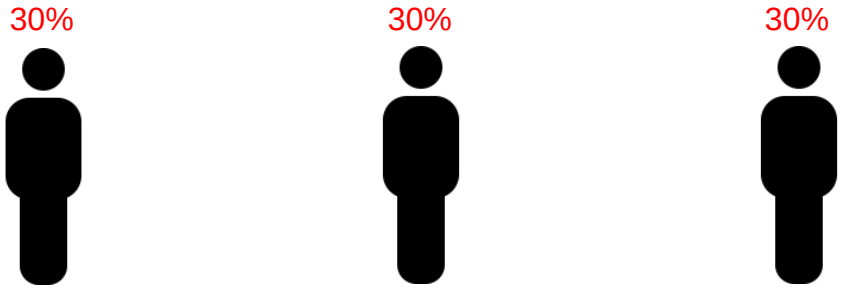
CSC411- Ensemble methods
Gradient Boost Tree

What is ensemble ?

Why ensemble?

When three people are walking together,
I am sure to find teachers among them.

Three stooges equal to one master



Ensemble error rate = $\binom{2}{3}(0.3)^2(0.7)^1 + \binom{3}{3}(0.3)^3(0.7)^0 = 21.6\%$

- If the individual error rate is 60% , then the ensemble error rate = 64.8%
- Ensemble error rate reduce to 2.6% (individual 30%) or increase to 82.6%(individual 60%) if there are 21 person.
- We want each individual accurate and make different errors.

Type of ensemble methods

Bayesian voting

Bagging
(bootstrapping aggregation)

Boosting

Stacking

Recap: Supervised Learning

- Notations: $x_i \in \mathbf{R}^d$ i-th training example
- **Model**: how to make prediction $\hat{y}_i$ given x_i
  - Linear model: $\hat{y}_i = \sum_j w_j x_{ij}$ (include linear/logistic regression)
  - The prediction score $\hat{y}_i$ can have different interpretations depending on the task
    - Linear regression: $\hat{y}_i$ is the predicted score
    - Logistic regression: $1/(1+exp(-\hat{y}_i))$ is predicted the probability of the instance being positive
    - Others… for example in ranking $\hat{y}_i$ can be the rank score
- **Parameters**: the things we need to learn from data
  - Linear model: $\Theta = \{w_j | j = 1, \cdots, d\}$

Objective Function

- Objective function that is everywhere

$$Obj(\Theta) = L(\Theta) + \Omega(\Theta)$$

Training Loss measures how well model fit on training data

Regularization, measures complexity of model

- Loss on training data: $L = \sum_{i=1}^{n} l(y_i, \hat{y}_i)$
  - Square loss: $l(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$
  - Logistic loss: $l(y_i, \hat{y}_i) = y_i \ln(1 + e^{-\hat{y}_i}) + (1 - y_i) \ln(1 + e^{\hat{y}_i})$
- Regularization: how complicated the model is?
  - L2 norm: $\Omega(w) = \lambda \|w\|^2$
  - L1 norm (lasso): $\Omega(w) = \lambda \|w\|_1$

Objective Function - GBT

- 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, to find f (since they are trees, instead of just numerical vectors)
- 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

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

Our New Goal

- Objective, with constants removed

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

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

- Why spending so much efforts to derive the objective, why not just grow trees …
  - Theoretical benefit: know what we are learning, convergence
  - **Engineering** benefit, recall the elements of supervised learning
    - g_i and h_i comes from definition of loss function
    - The learning of function only depend on the objective via g_i and h_i
    - Think of how you can separate modules of your code when you are asked to implement boosted tree for both square loss and logistic loss

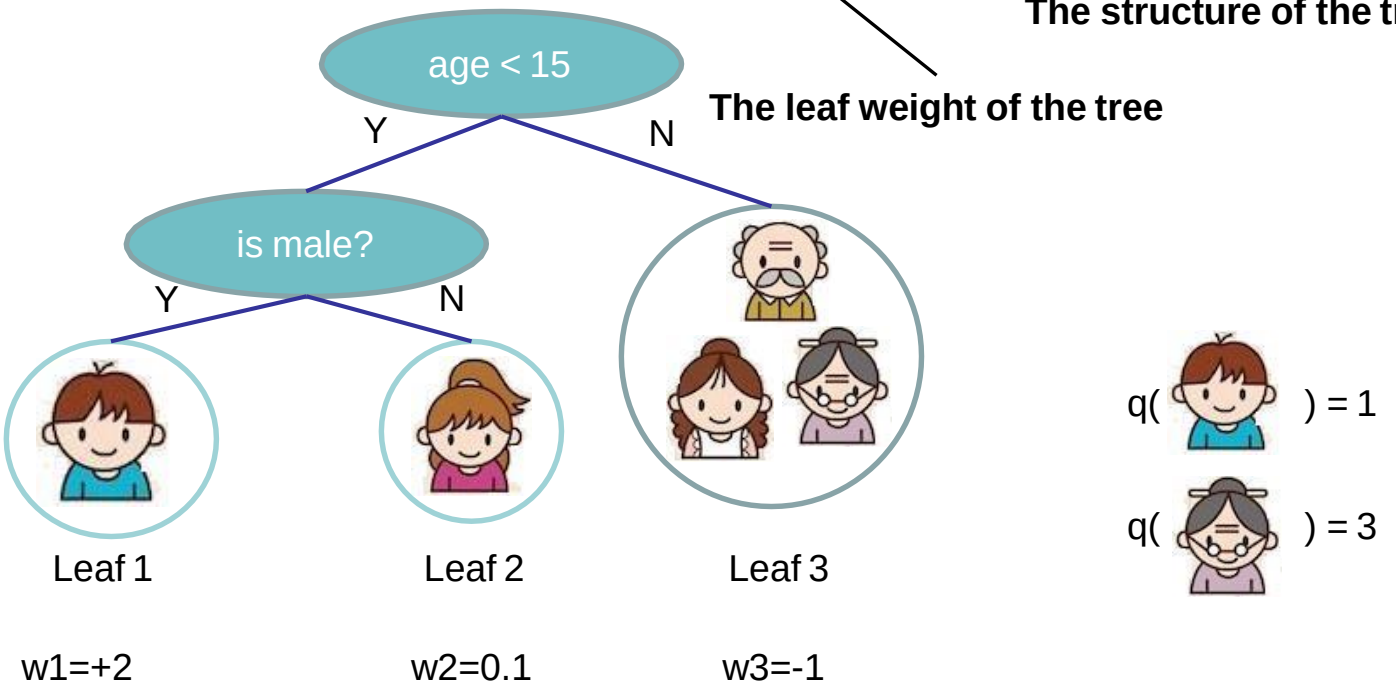
Refine the definition of tree

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

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

The structure of the tree

The leaf weight of the tree

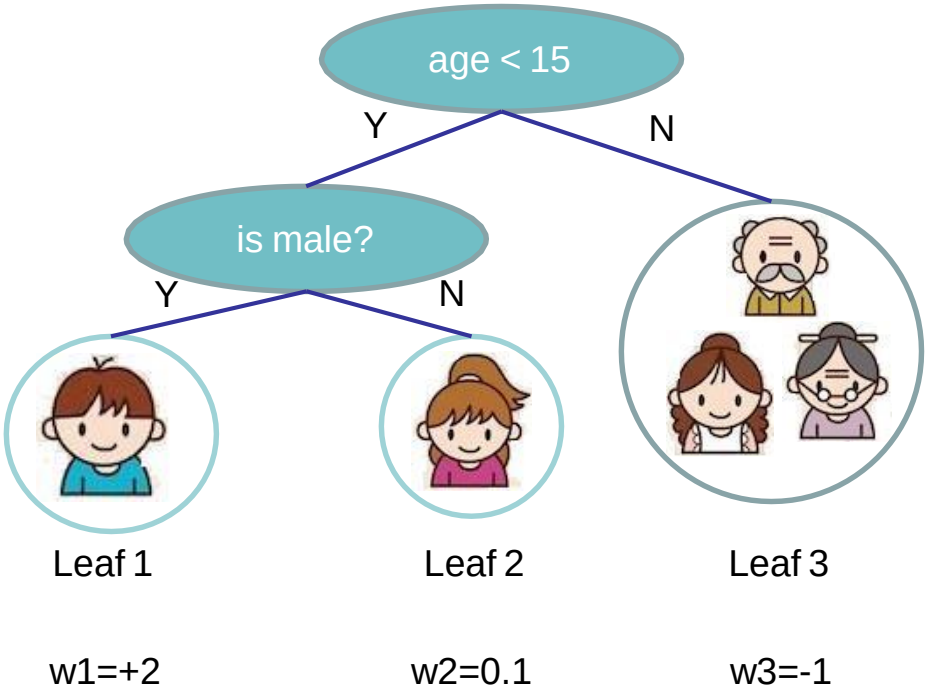


Define Complexity of a Tree

- Define complexity as (this is not the only possible definition)

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

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



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

Revisit the Objectives

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

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

- This is sum of T independent quadratic functions

The Structure Score

- Two facts about single variable quadratic function

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

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

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

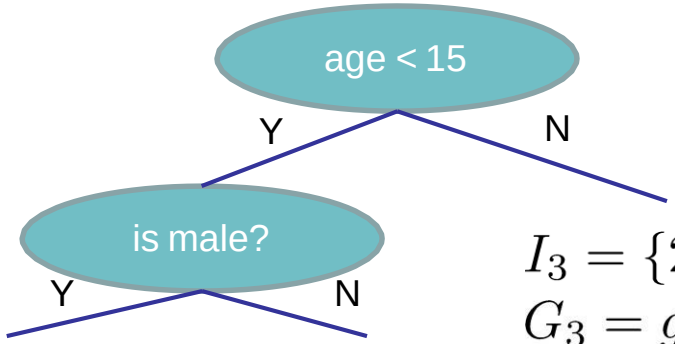
- Assume the structure of tree (q(x)) is fixed, the optimal weight in each leaf, and the resulting objective value are

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

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



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

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

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

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

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 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

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

The complexity cost by introducing additional leaf

the score of left child

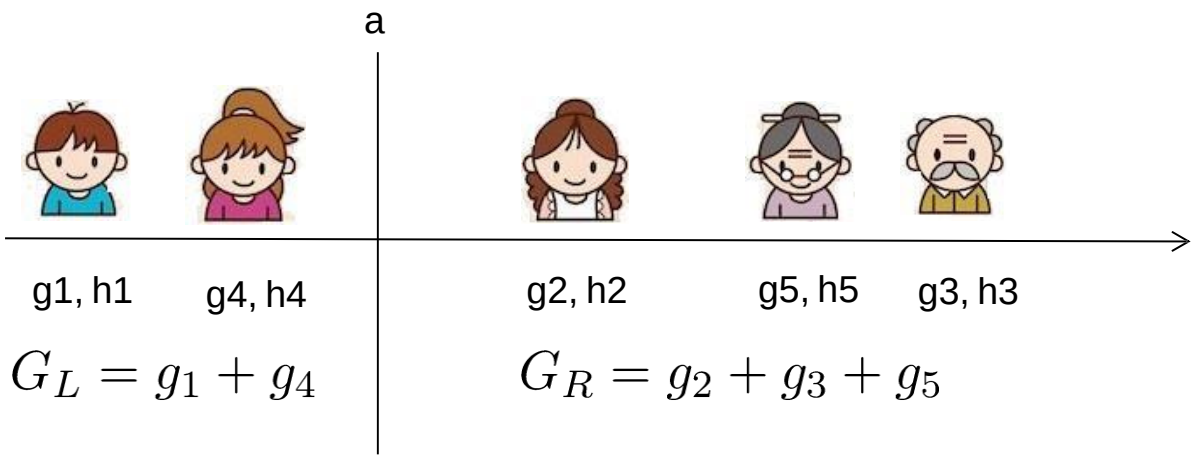
the score of right child

the score of if we do not split

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

Efficient Finding of the Best Split

- 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

An Algorithm for Split Finding

- 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

- Time Complexity growing a tree of depth K
  - It is O(n d K log n): or each level, need O(n log n) time to sort
    There are d features, and we need to do it for K level
  - This can be further optimized (e.g. use approximation or caching the sorted features)
  - Can scale to very large dataset

What about Categorical Variables?

- Some tree learning algorithm handles categorical variable and continuous variable separately
  - We can easily use the scoring formula we derived to score split based on categorical variables.
- Actually it is not necessary to handle categorical separately.
  - We can encode the categorical variables into numerical vector using one-hot encoding. Allocate a #categorical length vector

$$z_j = \begin{cases} 1 & \text{if } x \text{ is in category } j \\ 0 & otherwise \end{cases}$$

  - The vector will be sparse if there are lots of categories, the learning algorithm is preferred to handle sparse data

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 predictivness
- 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

Recap: 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