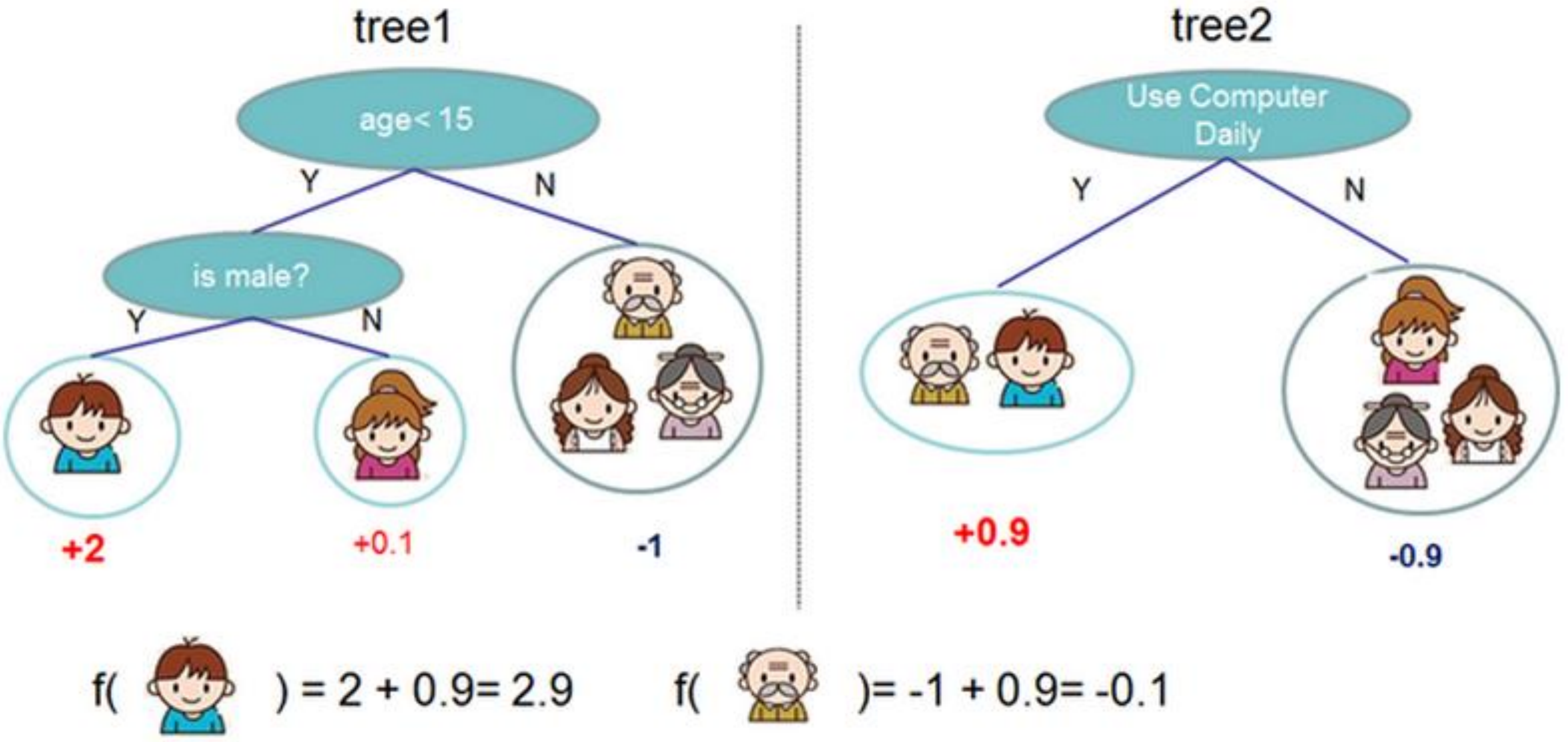
Xgboost


tree1
age< 15
Y
N
is male?
Y
N
+2
+0.1
-1
tree2
Use Computer Daily
Y
N
+0.9
-0.9
f( ) = 2 + 0.9= 2.9
f( )= -1 + 0.9= -0.1

Xgboost

$\hat{y}_i = \sum_j w_j x_{ij}$

目标函数：$l(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$

如何最优函数解？ $F^*(\vec{x}) = \arg\min E_{(x,y)}[L(y, F(\vec{x}))]$

集成算法的表示： $\hat{y}_i = \sum_{k=1}^{K} f_k(x_i), \quad f_k \in \mathcal{F}$

Xgboost

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

加入一个新的函数

第**t**轮的模型预测

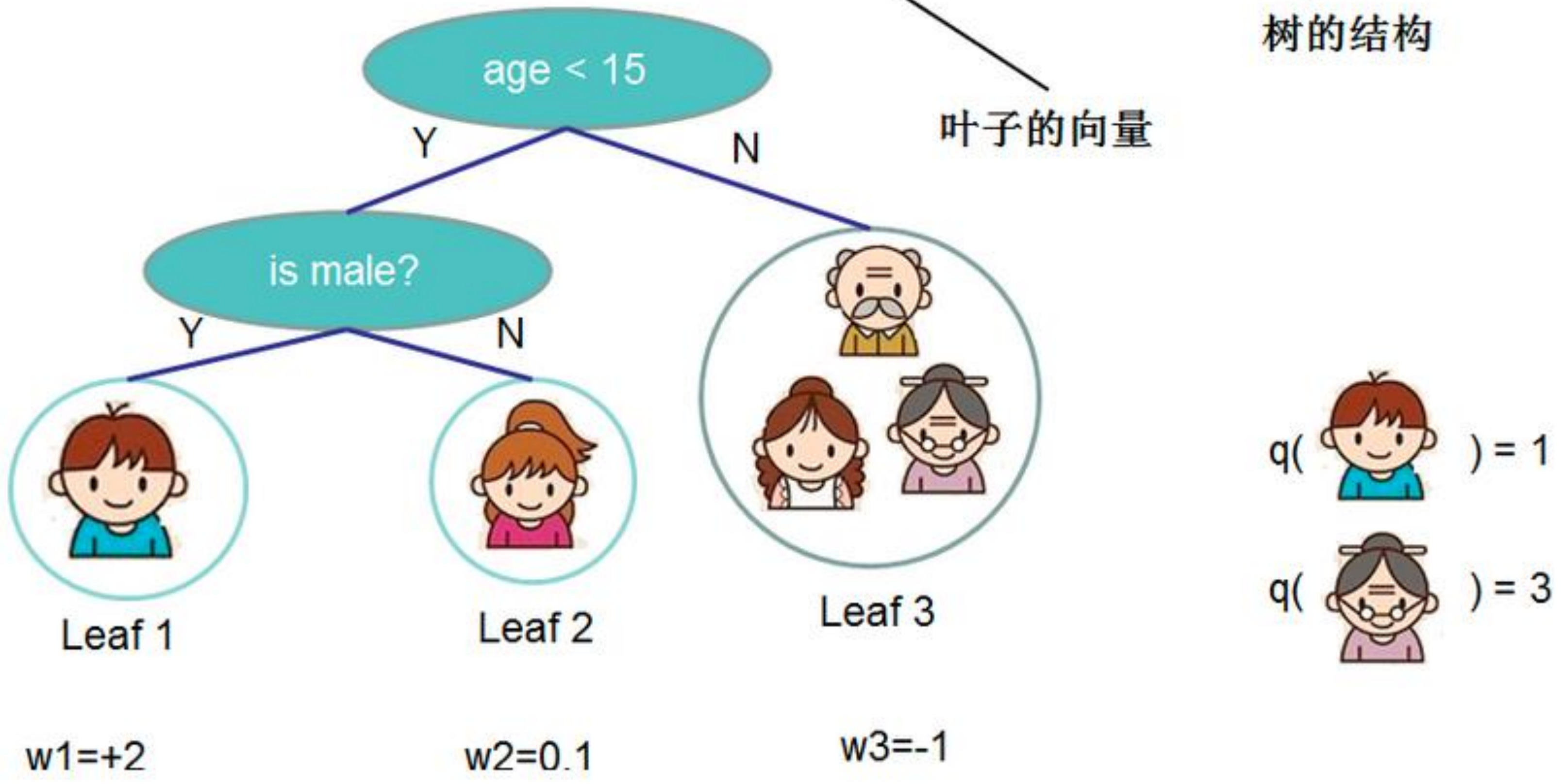
保留前面**t-1**轮的模型预测

Xgboost

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

树的结构

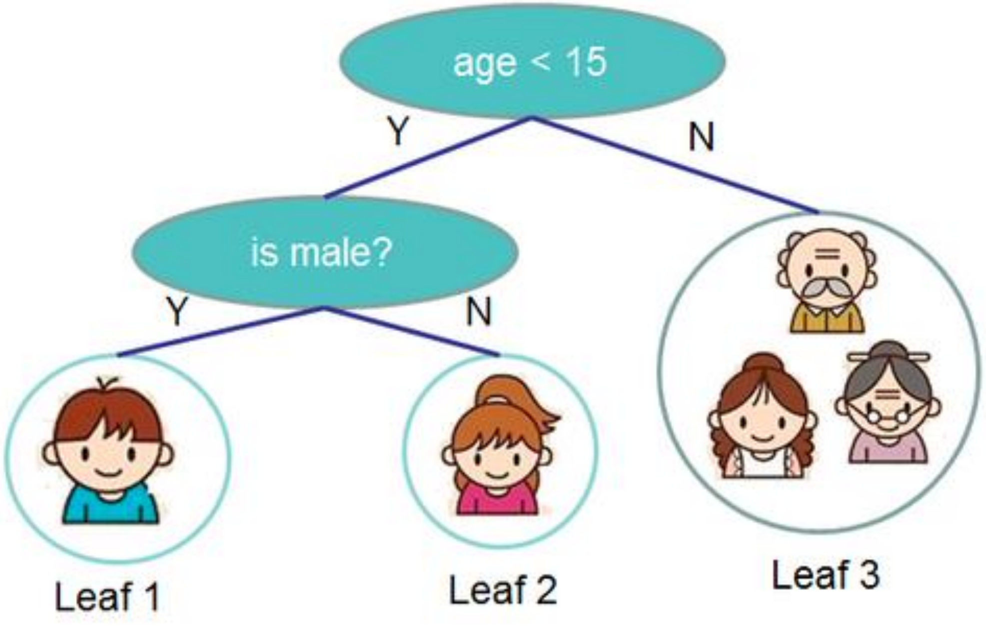
叶子的向量



Xgboost

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

叶子的个数　　　　w的L2模平方



w1=+2　　w2=0.1　　w3=-1

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

Xgboost

现在还剩下一个问题，我们如何选择每一轮加入什么f呢？答案是非常直接的，选取一个f来使得我们的目标函数尽量最大地降低

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

目标：找到 f_t 来优化这一目标

Xgboost

$$
\begin{aligned}
Obj^{(t)} &= \sum_{i=1}^{n} \left(y_i - (\hat{y}_i^{(t-1)} + f_t(x_i))\right)^2 + \Omega(f_t) + const \\
&= \sum_{i=1}^{n} \left[2(\hat{y}_i^{(t-1)} - y_i) f_t(x_i) + f_t(x_i)^2\right] + \Omega(f_t) + const
\end{aligned}
$$

一般叫做残差

Xgboost

- 目标 $Obj^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) + constant$
- 用泰勒展开来近似我们原来的目标
  - 泰勒展开：$f(x+\Delta x) \simeq f(x) + f'(x)\Delta x + \frac{1}{2}f''(x)\Delta x^2$
  - 定义：$g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)}), \quad h_i = \partial^2_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$

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

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

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

Xgboost

样本上遍历

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

叶子节点上遍历

Xgboost

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

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

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

$$= \sum_{j=1}^{T}\left[G_j w_j + \frac{1}{2}(H_j + \lambda)w_j^2\right] + \gamma T$$

Xgboost

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

$$= \sum_{j=1}^{T}[G_j w_j + \frac{1}{2}(H_j + \lambda)w_j^2] + \gamma T$$

$$\frac{\partial J(f_t)}{\partial w_j} = G_j + (H_j + \lambda)w_j = 0$$

$$w_j = -\frac{G_j}{H_j + \lambda}$$

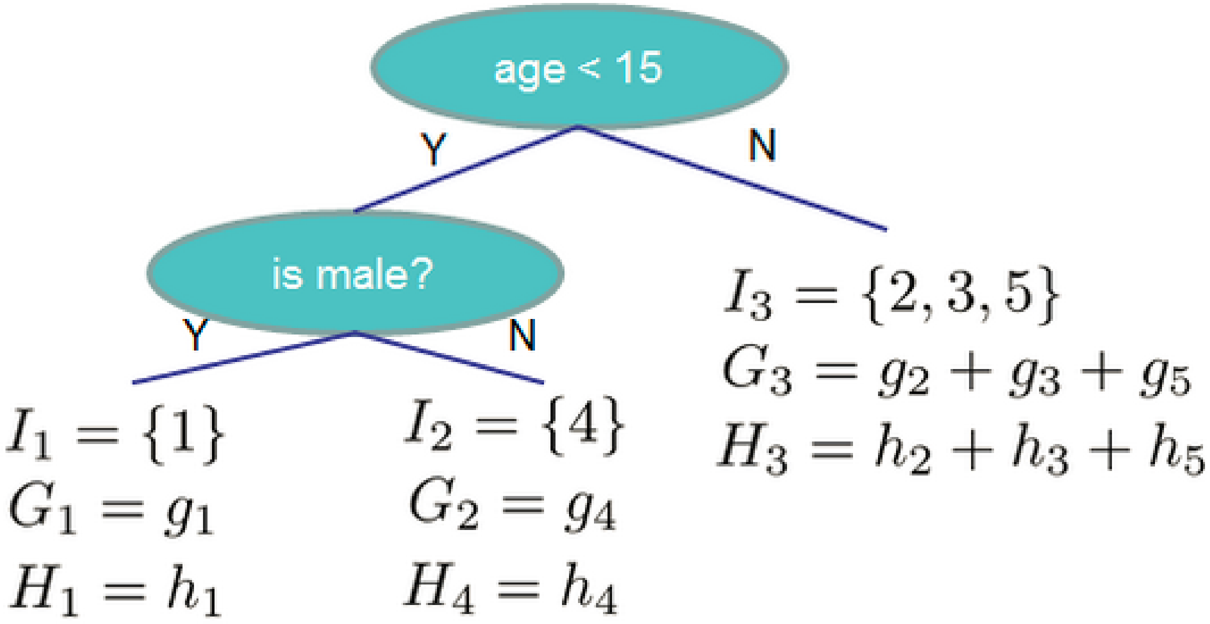
带回原目标函数

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

Xgboost

Obj代表了当我们指定一个树的结构的时候，我们在目标上面最多减少多少。我们可以把它叫做结构分数(structure score)。你可以认为这个就是类似吉尼系数一样更加一般的对于树结构进行打分的函数。下面是一个具体的打分函数计算的例子

样本号	梯度数据
1	g1, h1
2	g2, h2
3	g3, h3
4	g4, h4
5	g5, h5



$$Obj = -\frac{1}{2} \sum_j \frac{G_j^2}{H_j + \lambda} + 3\gamma$$

这个分数越小，代表这个树的结构越好

Xgboost

加入新叶子节点引入的复杂度代价

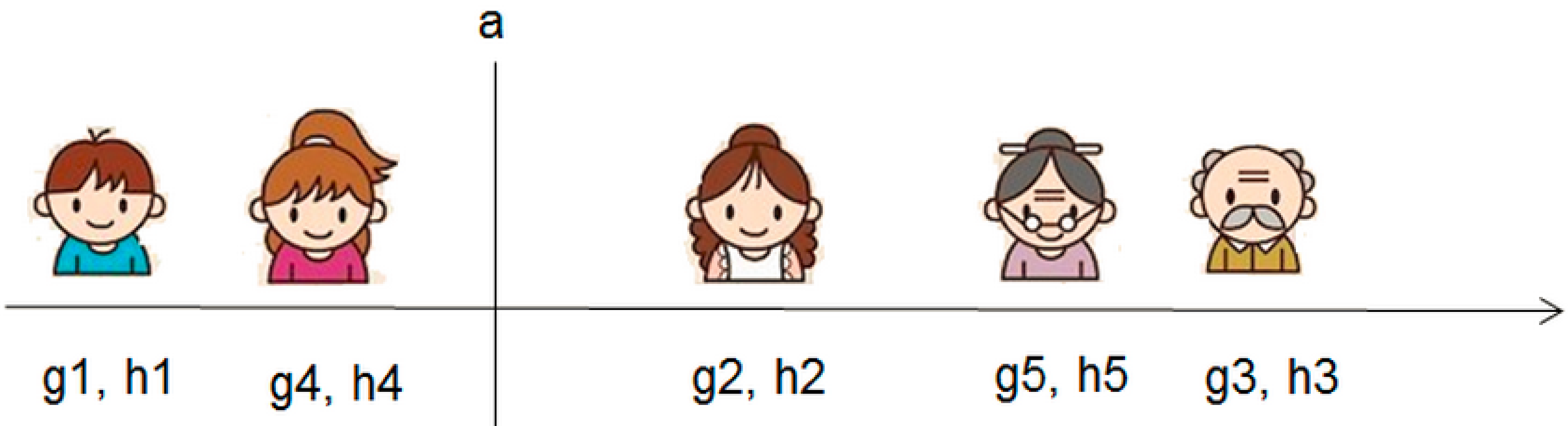
$$Gain = \frac{1}{2}\left[\frac{G_L^2}{H_L+\lambda} + \frac{G_R^2}{H_R+\lambda} - \frac{(G_L+G_R)^2}{H_L+H_R+\lambda}\right] - \gamma$$

左子树分数

不分割我们可以拿到的分数

右子树分数

对于每次扩展，我们还是要枚举所有可能的分割方案，如何高效地枚举所有的分割呢？我假设我们要枚举所有 $x < a$ 这样的条件，对于某个特定的分割a我们要计算a左边和右边的导数和。



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