# Lecture 13: 20 May, 2021

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Data Mining and Machine Learning
April–July 2021

# Limitations of classification models

Recall

- Bias : Expressiveness of model limits classification
- Variance: Variation in model based on sample of training data

Overcoming limitations

- Bagging is an effective way to overcome high variance
  - Ensemble models
    - Sequence of models based on independent bootstrap samples
    - Use voting to get an overall classifier
- How can we cope with high bias?

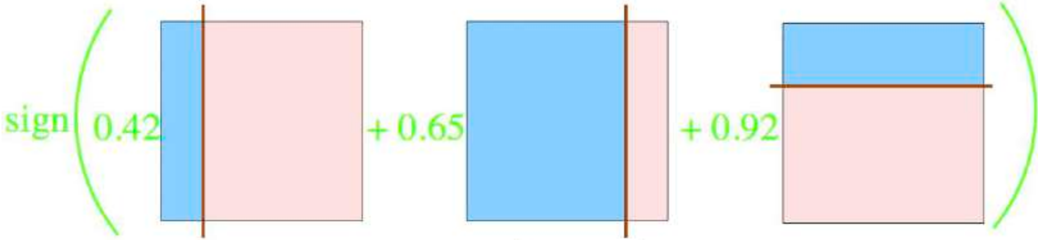
- Initially, all data items have equal weight
- Build a new model and compute its weighted error
- Discard if error rate is above 50%
- Damping factor — reduce weight of correct inputs
- Reweight data items and normalize
- Final classifier

$$f_{\text{final}}(x) = \arg\max_{y \in Y} \sum_{t : f_t(x) = y} \log \frac{1}{\beta_t}$$

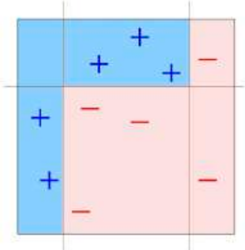
```
AdaBoost(D, Y, BaseLeaner, k)
  Initialize D_1(w_i) ← 1/n for all i;
  for t = 1 to k do
      f_t ← BaseLearner(D_t);
      e_t ← Σ_{i: f_t(D_t(x_i)) ≠ y_i} D_t(w_i);
      if e_t > ½ then
          k ← k – 1;
          exit-loop
      else
          β_t ← e_t / (1 – e_t);
          D_{t+1}(w_i) ← D_t(w_i) × { β_t  if f_t(D_t(x_i)) = y_i
                                    { 1    otherwise               ;
          D_{t+1}(w_i) ← D_{t+1}(w_i) / Σ_{i=1}^{n} D_{t+1}(w_i)
```

# Boosting: An example

- Final classifier is weighted sum of three weak classifiers




- Pictorially



# Gradient Boosting

- AdaBoost uses weights to build new weak learners that compensate for earlier errors
- Gradient boosting follows a different approach
  - Shortcomings of the current model are defined in terms of gradients
  - Gradient boosting = Gradient descent + boosting

# Gradient Boosting for Regression

- Training data $(x_1, y_1, (x_2, y_2), \ldots, (x_n, y_n)$
- Fit a model $F(x)$ to minimize square loss
- The model $F$ we build is good, but not perfect
  - $y_1 = 0.9$, $F(x_1) = 0.8$
  - $y_2 = 1.3$, $F(x_2) = 1.4$
  - ...
- Add an additional model $h$, so that new prediction is $F(x) + h(x)$

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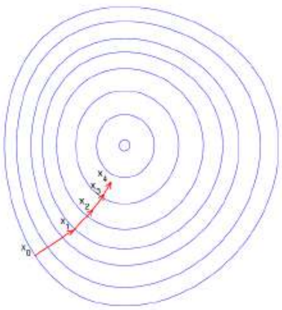
  - $\ldots$
- Add an additional model $h$, so that new prediction is $F(x) + h(x)$
- What should $h$ look like?
- For each $x_i$, want $F(x_i) + h(x_i) = y_i$
- $h(x_i) = y_i - F(x_i)$
- Fit a new model $h$ (typically a regression tree) to the residuals $y_i - F(x_i)$
- If $F + h$ is not satisfactory, build another model $h'$ to fit residuals $y_i - [F(x_i) + h(x_i)]$
- Why should this work?

# Residuals and gradients

## Gradient descent

- Move parameters against the gradient with respect to loss function

$$\theta_i \leftarrow \theta_i - \frac{\partial J}{\partial \theta_i}$$




- Individual loss: $L(y, F(x)) = (y - F(x))^2/2$
- Minimize overall loss: $J = \sum_i L(y_i, F(x_i))$
- $\dfrac{\partial J}{\partial F(x_i)} = F(x_i) - y$
- Residual $y_i - F(x_i)$ is negative gradient
- Fitting $h$ to residual is same as fitting $h$ to negative gradient
- Updating $F$ using residual is same as updating $F$ based on negative gradient

# Residuals and gradients

- Residuals are a special case — gradients for square loss
- Can use other loss functions, and fit $h$ to corresponding gradient
- Square loss gets skewed by outliers
- More robust loss functions with outliers
  - Absolute loss $|y - f(x)|$
  - Huber loss

$$L(y,F) = \begin{cases} \frac{1}{2}(y-F)^2, & |y-F| \leq \delta \\ \delta(|y-F| - \delta/2), & |y-F| > \delta \end{cases}$$

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- More generally, boosting with respect to gradient rather than just residuals
- Given any differentiable loss function $L$,
  - Start with an initial model $F$
  - Calculate negative gradients

$$-g(x_i) = \frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}$$

  - Fit a regression tree $h$ to negative gradients $-g(x_i)$
  - Update $F$ to $F + \rho h$
  - $\rho$ is the learning rate

## Regression Trees

- Predict age based on given attributes

| Person ID | Age | Likes Gardening | Plays Video Games | Likes Hats |
|---|---|---|---|---|
| 1 | 13 | FALSE | TRUE | TRUE |
| 2 | 14 | FALSE | TRUE | FALSE |
| 3 | 15 | FALSE | TRUE | FALSE |
| 4 | 25 | TRUE | TRUE | TRUE |
| 5 | 35 | FALSE | TRUE | TRUE |
| 6 | 49 | TRUE | FALSE | FALSE |
| 7 | 68 | TRUE | TRUE | TRUE |
| 8 | 71 | TRUE | FALSE | FALSE |
| 9 | 73 | TRUE | FALSE | TRUE |

# Regression Trees

- Predict age based on given attributes
- Build a regression tree using CART algorithm

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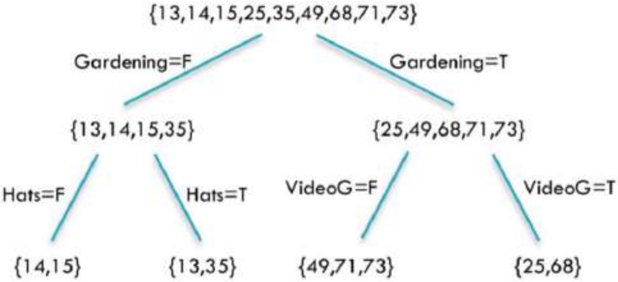
# Regression Trees




- **LikesHats** seems irrelevant, yet pops up

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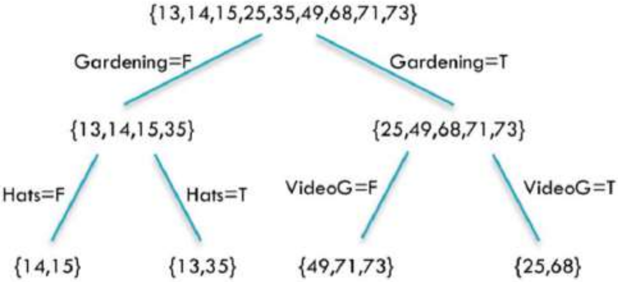


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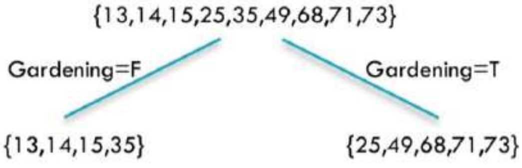
- **LikesHats** seems irrelevant, yet pops up
- Can we do better?

# Residuals




Tree 1

| PersonID | Age | Tree1 Prediction | Tree1 Residual |
|---|---|---|---|
| 1 | 13 | 19.25 | -6.25 |
| 2 | 14 | 19.25 | -5.25 |
| 3 | 15 | 19.25 | -4.25 |
| 4 | 25 | 57.2 | -32.2 |
| 5 | 35 | 19.25 | 15.75 |
| 6 | 49 | 57.2 | -8.2 |
| 7 | 68 | 57.2 | 10.8 |
| 8 | 71 | 57.2 | 13.8 |
| 9 | 73 | 57.2 | 15.8 |

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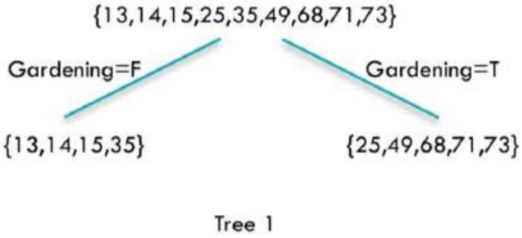


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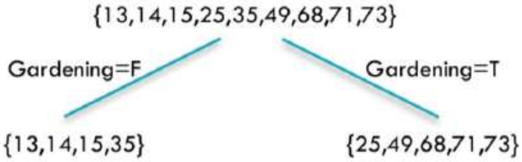


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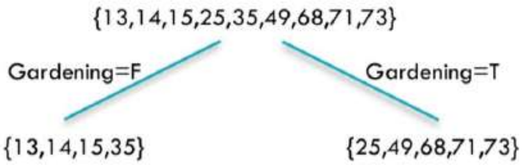


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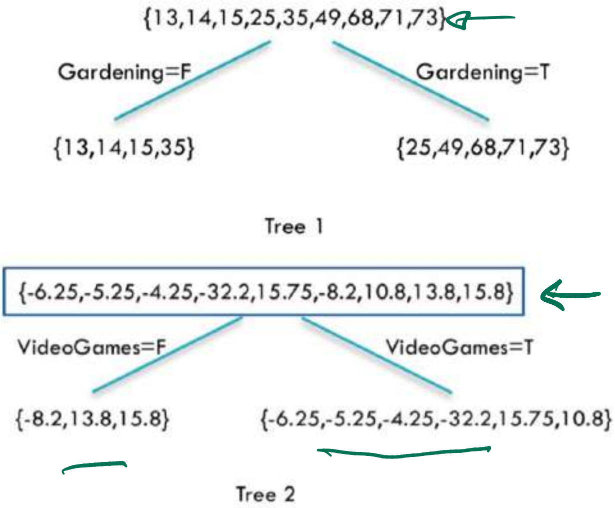


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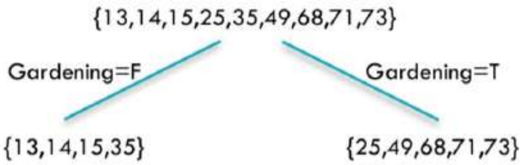


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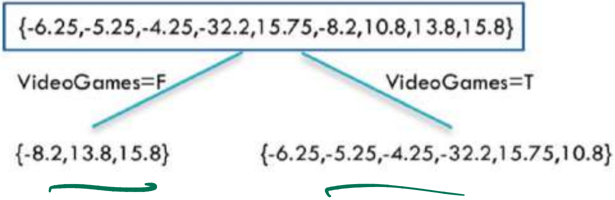
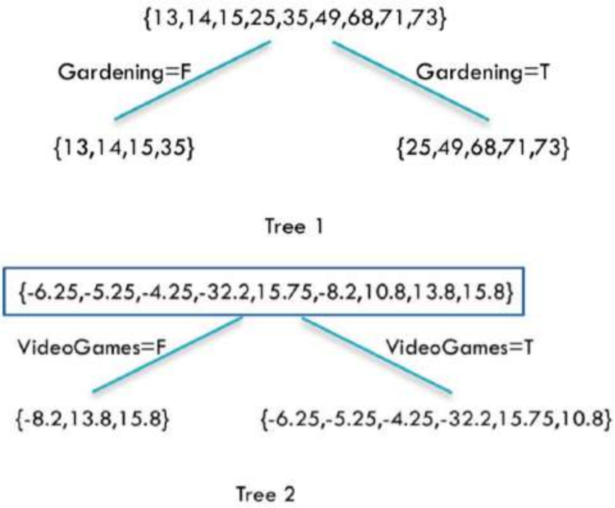



Tree 2

| Person ID | Age | Tree1 Prediction | Tree1 Residual | Tree2 Prediction | Combined | Final Residual |
|---|---|---|---|---|---|---|
| 1 | 13 | 19.25 | -6.25 | -3.567 | 15.68 | -2.683 |
| 2 | 14 | 19.25 | -5.25 | -3.567 | 15.68 | -1.683 |
| 3 | 15 | 19.25 | -4.25 | -3.567 | 15.68 | -0.6833 |
| 4 | 25 | 57.2 | -32.2 | -3.567 | 53.63 | -28.63 |
| 5 | 35 | 19.25 | 15.75 | -3.567 | 15.68 | +19.32 |
| 6 | 49 | 57.2 | -8.2 | 7.133 | 64.33 | -15.33 |
| 7 | 68 | 57.2 | 10.8 | -3.567 | 53.63 | +14.37 |
| 8 | 71 | 57.2 | 13.8 | 7.133 | 64.33 | +6.667 |
| 9 | 73 | 57.2 | 15.8 | 7.133 | 64.33 | +8.667 |

# Residuals

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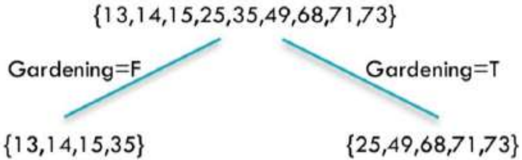


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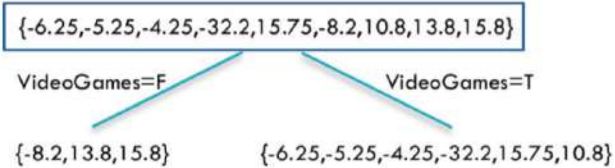


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| 3 | 15 | 19.25 | -4.25 | -3.567 | 15.68 | -0.6833 |
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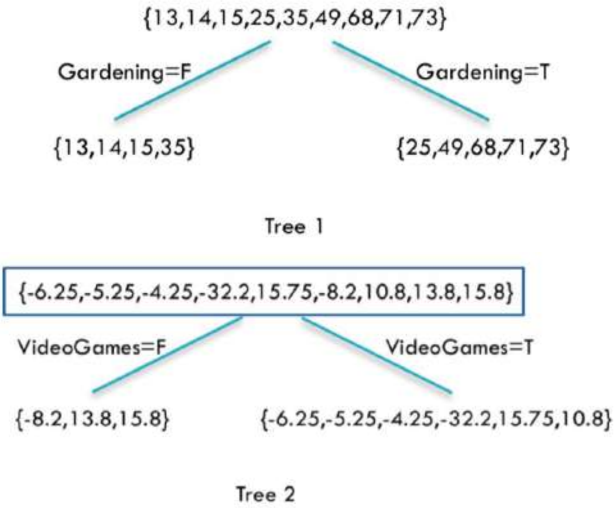


8x

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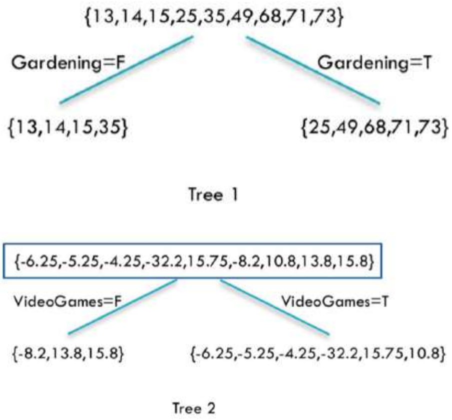
## General Strategy



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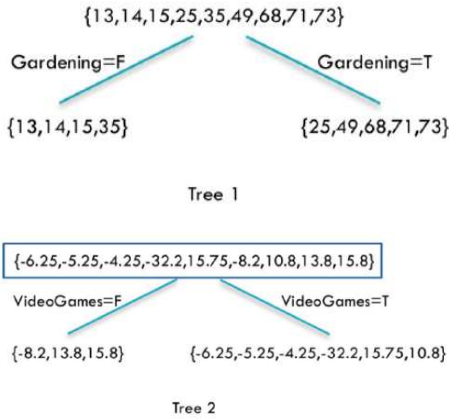
- Build tree 1, $F_1$



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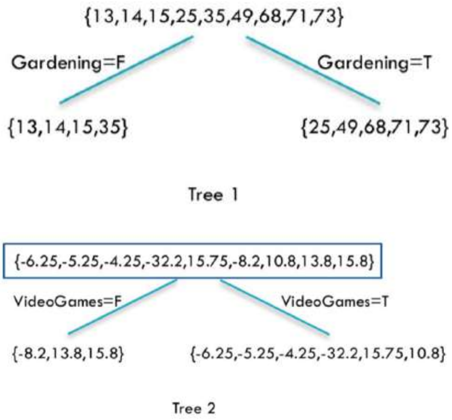

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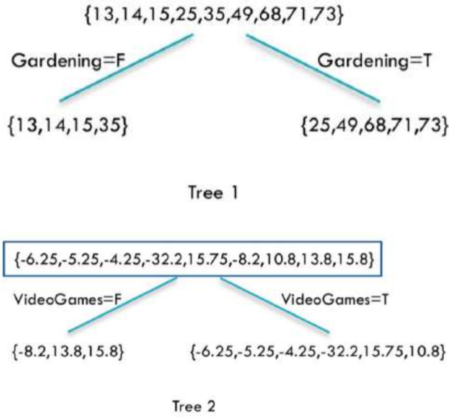

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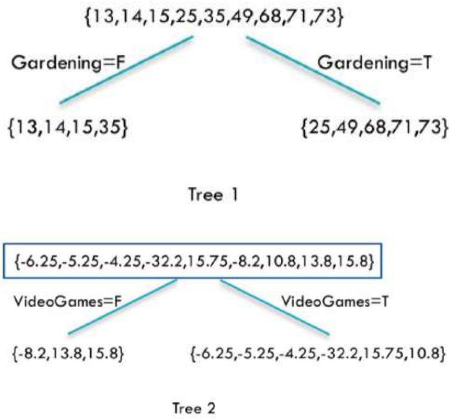

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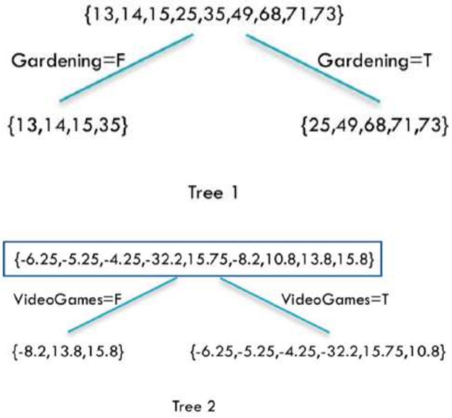
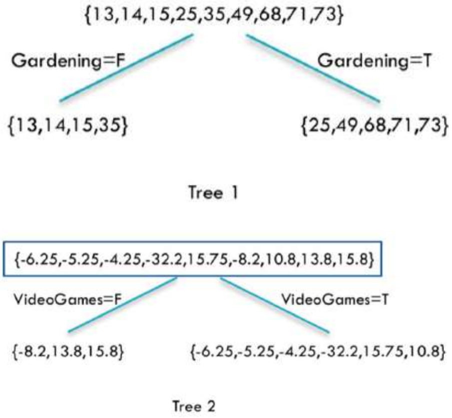
- . . .



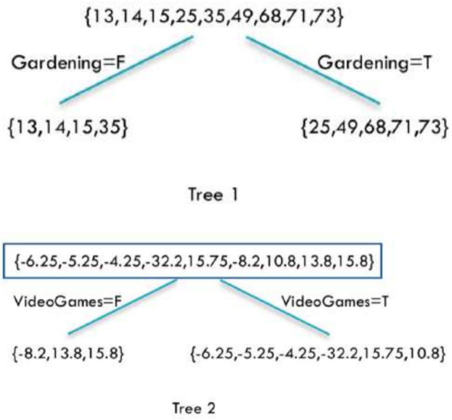
## Learning Rate



# Hyper Parameters

## Learning Rate

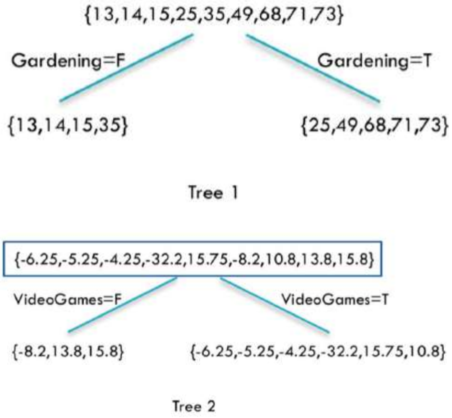
- $h_j$ fits residuals of $F_j$



# Hyper Parameters

## Learning Rate

- $h_j$ fits residuals of $F_j$
- $F_{j+1}(x) = F_J(x) + LR \cdot h_j(x)$
  - $LR$ controls contribution of residual
  - $LR = 1$ in our previous example



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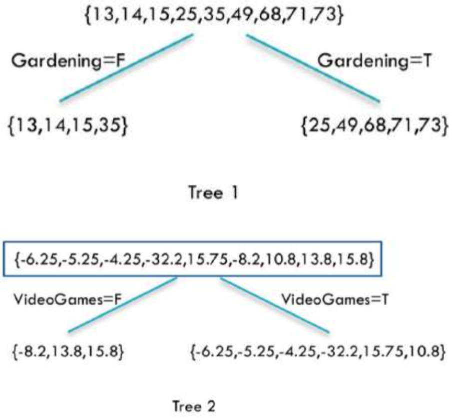
- $F_{j+1}(x) = F_J(x) + LR \cdot h_j(x)$
  - $LR$ controls contribution of residual
  - $LR = 1$ in our previous example
- Ideally, choose $LR$ separately for each residual to minimize loss function
  - Can apply different $LR$ to different leaves




Fixed Fixed

$F + g h \rightsquigarrow \underline{\underline{L}}$

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- For each $x$, classifier produces scores $\langle s_0, s_1 \rangle$ [0, 1]
- Use softmax to convert to probabilities:

For $j \in \{0, 1\}$, $p_j = \dfrac{e^{s_j}}{e^{s_0} + e^{s_1}}$

SOFTMAX

# Gradient Boosting for Classification

- Assume binary classification
- Original training outputs are $y \in \{0, 1\}$
- For each $x$, classifier produces scores $\langle s_0, s_1 \rangle$
- Use softmax to convert to probabilities:

  For $j \in \{0, 1\}$, $p_j = \dfrac{e^{s_j}}{e^{s_0} + e^{s_1}}$
- Use cross entropy as the loss function

  $L(y, F) = y \log(p_1) + (1 - y) \log(p_0)$

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- Compute negative gradients
- Fit regression trees to negative gradients to minimize cross entropy

Decision Stumps

One node tree