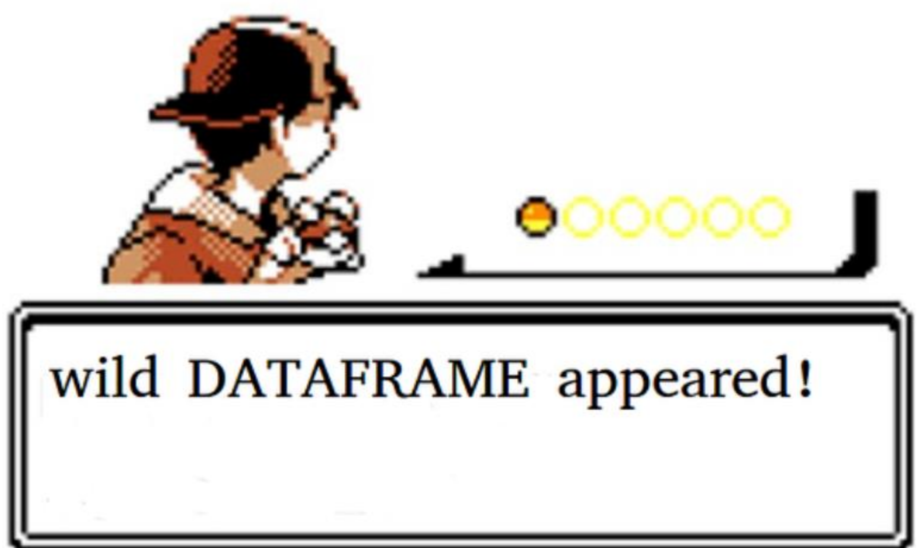
CISC 372
Advanced Data Analytics
L9 Gradient Boosting

	name	age	state	num_children	num_pets
0	john	23	iowa	2	0
1	mary	78	dc	2	4
2	peter	22	california	0	0
3	jeff	19	texas	1	5
4	bill	45	washington	2	0
5	lisa	33	dc	1	0



Tree[s]

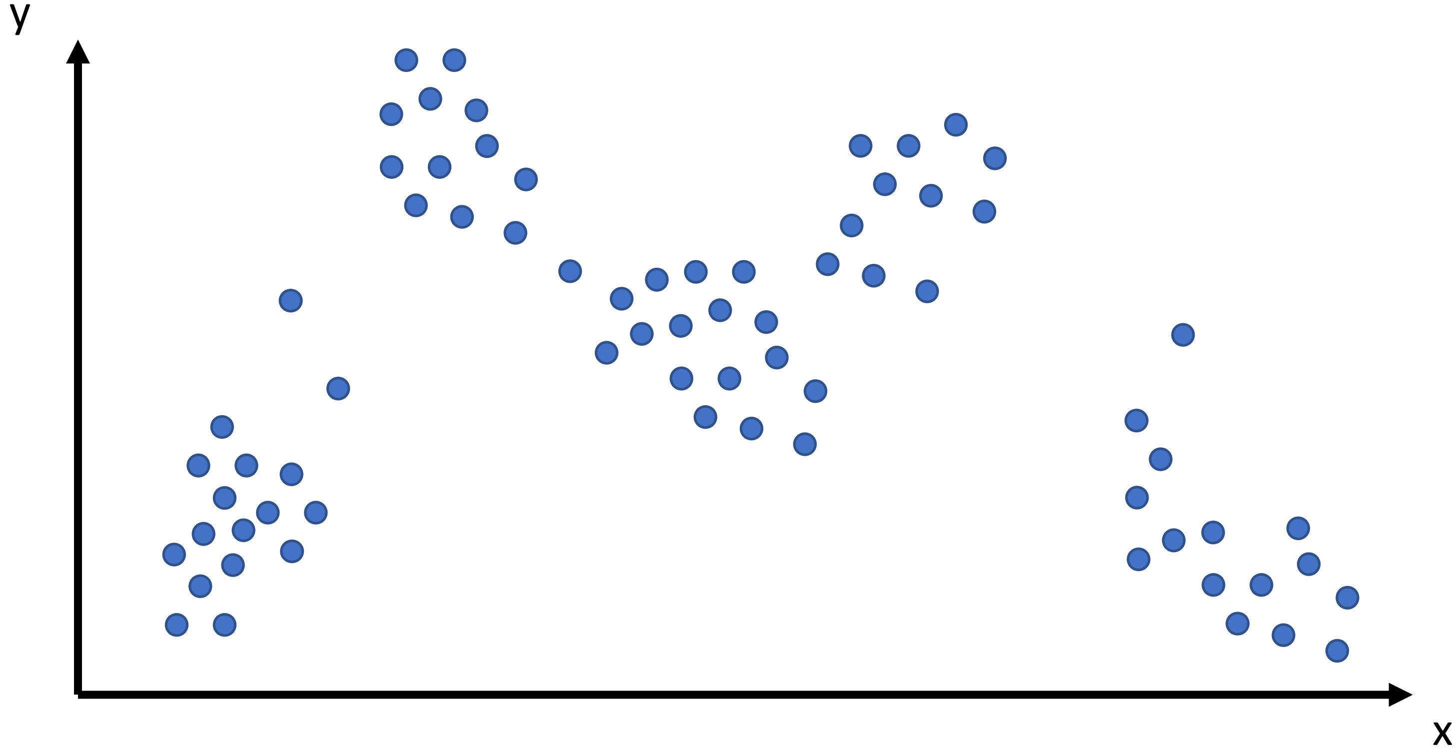
- Tree Induction
- Information Gain
- Gain Ratio (regularized information gain)
- Gini Index
- ID3, CART, C4.5
- Splitting Numeric Attribute
- Feature Selection (is difficult)
- Random Forest (the easy way)
  - Built-in bootstrap sampling

Today

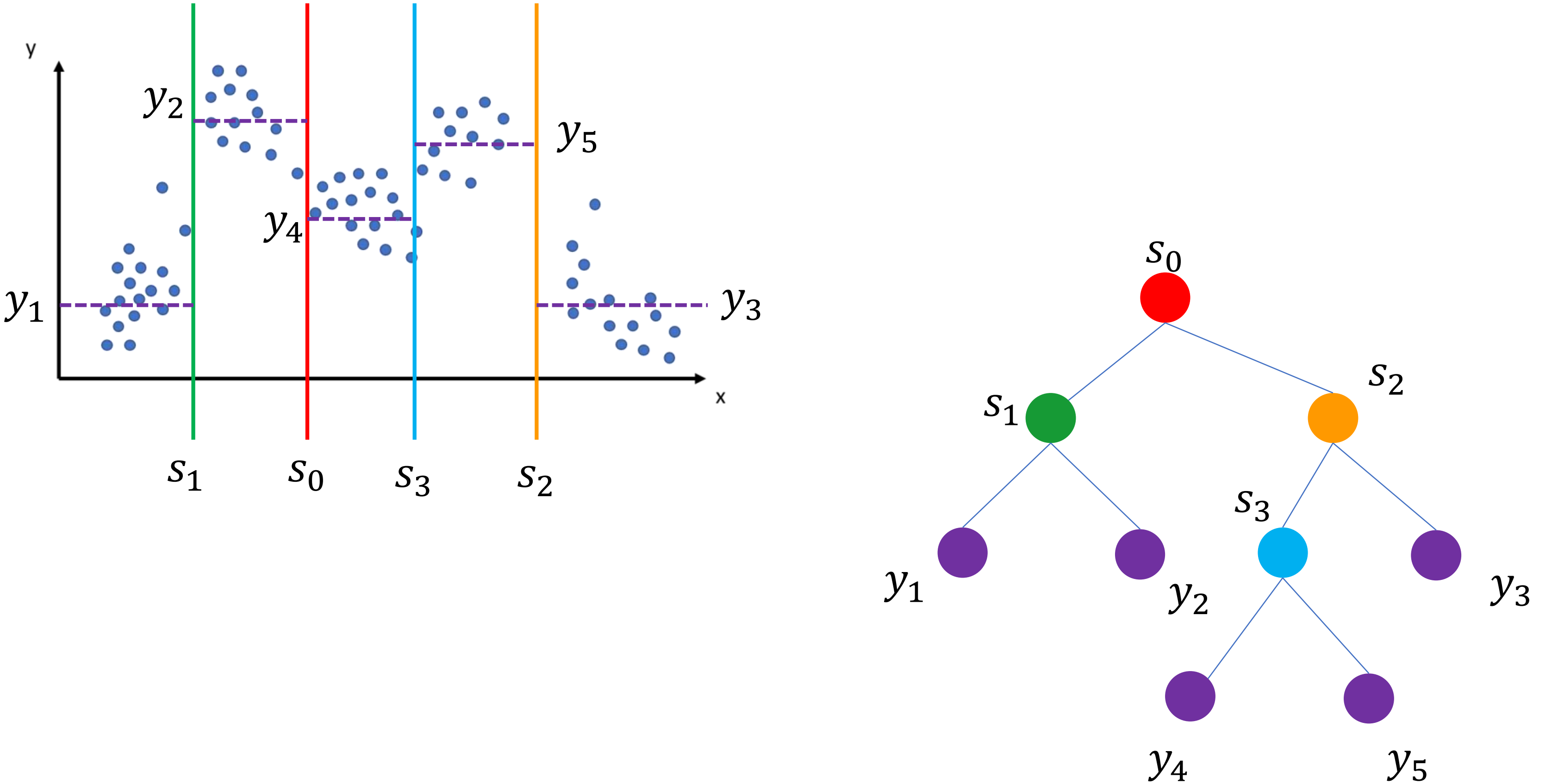
- Regression Tree (with CART)
- Tree Boosting
- XGBoost

Regression Tree (with CART)

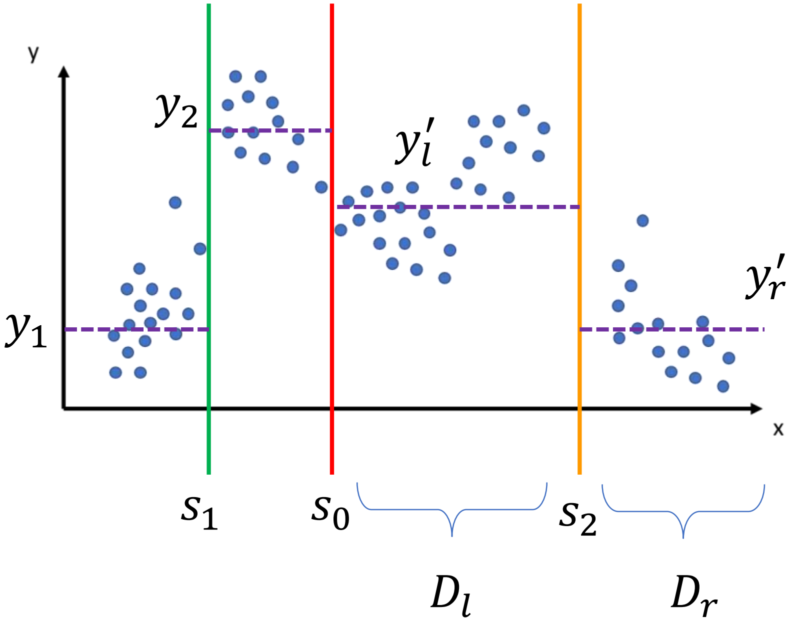
- When your class label and attributes are numeric data

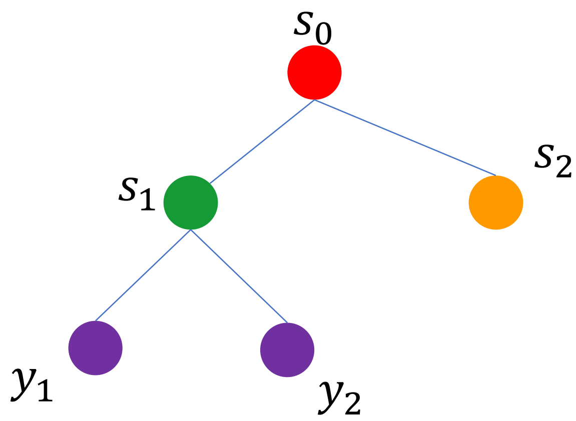


CART – Binary Tree



Regression Tree (with CART)

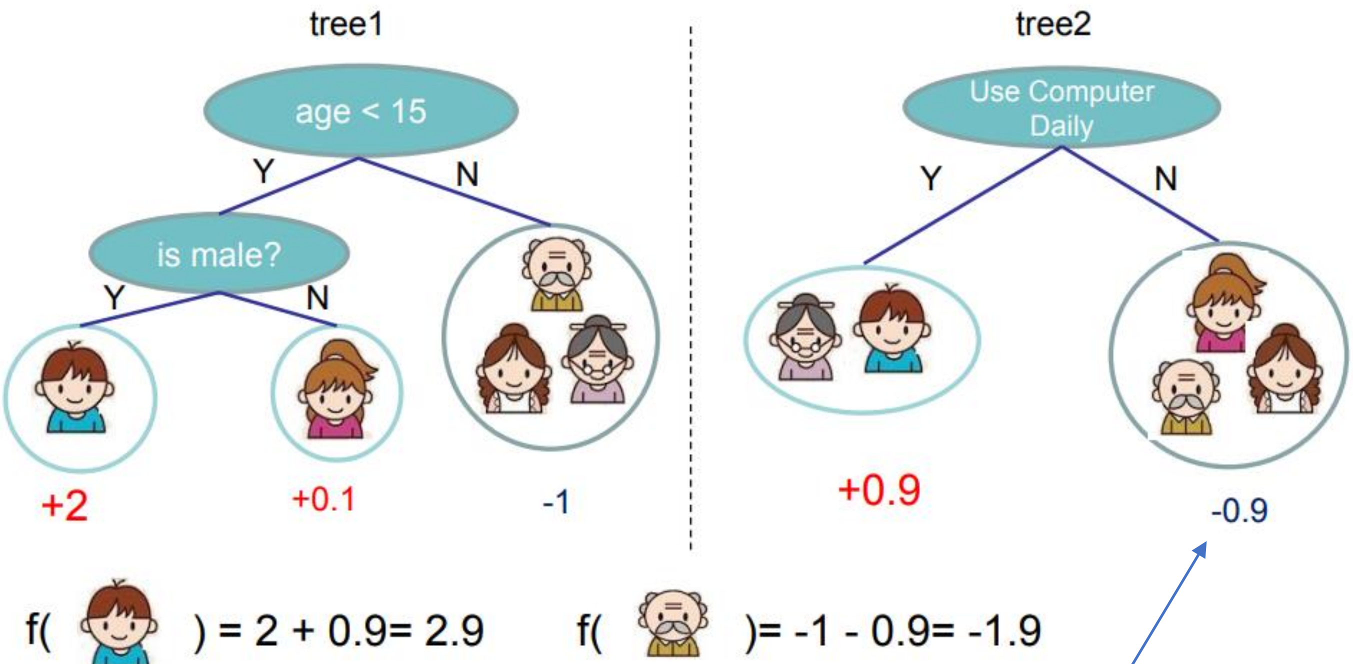




$$SSE = \sum_{i \in D_l} (y_i - y_l')^2 + \sum_{i \in D_r} (y_i - y_r')^2$$

Breiman, Leo, et al. Classification and regression trees. CRC press, 1984.

Tree Ensemble (Regression)

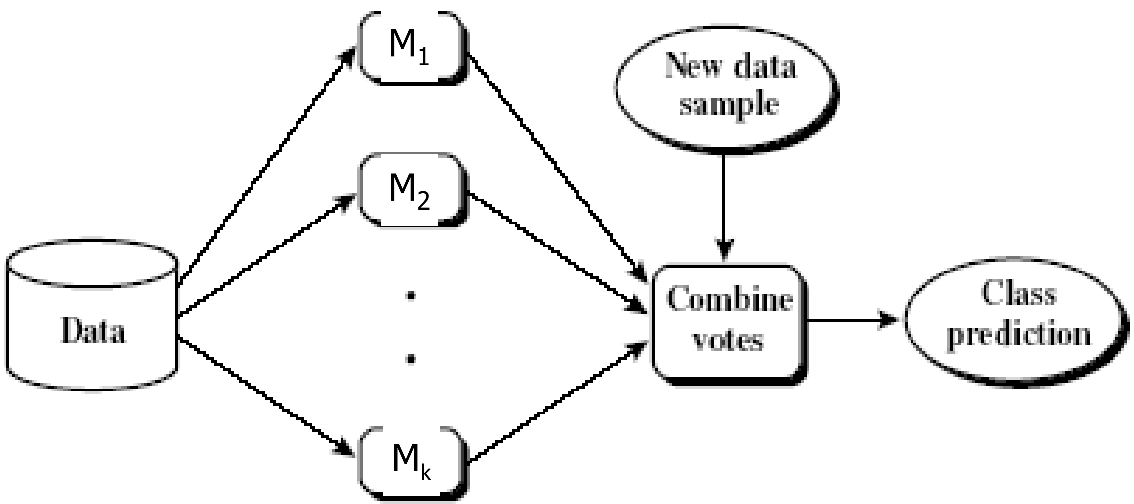


$$\hat{y}_i = \phi(\mathbf{x}_i) = \sum_{k=1}^{K} f_k(\mathbf{x}_i), \quad f_k \in \mathcal{F}, \quad \mathcal{F} = \{f(\mathbf{x}) = w_{q(\mathbf{x})}\}(q : \mathbb{R}^m \to T, w \in \mathbb{R}^T)$$

Chen, T., & Guestrin, C. (2016, August). Xgboost: A scalable tree boosting system. In *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining* (pp. 785-794).

Recalled: Boosting

- How should we learn the trees?
- Learn from the errors/mistakes that made in the last round



Recalled: Boosting

Weight
1
1
1
1
1

Rec ID	Attribs.	Class
100	…	Yes
101	…	Yes
102	…	Yes
103	…	No
104	…	No

Correct?
✓
✓
✗
✓
✓

Weight
1
1
1.2
1
1

Rec ID	Attribs.	Class
100	…	Yes
101	…	Yes
102	…	Yes
103	…	No
104	…	No

Correct?
✓
✗
✓
✓
✓

Tree Boosting

- How should we learn the trees?
- Supervised learning => optimization

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

Training loss

Regularization

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Tree Boosting

- Parameters?

$$\hat{y}_i = \phi(\mathbf{x}_i) = \sum_{k=1}^{K} f_k(\mathbf{x}_i), \quad f_k \in \mathcal{F}, \quad \mathcal{F} = \{f(\mathbf{x}) = w_{q(\mathbf{x})}\}(q : \mathbb{R}^m \to T, w \in \mathbb{R}^T)$$

It is intractable to learn all the trees at once.

Boosting: additive strategy

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Additive learning

- Let t denotes the time (round)

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

- Reduce the problem of: optimizing all the tree
- To: which tree do we want at each step?

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Boosting: additive strategy

- Objective at time step t (with MSE):

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

$$\begin{aligned}\text{obj}^{(t)} &= \sum_{i=1}^{n} (y_i - (\hat{y}_i^{(t-1)} + f_t(x_i)))^2 + \sum_{i=1}^{t} \Omega(f_i) \\ &= \sum_{i=1}^{n} [2(\hat{y}_i^{(t-1)} - y_i) f_t(x_i) + f_t(x_i)^2] + \Omega(f_t) + \text{constant}\end{aligned}$$

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Boosting: additive strategy

- Objective at time step t (general case):

$$\text{obj}^{(t)} = \sum_{i=1}^{n} l(y_i, \hat{y}_i^{(t)}) + \sum_{i=1}^{t} \Omega(f_i)$$

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

$$g_i = \partial_{\hat{y}_i^{(t-1)}} l(y_i, \hat{y}_i^{(t-1)})$$

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

In terms of MSE:

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

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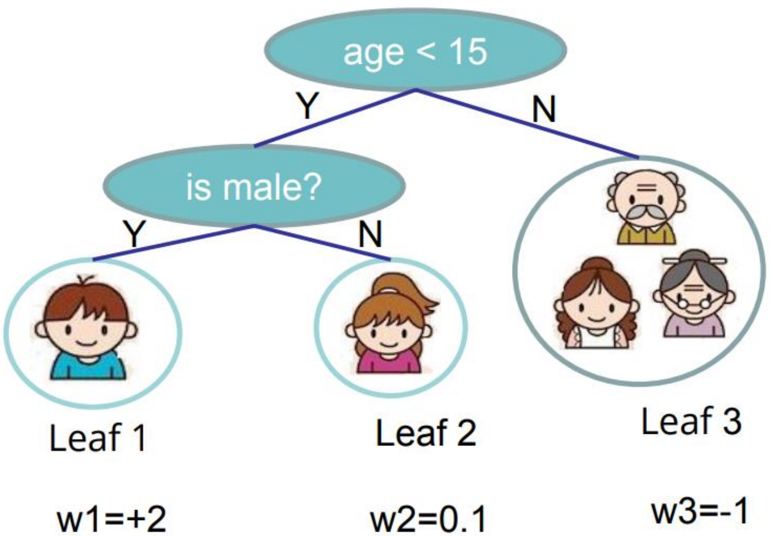
Tree Complexity

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

Number of leaves

L2 norm of leaf scores



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

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Structure Score

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

$$\text{obj}^{(t)} \approx \sum_{i=1}^{n} [g_i w_{q(x_i)} + \frac{1}{2} h_i w_{q(x_i)}^2] + \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} w_j^2$$

$$= \sum_{j=1}^{T} [(\sum_{i \in I_j} g_i) w_j + \frac{1}{2}(\sum_{i \in I_j} h_i + \lambda) w_j^2] + \gamma T$$

$I_j = \{i | q(x_i) = j\}$ is the set of indices of data points assigned to the j-th leaf.

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Structure Score

$$\text{obj}^{(t)} \approx \sum_{i=1}^{n}[g_i w_{q(x_i)} + \frac{1}{2}h_i w_{q(x_i)}^2] + \gamma T + \frac{1}{2}\lambda\sum_{j=1}^{T} w_j^2$$

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In terms of MSE:

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

$$G_j = \sum_{i\in I_j} g_i \qquad H_j = \sum_{i\in I_j} h_i$$

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

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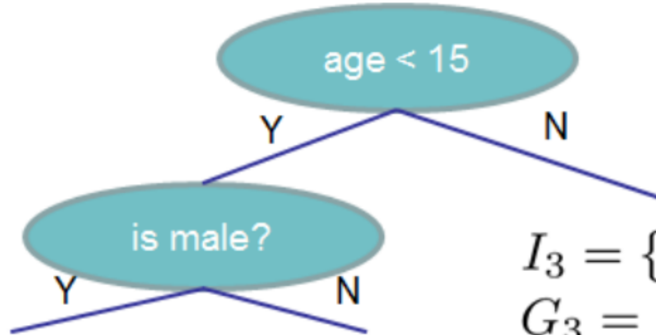
Instance index	gradient statistics
1	g1, h1
2	g2, h2
3	g3, h3
4	g4, h4
5	g5, h5



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

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

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

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

The smaller the score is, the better the structure is

In terms of MSE:

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

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Tree?

- Naïve approach:
  - Enumerate all possible trees
  - Calculate the score
  - Find the best Tree
  - Intractable

- Optimizing the Tree Structure Itself:

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

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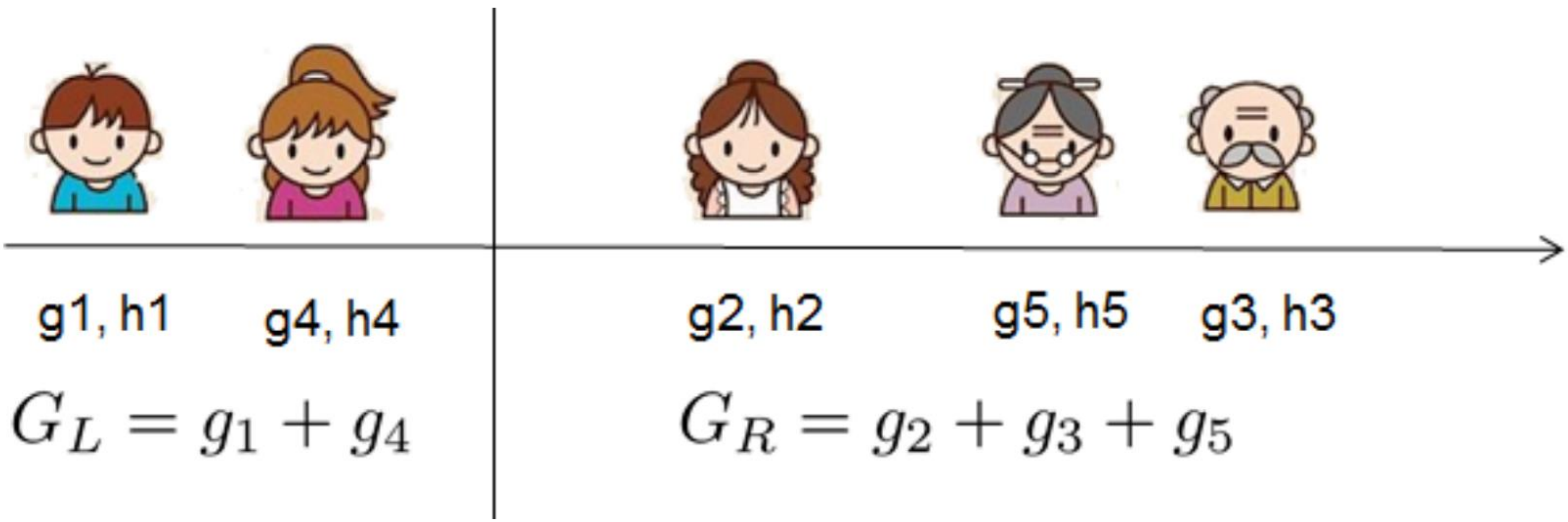
Search for Optimal Split

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



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

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What XGBoost can do for you

- Push the limit of computation resource
- Missing Value Handling
- Feature Selection

- You still need to
  - Feature Engineering
  - Tuning

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