

# Introduction to Boosted Trees

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# Outline

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- **Review of key concepts of supervised learning**  
监督学习的关键概念回顾
  - Regression Tree and Ensemble (What are we Learning)  
回归树与集成算法（我们在学习什么）
  - Gradient Boosting (How do we Learn)  
梯度提升（我们怎么学习）
  - Summary  
总结
-

# 监督学习的元素

## Elements in Supervised Learning

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- Notations:  $x_i \in \mathbb{R}^d$  i-th training example  
记号
  - **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:  $\Theta = \{w_j | j = 1, \dots, d\}$
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# Elements continued: Objective Function

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- 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):  $\Omega(w) = \lambda \|w\|_1$
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# Putting known knowledge into context

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- Ridge regression:  $\sum_{i=1}^n (y_i - w^T x_i)^2 + \lambda \|w\|^2$ 
  - Linear model, square loss, L2 regularization
- Lasso:  $\sum_{i=1}^n (y_i - w^T x_i)^2 + \lambda \|w\|_1$ 
  - Linear model, square loss, L1 regularization
- Logistic regression:
$$\sum_{i=1}^n [y_i \ln(1 + e^{-w^T x_i}) + (1 - y_i) \ln(1 + e^{w^T x_i})] + \lambda \|w\|^2$$
  - Linear model, logistic loss, L2 regularization
- The conceptual separation between model, parameter, objective also gives you **engineering benefits**.
  - Think of how you can implement SGD for both ridge regression and logistic regression 解耦，代码复用性高

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模型、参数、目标之间的概念分离带来了工程效益

# Objective and Bias Variance Trade-off

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

**Training Loss** measures how well model fit on training data

**Regularization**, measures complexity of model

为什么我们要在目标中包含两个成分？

- Why do we want to contain two component in the objective?

优化训练损失鼓励模型拟合程度

- Optimizing training loss encourages **predictive** models

- Fitting well in training data at least get you close to training data which is hopefully close to the underlying distribution

优化正则化鼓励简单模型

- Optimizing regularization encourages **simple** models

- Simpler models tends to have smaller variance in future predictions, making prediction **stable**
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  - **Regression Tree and Ensemble (What are we Learning)**  
回归树与集成算法（我们在学习什么）
  - Gradient Boosting (How do we Learn)  
用了一套通用的解决方案——梯度提升
  - Summary
-

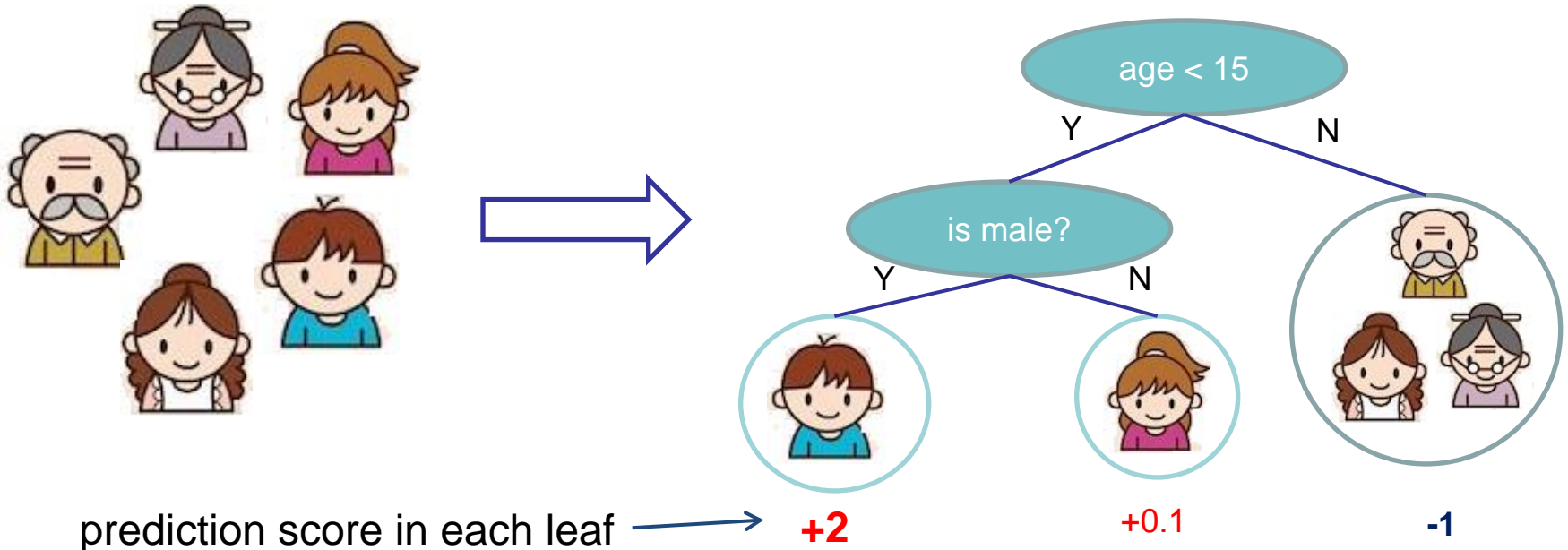
# Regression Tree (CART)

CART

- regression tree (also known as classification and regression tree):
  - Decision rules same as in decision tree
  - Contains one score in each leaf value

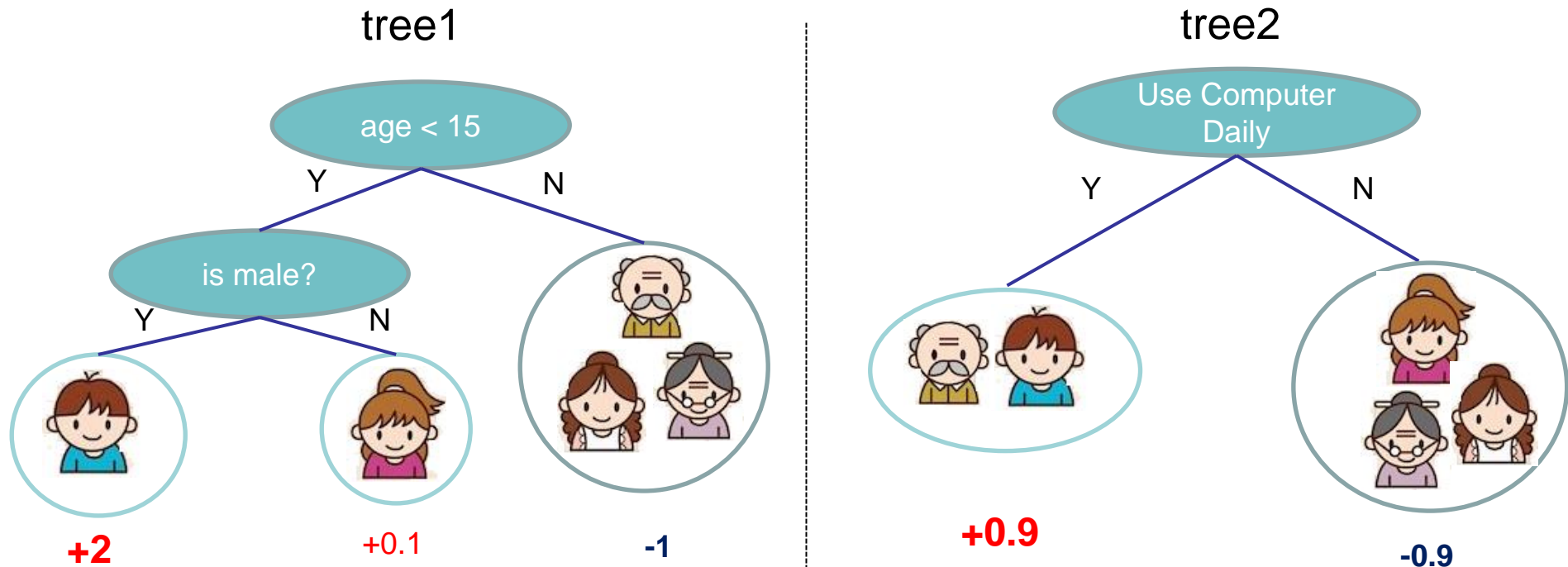
Input: age, gender, occupation, ...

Does the person like computer games





# Regression Tree Ensemble



$$f(\text{boy icon}) = 2 + 0.9 = 2.9$$

$$f(\text{old man icon}) = -1 + 0.9 = -0.1$$

Prediction of is sum of scores predicted by each of the tree

预测值是每棵树分数的和

# Tree Ensemble methods

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- Very widely used, look for GBM, random forest...
  - Almost half of data mining competition are won by using some variants of tree ensemble methods

使用广泛，例如梯度提升模型，随机森林

- Invariant to scaling of inputs, so you do not need to do careful features normalization.

不需特征缩放，所以你不需要做仔细的特征归一化

- Learn higher order interaction between features.

学习特征之间的高阶交互

- Can be scalable, and are used in Industry

可扩展性，用于工业

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# 集成算法实际应用：模型与参数

## Put into context: Model and Parameters

- Model: assuming we have K trees

$$\hat{y}_i = \sum_{k=1}^K f_k(x_i), \quad f_k \in \mathcal{F}$$

Space of functions containing all Regression trees

F：假设空间，包含了所有回归树

*Think: regression tree is a function that maps the attributes to the score*

思想：回归树是一个函数，他将特征、属性向量映射为一个分数

- Parameters

- Including structure of each tree, and the score in the leaf

每棵树的结构，以及叶子上的分数

- Or simply use function as parameters

$$\Theta = \{f_1, f_2, \dots, f_K\}$$

- Instead learning weights in  $\mathbf{R}^d$ , we are learning functions(trees)

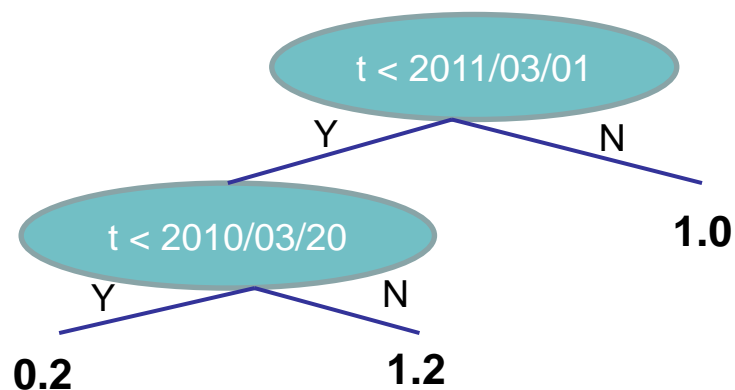
也可以换个角度，认为不是学习这些参数，而是学习多个函数

# 单变量时，树的学习

## Learning a tree on single variable

- How can we learn functions?
- Define objective (loss, regularization), and optimize it!!
- Example:
  - Consider regression tree on single input  $t$  (time)
  - I want to predict whether I like romantic music at time  $t$

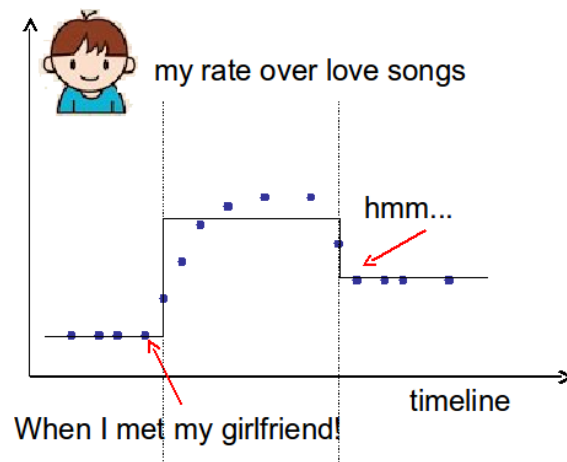
The model is regression tree that splits on time



Equivalently

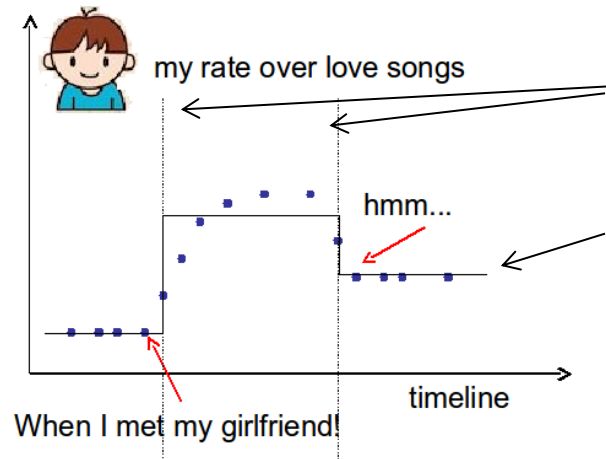


Piecewise step function over time



# Learning a step function 学习阶跃函数

- Things we need to learn



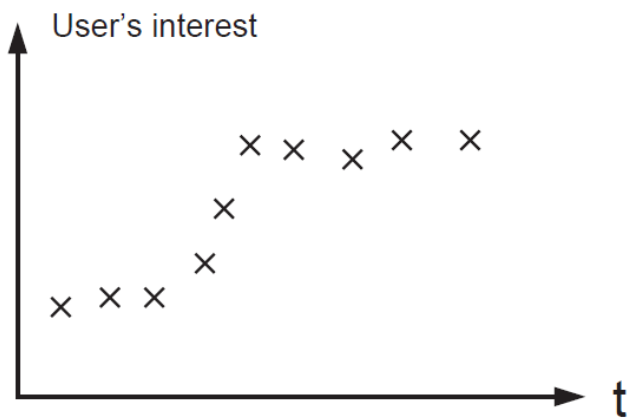
Splitting Positions

The Height in each segment

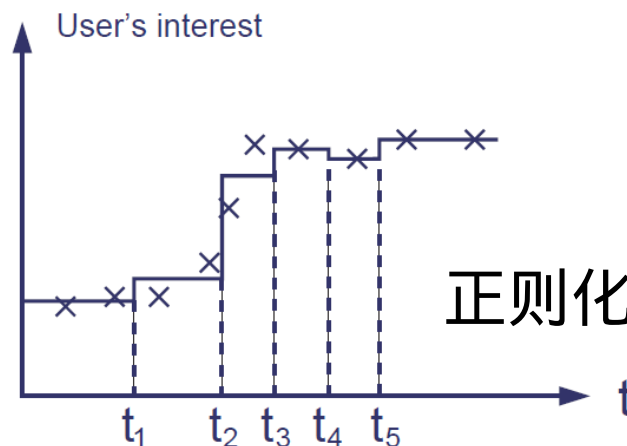
划分点位置、每个分段上的高度（取值）

- Objective for single variable regression tree(step functions)
  - Training Loss: How will the function fit on the points?
  - Regularization: How do we define complexity of the function?
    - ◆ Number of splitting points,  $l_2$  norm of the height in each segment?

# 视觉上学习阶跃函数 Learning step function (visually)

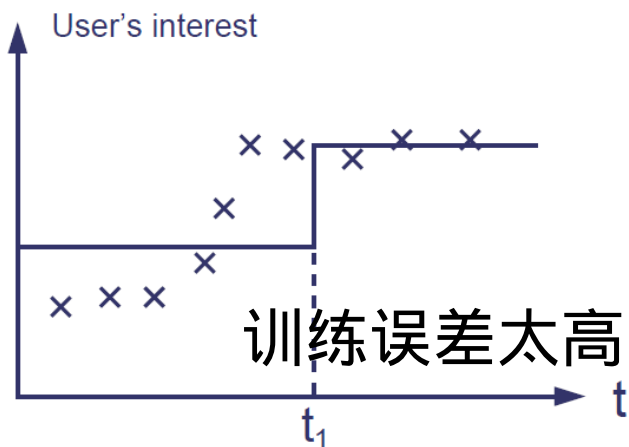


Observed user's interest on topic k against time t



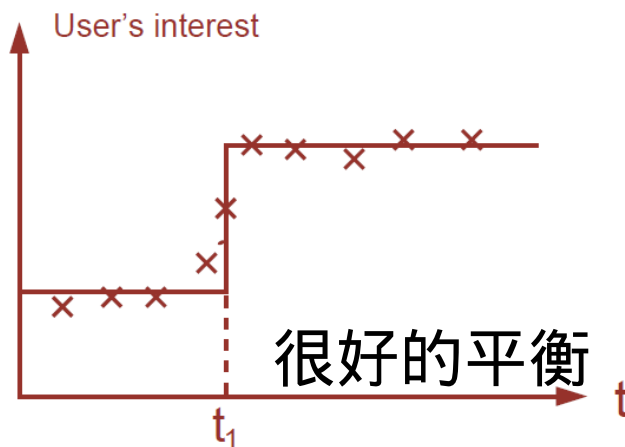
正则化项太高

☒ Too many splits,  $\Omega(f)$  is high



训练误差太高

☒ Wrong split point,  $L(f)$  is high



很好的平衡

☒ Good balance of  $\Omega(f)$  and  $L(f)$

# Coming back: Objective for Tree Ensemble

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- Model: assuming we have K trees

$$\hat{y}_i = \sum_{k=1}^K f_k(x_i), \quad f_k \in \mathcal{F}$$

- Objective

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

Training loss

Complexity of the Trees

- Possible ways to define  $\Omega$  ?
    - Number of nodes in the tree, depth
    - L2 norm of the leaf weights
    - ... detailed later
-

# Objective vs Heuristic 目标函数 VS 启发式学习

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- When you talk about (decision) trees, it is usually heuristics
    - Split by information gain
    - Prune the tree
    - Maximum depth
    - Smooth the leaf values
  - Most heuristics maps well to objectives, taking the formal (objective) view let us know what we are learning
    - Information gain -> training loss
    - Pruning -> regularization defined by #nodes 不需要了解
    - Max depth -> constraint on the function space
    - Smoothing leaf values -> L2 regularization on leaf weights
-



# 回归树不仅仅是用来做回归的 Regression Tree is not just for regression!

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- Regression tree ensemble defines how you make the prediction score, it can be used for
    - Classification, Regression, Ranking....
    - ....
  - It all depends on how you define the objective function!
  - So far we have learned:
    - Using Square loss  $l(y_i, \hat{y}_i) = (y_i - \hat{y}_i)^2$  回归
      - ♦ Will results in common gradient boosted machine
    - Using Logistic loss  $l(y_i, \hat{y}_i) = y_i \ln(1 + e^{-\hat{y}_i}) + (1 - y_i) \ln(1 + e^{\hat{y}_i})$ 
      - ♦ Will results in LogitBoost 分类
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## Take Home Message for this section

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- Bias-variance tradeoff is everywhere 偏差和方差的平衡无处不在
  - The loss + regularization objective pattern applies for regression tree learning (function learning)  
损失+正则化目标模式适用于回归树学习（函数学习）
  - We want **predictive** and **simple** functions  
我们需要训练误差小并且简单的函数。
  - This defines what we want to learn (objective, model).  
这就定义了我们想要学习的东西（目标，模型）
  - But how do we learn it?
    - Next section
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# So How do we Learn?

- 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)  
我们不能使用诸如SGD之类的方法来找到 $f$

- Solution: **Additive Training (Boosting)**

- Start from constant prediction, add a new function each time  
从常数预测开始，每次添加一个新函数

$$\hat{y}_i^{(0)} = 0$$

$$\hat{y}_i^{(1)} = f_1(x_i) = \hat{y}_i^{(0)} + f_1(x_i)$$

$$\hat{y}_i^{(2)} = f_1(x_i) + f_2(x_i) = \hat{y}_i^{(1)} + f_2(x_i)$$

...

$$\hat{y}_i^{(t)} = \sum_{k=1}^t f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i)$$

New function

Model at training round  $t$

Keep functions added in previous round

保留前面轮次中添加的函数

# Additive Training 加法模型训练

- 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  $t$

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

这里和GBDT不一样

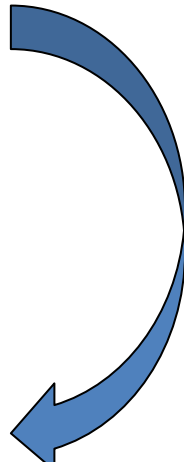
Goal: find  $f_t$  to minimize this

- 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

# 损失的泰勒展开逼近 Taylor Expansion Approximation of Loss

- Goal  $Obj^{(t)} = \sum_{i=1}^n l(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)) + \Omega(f_t) + constant$ 
    - Seems still complicated except for the case of square loss
  - Take Taylor expansion of the objective 对目标函数泰勒展开
    - Recall  $f(x + \Delta x) \simeq f(x) + f'(x)\Delta x + \frac{1}{2}f''(x)\Delta x^2$
    - Define  $g_i = \partial_{\hat{y}^{(t-1)}} l(y_i, \hat{y}^{(t-1)})$ ,  $h_i = \partial_{\hat{y}^{(t-1)}}^2 l(y_i, \hat{y}^{(t-1)})$
- 

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

令  $x - x_0 = x$  , 将  $x$  视为静态的 , 将  $x + x$  视为动态的

- *If you are not comfortable with this, think of square loss*

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

- Compare what we get to previous slide

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思考：为什么要用泰勒展开？

# Our New Goal 新目标函数

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

- Why spending s much efforts to derive the objective, why not just grow trees ... 为什么花这么多的精力来推导目标函数，为什么不直接建树呢？

- Theoretical benefit: know what we are learning, convergence  
理论上的好处：知道我们在学习什么，知道什么时候收敛

- **Engineering** benefit, recall the elements of supervised learning

- ♦  $g_i$  and  $h_i$  comes from definition of loss function

$g$ 和 $h$ 来自损失函数的定义

- ♦ The learning of function only depend on the objective via  $g_i$  and  $h_i$   
函数的学习只依赖于与 $g$ 和 $h$ 有关的目标

- ♦ 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

当你被要求使用平方损失和逻辑损失的提升树时，请考虑如何分离代码的模块

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# Refine the definition of tree 精炼树的定义

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

我们通过叶子的分数向量 $w$ 和叶子索引映射函数 $q(x)$ 来定义树，叶子索引映射函数可以将实例映射到叶节点

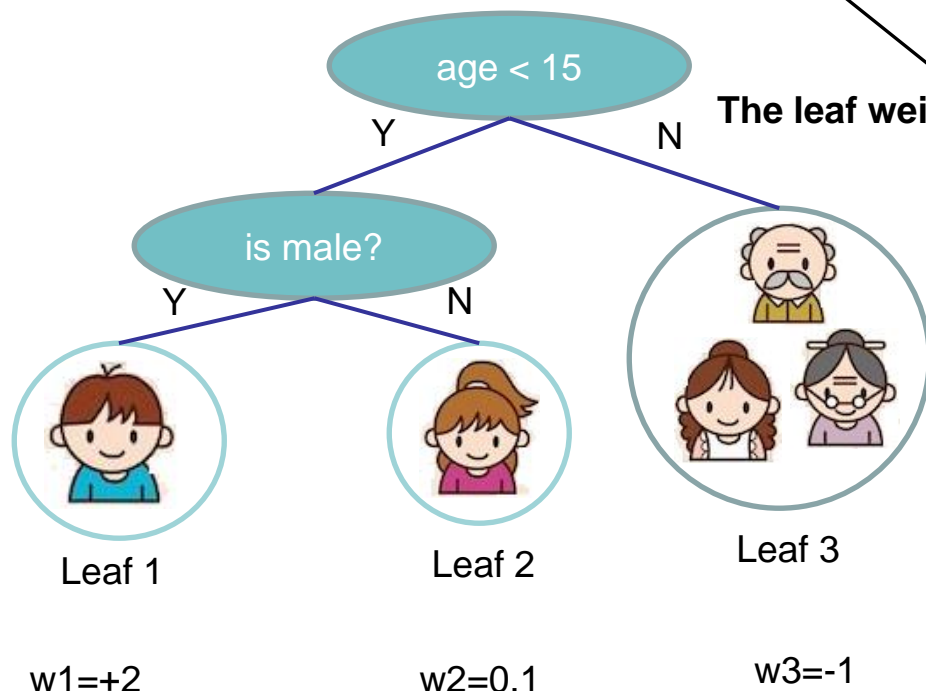
$$f_t(x) = w_{q(x)}, \quad w \in \mathbf{R}^T, \quad q: \mathbf{R}^d \rightarrow \{1, 2, \dots, T\}$$

$T$ : 叶子编号

The structure of the tree

The leaf weight of the tree

$w$ : 叶子节点的分数向量



$$q(\text{boy icon}) = 1$$

$$q(\text{elderly woman icon}) = 3$$

$q(x)$ 是叶子索引映射函数（其实就是树结构），输入一个样本，返回样本所在叶子索引



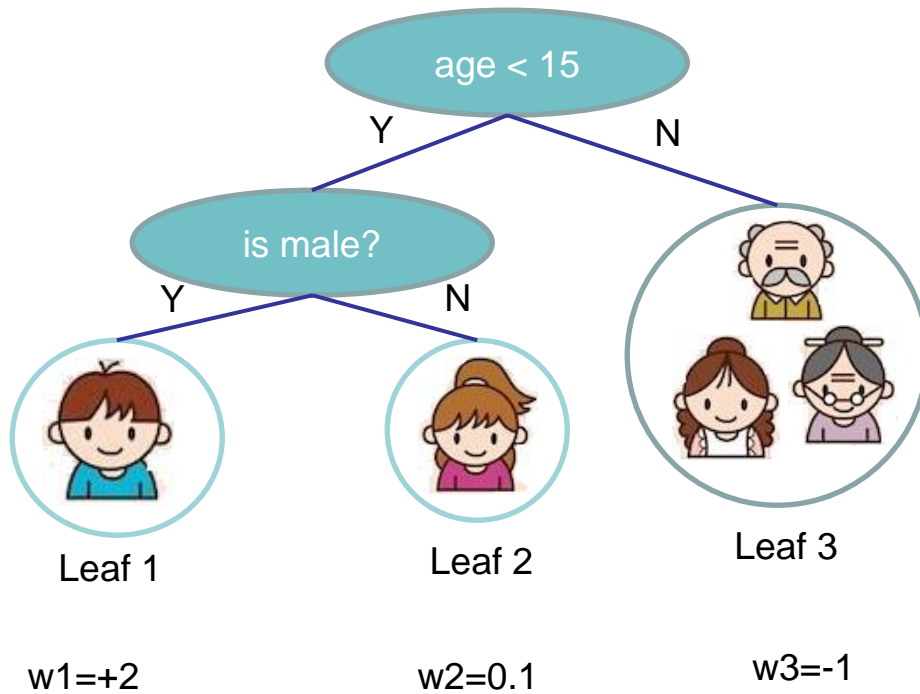
# Define the Complexity of Tree 定义树的复杂度

- 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 重新审视目标函数

- Define the instance set in leaf  $j$  as  $I_j = \{i | q(x_i) = j\}$   
定义叶子  $j$  上的样本集合为  $I_j$ .
- Regroup the objective by each leaf 用每一个叶子重新组合目标函数

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

- This is sum of  $T$  independent quadratic functions  
这是  $T$  个独立的二次函数的求和

$q(x)$  是叶子索引映射函数，输入一个样本，返回样本所在叶子索引。 $I_j$  是叶子索引为  $j$  的所有样本的序号的集合。

# The Structure Score 结构分数

- Two facts about single variable quadratic function

## 单变量二次函数的两个事实

$$\operatorname{argmin}_x Gx + \frac{1}{2}Hx^2 = -\frac{G}{H}, \quad H > 0 \qquad \min_x Gx + \frac{1}{2}Hx^2 = -\frac{1}{2}\frac{G^2}{H}$$

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

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

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

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

**This measures how good a tree structure is!**




假设树的结构 (qx) 确定了, 每个叶子最优的权重和最终的目标函数值就确定了

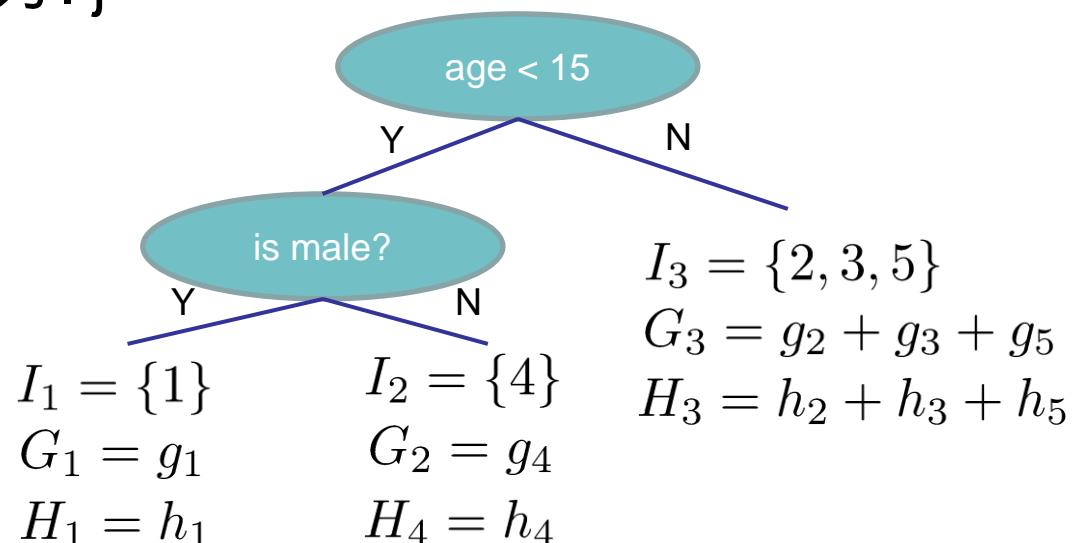
[illegible]

# The Structure Score Calculation 结构分数计算

定义叶子j上的样本集合为 $I_j$

Instance index      gradient statistics

1		$g_1, h_1$
2		$g_2, h_2$
3		$g_3, h_3$
4		$g_4, h_4$
5		$g_5, h_5$



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

The smaller the score is, the better the structure is

Obj分数越小，结构越好

# Searching Algorithm for Single Tree

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- Enumerate the possible tree structures  $q$  枚举可能的树结构 $q$
- Calculate the structure score for the  $q$ , using the scoring eq.

$$Obj = -\frac{1}{2} \sum_{j=1}^T \frac{G_j^2}{H_j + \lambda} + \gamma T \quad \text{使用评分方程计算} q \text{的结构得分}$$

- Find the best tree structure, and use the optimal leaf weight

$$w_j^* = -\frac{G_j}{H_j + \lambda} \quad \text{寻找到最优树结构后, 就能求最优叶子权重}$$

- But... there can be infinite possible tree structures..  
但是.....可以有无限的可能的树结构
-

# Greedy Learning of the Tree 树的贪婪学习

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- In practice, we grow the tree greedily 在实践中，我们贪婪地建树
  - Start from tree with depth 0
  - 对于树的每个叶节点，尝试添加一个划分。加入划分后目标函数的变化为
  - For each leaf node of the tree, try to add a split. The change of objective after adding the split is

$$Gain = \frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} - \gamma$$

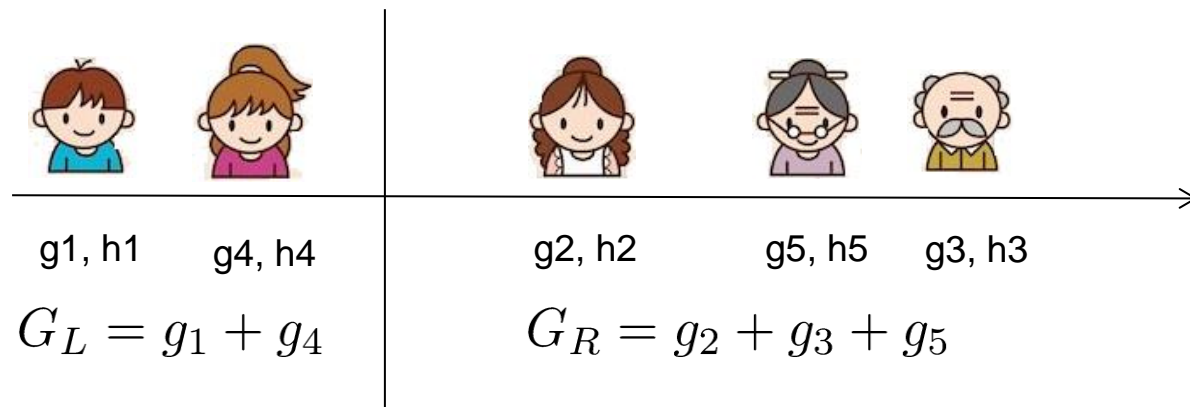
the score of left child      the score of right child      the score of if we do not split      The complexity cost by introducing additional leaf  
额外增加的代价

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

疑问：如何找到最优划分点呢？

# Efficient Finding of the Best Split 高效地寻找最优化分点

- What is the gain of a split rule  $x_j < a$  ? Say  $x_j$  is age  
选择划分规则  $x_j < a$  的增益是什么？比方说  $x_j$  是年龄



- 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

我们所需要的是两边的 $g$ 和 $h$ 的总和，并计算

在排序实例上的进行从左到右线性扫描，足以决定在该特征上的最佳划分。

# An Algorithm for Split Finding 寻找划分点算法

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- 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

对于每个节点，枚举所有特征

对于每个特征，按特征值对实例进行排序。

使用线性扫描来确定该特征的最佳分割。

采取所有特征中最佳分割方案

时间复杂性分析：深度K树

$O(n d K \log n)$ ：每个级别，需要 $O(n \log n)$ 排序。有D特征，我们需要做K层

这可以进一步优化（例如使用近似或缓存排序的特征）

可以扩展到非常大的数据集

- 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
-



那类别型变量呢

# What about Categorical Variables?

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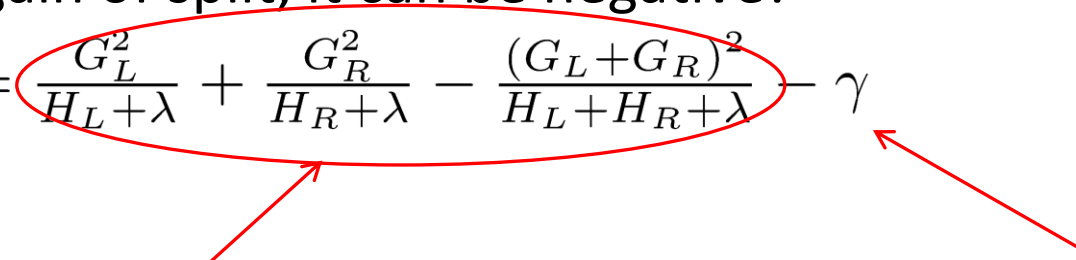
- Some tree learning algorithm handles categorical variable and continuous variable separately
  - 一些树学习算法分别处理类别变量和连续变量
    - We can easily use the scoring formula we derived to score split based on categorical variables.
- Actually it is not necessary to handle categorical separately.
  - We can encode the categorical variables into numerical vector using one-hot encoding. Allocate a #categorical length vector

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

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

# Pruning and Regularization 剪枝和正则化

- Recall the gain of split, it can be negative! 回顾划分后的信息增益，他不能是负的

$$Gain = \frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} - \frac{(G_L + G_R)^2}{H_L + H_R + \lambda} - \gamma$$


- 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 如果最佳分裂具有负增益，则停止分裂
    - But maybe a split can benefit future splits.. 但是分裂可能会有利于未来的分裂
  - Post-Prunning 将一棵树生长到最大深度，递归地修剪所有负增益的叶子划分点。
    - Grow a tree to maximum depth, recursively prune all the leaf splits with negative gain

# Recap: Boosted Tree Algorithm 概括

- Add a new tree in each iteration 每一轮增加一棵新树
- Beginning of each iteration, calculate 每一轮的开始，计算

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

- Use the statistics to greedily grow a tree  $f_t(x)$  使用贪婪算法构建树

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

- Add  $f_t(x)$  to the model  $\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + f_t(x_i)$  将构建好的模型加入加法模型
  - Usually, instead we do  $y^{(t)} = y^{(t-1)} + \epsilon f_t(x_i)$
  - $\epsilon$  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

这意味着我们不会在每一步都做充分的优化，并为未来的回合保留机会，这有助于防止过拟合

! !

# Outline

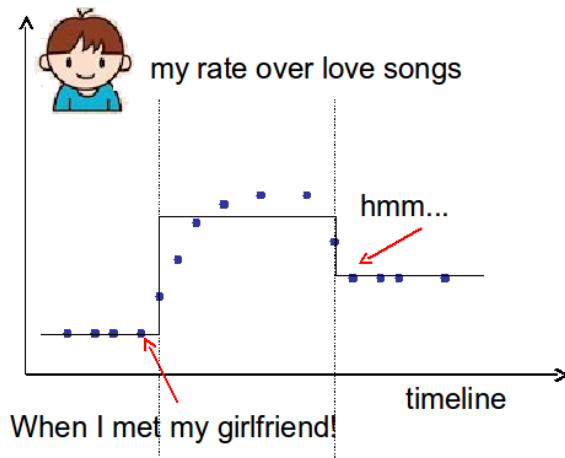
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- Review of key concepts of supervised learning
  - Regression Tree and Ensemble (What are we Learning)
  - Gradient Boosting (How do we Learn)
  - **Summary**
-

# Questions to check if you really get it

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- How can we build a boosted tree classifier to do weighted regression problem, such that each instance have a importance weight?
- Back to the time series problem, if I want to learn step functions over time. Is there other ways to learn the time splits, other than the top down split approach?



# Questions to check if you really get it

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- How can we build a boosted tree classifier to do weighted regression problem, such that each instance have a importance weight?
  - Define objective, calculate  $g_i, h_i$ , feed it to the old tree learning algorithm we have for un-weighted version

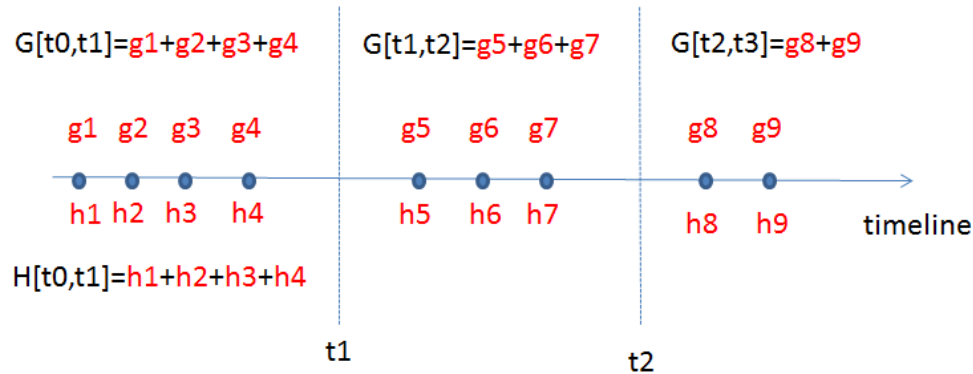
$$l(y_i, \hat{y}_i) = \frac{1}{2}a_i(\hat{y}_i - y_i)^2 \quad g_i = a_i(\hat{y}_i - y_i) \quad h_i = a_i$$

- Again think of separation of model and objective, how does the theory can help better organizing the machine learning toolkit
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# Questions to check if you really get it

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- Time series problem



- All that is important is the structure score of the splits

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

- Top-down greedy, same as trees
  - Bottom-up greedy, start from individual points as each group, greedily merge neighbors
  - Dynamic programming, can find optimal solution for this case
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# Summary

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- The separation between model, objective, parameters can be helpful for us to understand and customize learning models
- The bias-variance trade-off applies everywhere, including learning in functional space

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

- We can be formal about what we learn and how we learn. Clear understanding of theory can be used to guide cleaner implementation.
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# Reference

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- Greedy function approximation a gradient boosting machine. *J.H. Friedman*
    - *First paper about gradient boosting*
  - *Stochastic Gradient Boosting. J.H. Friedman*
    - *Introducing bagging trick to gradient boosting*
  - *Elements of Statistical Learning. T. Hastie, R. Tibshirani and J.H. Friedman*
    - *Contains a chapter about gradient boosted boosting*
  - Additive logistic regression a statistical view of boosting. *J.H. Friedman T. Hastie R. Tibshirani*
    - *Uses second-order statistics for tree splitting, which is closer to the view presented in this slide*
  - Learning Nonlinear Functions Using Regularized Greedy Forest. *R. Johnson and T. Zhang*
    - *Proposes to do fully corrective step, as well as regularizing the tree complexity. The regularizing trick is closed related to the view present in this slide*
  - Software implementing the model described in this slide: <https://github.com/tqchen/xgboost>
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