Lecture 12: 3 March, 2022

Madhavan Mukund

https://www.cmi.ac.in/~madhavan

Data Mining and Machine Learning
January–May 2022

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), ..., (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 $F(x) + h(x)$

Gradient Boosting for Regression

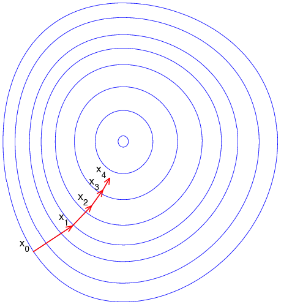
- Training data (x_1, y_1), (x_2, y_2), ..., (x_n, y_n)
- Fit a model $F(x)$ to minimize square loss
- The model F we build is good, but not perfect
  - $y_1 = 0.9$, $F(x_1) = 0.8$
  - $y_2 = 1.3$, $F(x_2) = 1.4$
  - ...
- Add an additional model h, so that new prediction is $F(x) + h(x)$
- What should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

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

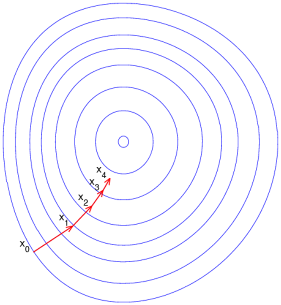


Residuals and gradients

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

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

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

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

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

- More generally, boosting with respect to gradient rather than just residuals
- Given any differential 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 $F + \rho h$
  - ρ is the learning rate

Regression Trees

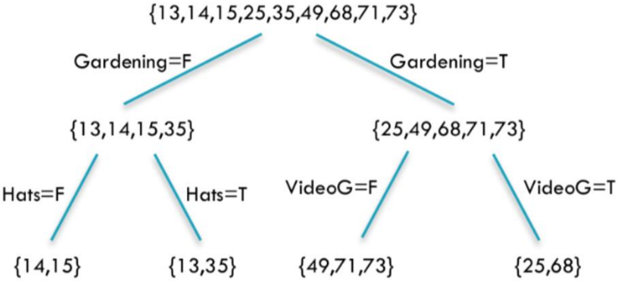
- Predict age based on given attributes

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

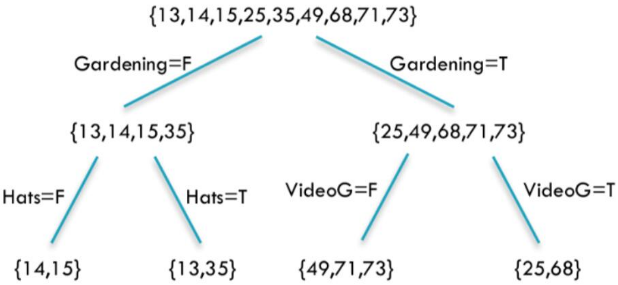
- Predict age based on given attributes
- Build a regression tree using CART algorithm

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



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

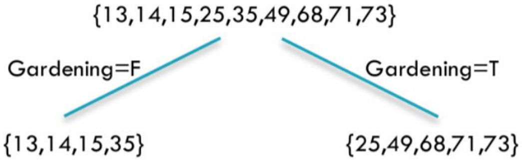
Person ID	Age	Likes Gardening	Plays Video Games	Likes Hats
1	13	FALSE	TRUE	TRUE
2	14	FALSE	TRUE	FALSE
3	15	FALSE	TRUE	FALSE
4	25	TRUE	TRUE	TRUE
5	35	FALSE	TRUE	TRUE
6	49	TRUE	FALSE	FALSE
7	68	TRUE	TRUE	TRUE
8	71	TRUE	FALSE	FALSE
9	73	TRUE	FALSE	TRUE



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

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

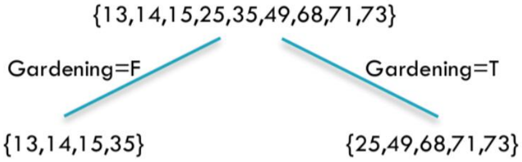
Residuals



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

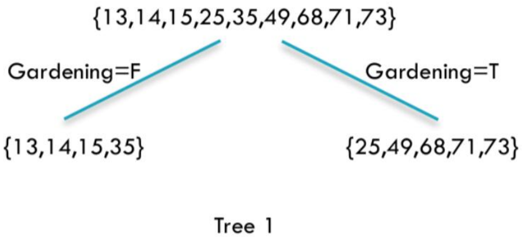
Residuals



Tree 1

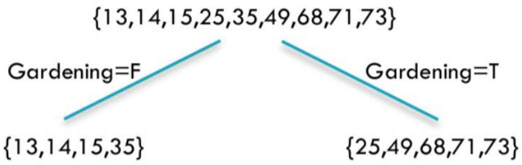
PersonID	Age	Tree1 Prediction	Tree1 Residual
1	13	19.25	-6.25
2	14	19.25	-5.25
3	15	19.25	-4.25
4	25	57.2	-32.2
5	35	19.25	15.75
6	49	57.2	-8.2
7	68	57.2	10.8
8	71	57.2	13.8
9	73	57.2	15.8

Residuals



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

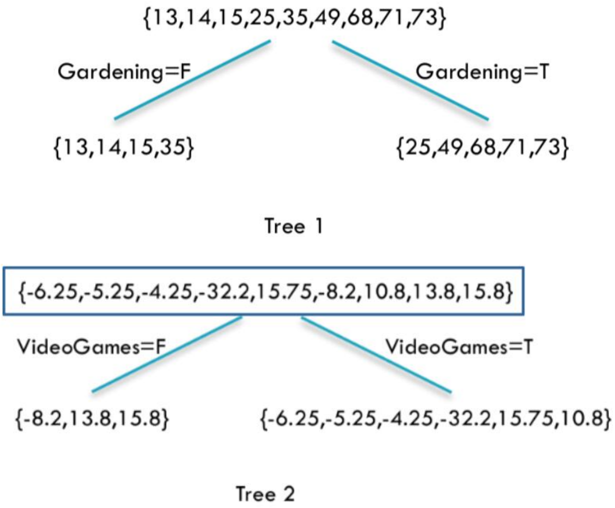
Residuals



Tree 1

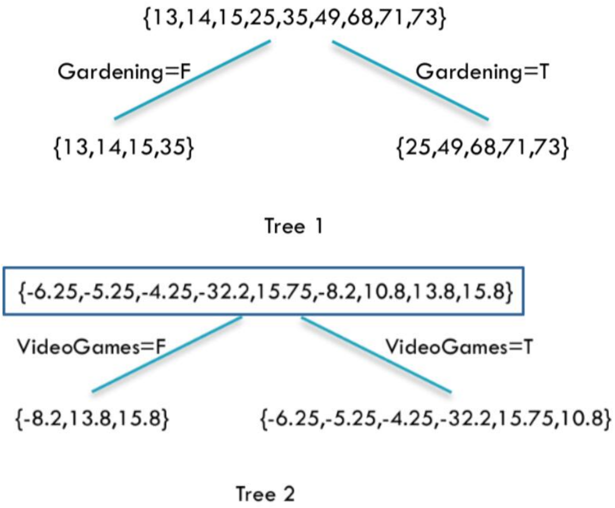
PersonID	Age	Tree1 Prediction	Tree1 Residual
1	13	19.25	-6.25
2	14	19.25	-5.25
3	15	19.25	-4.25
4	25	57.2	-32.2
5	35	19.25	15.75
6	49	57.2	-8.2
7	68	57.2	10.8
8	71	57.2	13.8
9	73	57.2	15.8

Residuals



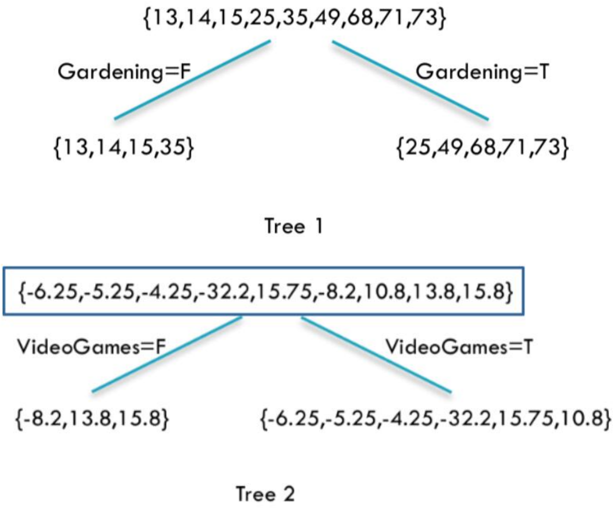
PersonID	Age	Tree1 Prediction	Tree1 Residual
1	13	19.25	-6.25
2	14	19.25	-5.25
3	15	19.25	-4.25
4	25	57.2	-32.2
5	35	19.25	15.75
6	49	57.2	-8.2
7	68	57.2	10.8
8	71	57.2	13.8
9	73	57.2	15.8

Residuals



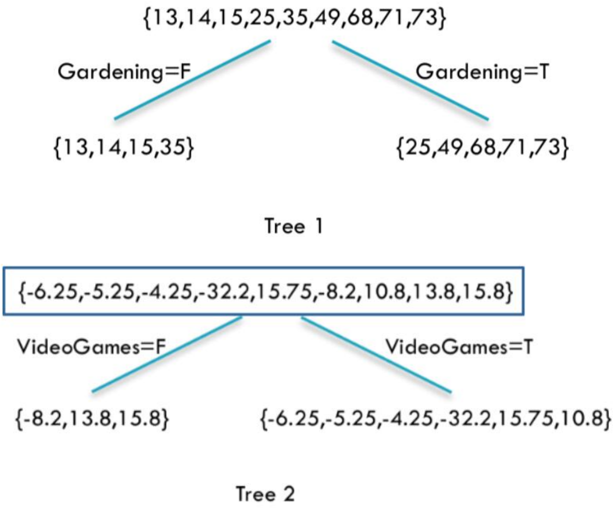
Person ID	Age	Tree1 Prediction	Tree1 Residual	Tree2 Prediction	Combined	Final Residual
1	13	19.25	-6.25	-3.567	15.68	-2.683
2	14	19.25	-5.25	-3.567	15.68	-1.683
3	15	19.25	-4.25	-3.567	15.68	-0.6833
4	25	57.2	-32.2	-3.567	53.63	-28.63
5	35	19.25	15.75	-3.567	15.68	+19.32
6	49	57.2	-8.2	7.133	64.33	-15.33
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



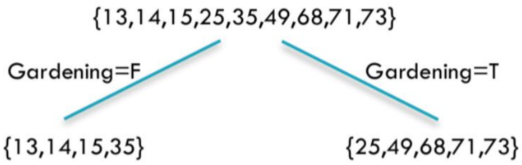
Person ID	Age	Tree1 Prediction	Tree1 Residual	Tree2 Prediction	Combined	Final Residual
1	13	19.25	-6.25	-3.567	15.68	-2.683
2	14	19.25	-5.25	-3.567	15.68	-1.683
3	15	19.25	-4.25	-3.567	15.68	-0.6833
4	25	57.2	-32.2	-3.567	53.63	-28.63
5	35	19.25	15.75	-3.567	15.68	+19.32
6	49	57.2	-8.2	7.133	64.33	-15.33
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

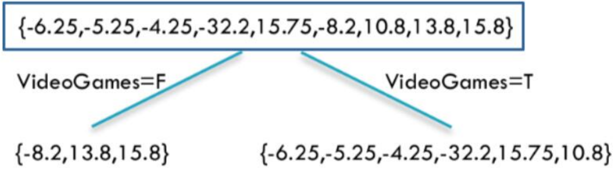


Person ID	Age	Tree1 Prediction	Tree1 Residual	Tree2 Prediction	Combined	Final Residual
1	13	19.25	-6.25	-3.567	15.68	-2.683
2	14	19.25	-5.25	-3.567	15.68	-1.683
3	15	19.25	-4.25	-3.567	15.68	-0.6833
4	25	57.2	-32.2	-3.567	53.63	-28.63
5	35	19.25	15.75	-3.567	15.68	+19.32
6	49	57.2	-8.2	7.133	64.33	-15.33
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



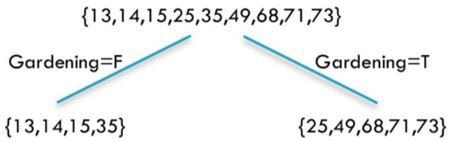
Tree 1



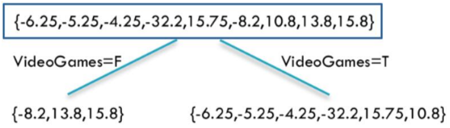
Tree 2

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

General Strategy



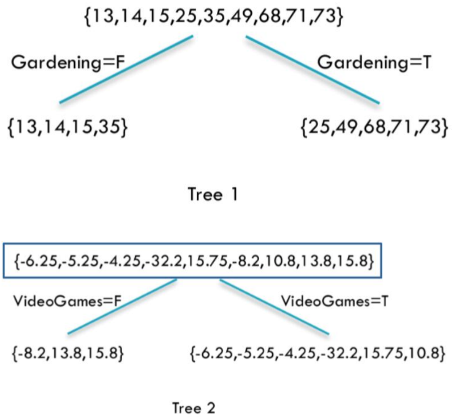
Tree 1



Tree 2

General Strategy

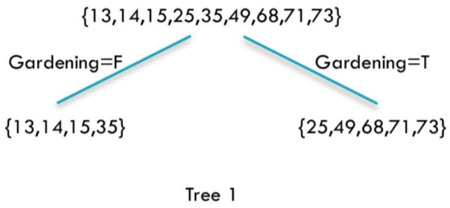
- Build tree 1, F_1

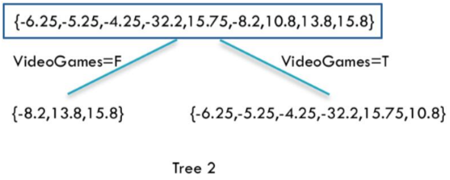


Gradient Boosting

General Strategy

- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$

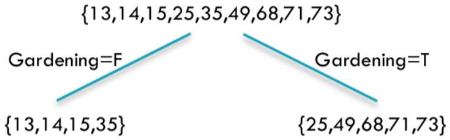




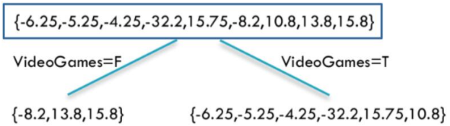
Gradient Boosting

General Strategy

- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$
- Create a new model $F_2(x) = F_1(x) + h_1(x)$



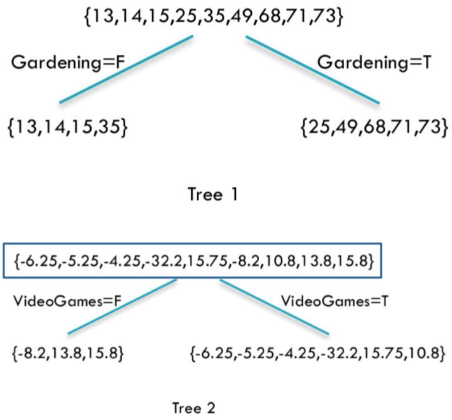
Tree 1



Tree 2

General Strategy

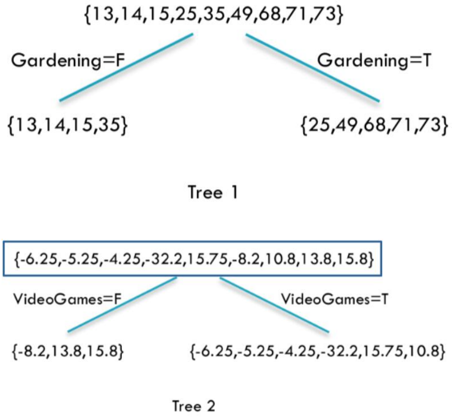
- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$
- Create a new model $F_2(x) = F_1(x) + h_1(x)$
- Fit a model to residuals, $h_2(x) = y - F_2(x)$



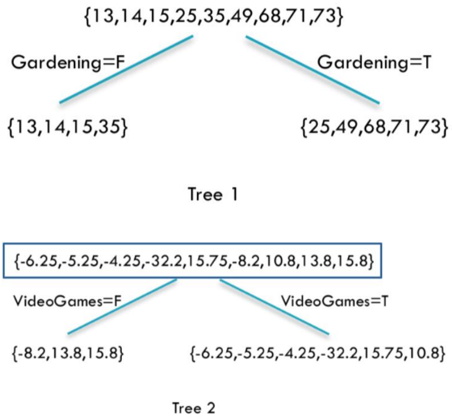
Gradient Boosting

General Strategy

- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$
- Create a new model $F_2(x) = F_1(x) + h_1(x)$
- Fit a model to residuals, $h_2(x) = y - F_2(x)$
- Create a new model $F_3(x) = F_2(x) + h_2(x)$
- ...



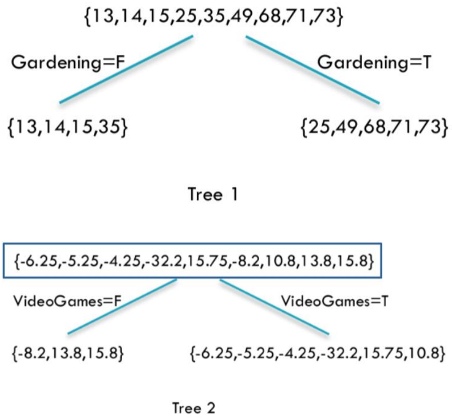
Learning Rate



Hyper Parameters

Learning Rate

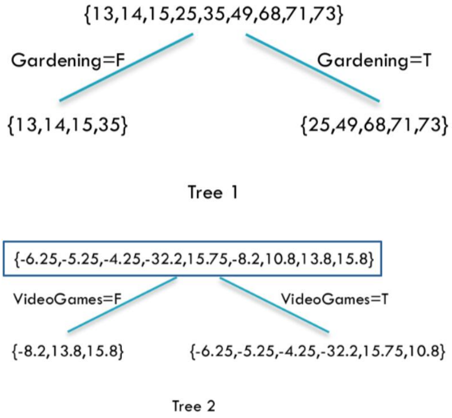
- h_j fits residuals of F_j



Hyper Parameters

Learning Rate

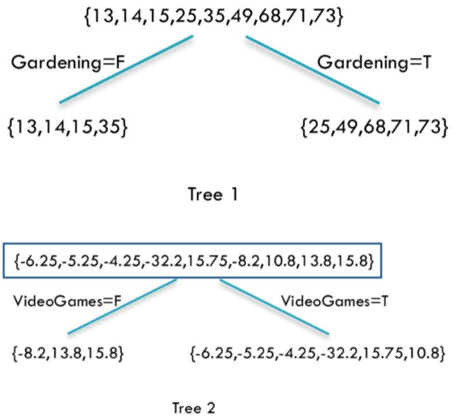
- h_j fits residuals of F_j
- $F_{j+1}(x) = F_J(x) + LR \cdot h_j(x)$
  - LR controls contribution of residual
  - $LR = 1$ in our previous example



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
- Ideally, choose LR separately for each residual to minimize loss function
  - Can apply different LR to different leaves



Gradient Boosting for Classification

- Assume binary classification

Gradient Boosting for Classification

- Assume binary classification
- Original training outputs are $y \in \{0, 1\}$

Gradient Boosting for Classification

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

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

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

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

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

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

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

  $L(y, F) = y \log(p_1) + (1 - y) \log(p_0)$
- Compute negative gradients
- Fit regression trees to negative gradients to minimize cross entropy