# Lecture 12: 27 February, 2025

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Data Mining and Machine Learning
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# Limitations of classification models

Recall

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

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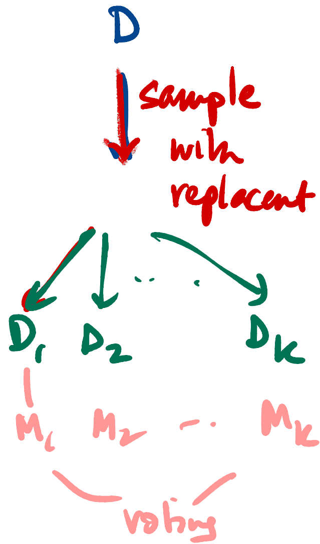
Overcoming limitations

- 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?



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  - Build an ensemble of models to average out mistakes

# Dealing with bias

- A biased model always makes mistakes
  - Build an ensemble of models to average out mistakes
- Mistakes should be compensated across models in the ensemble
  - How to build a sequence of models, each biased a different way?
  - Again, we assume we have only one set of training data

# Boosting

- Build a sequence of weak classifiers $M_1, M_2, \ldots, M_n$ on inputs $D_1, D_2, \ldots, D_n$
  - A weak classifier is any classifier that has error rate strictly below 50%

Each weak classifier is correct > 50%

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  - Initially all weights equal, $D_1$
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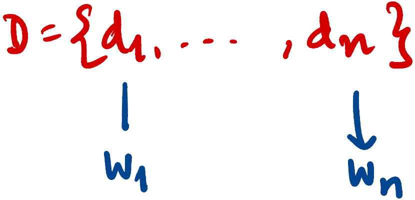
"reputation" of $M_i$

- Ensemble output
  - Individual classification outcomes are $\{-1, +1\}$
  - Unknown input $x$: ensemble outcome is weighted sum $\sum_{i=1}^{n} \alpha_i M_i(x)$
  - Check if weighted sum is negative/positive

# The boosting algorithm — Adaboost

- Initially, all data items have equal weight




**AdaBoost**($D$, $Y$, BaseLeaner, $k$)

1. Initialize $D_1(w_i) \leftarrow 1/n$ for all $i$;
2. **for** $t = 1$ to $k$ **do**
3. $f_t \leftarrow$ BaseLearner($D_t$);
4. $e_t \leftarrow \sum_{i: f_t(D_t(\mathbf{x}_i)) \neq y_i} D_t(w_i)$;
5. **if** $e_t > ½$ **then**
6. $k \leftarrow k - 1$;
7. exit-loop
8. **else**
9. $\beta_t \leftarrow e_t / (1 - e_t)$;
10. $D_{t+1}(w_i) \leftarrow D_t(w_i) \times \begin{cases} \beta_t & \text{if } f_t(D_t(\mathbf{x}_i)) = y_i \\ 1 & \text{otherwise} \end{cases}$;
11. $D_{t+1}(w_i) \leftarrow \dfrac{D_{t+1}(w_i)}{\sum_{i=1}^{n} D_{t+1}(w_i)}$

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**if** $e_t > \frac{1}{2}$ **then**

$k \leftarrow k - 1$;

exit-loop

**else**

$\beta_t \leftarrow e_t / (1 - e_t)$;

$D_{t+1}(w_i) \leftarrow D_t(w_i) \times \begin{cases} \beta_t & \text{if } f_t(D_t(\mathbf{x}_i)) = y_i \\ 1 & \text{otherwise} \end{cases}$;

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- 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

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

reputation

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Initialize D_1(w_i) ← 1/n for all i;
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                                   { 1     otherwise ;
        D_{t+1}(w_i) ← D_{t+1}(w_i) / Σ_{i=1}^{n} D_{t+1}(w_i)
```

Multiplicative weight update

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  - Pick model with lowest error rate on $D_{j+1}$ as $M_{j+1}$
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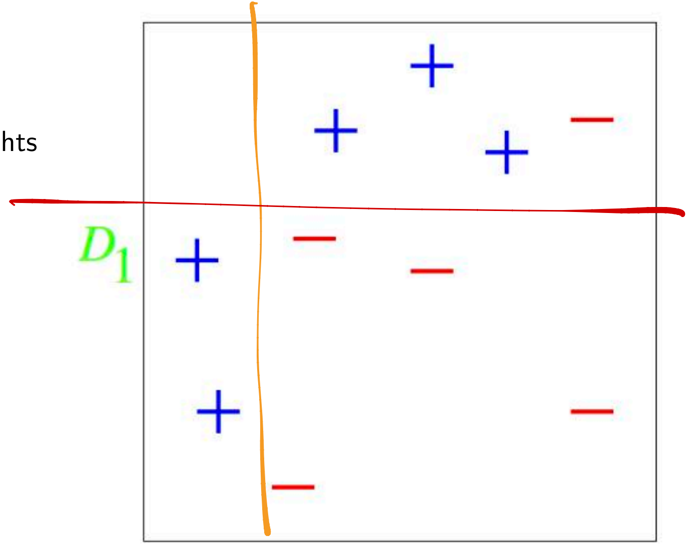
  - Reweight all training data based on error rate of $M_{j+1}$
- Note that same model $M$ may be picked in multiple iterations, assigned different weights $\alpha$

# Boosting: An example

- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights



## Boosting: An example

- Weak classifiers are horizontal and vertical lines
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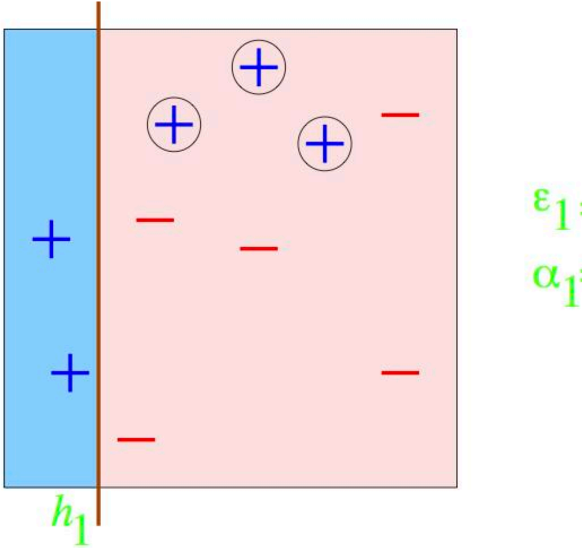
- First separator: vertical line



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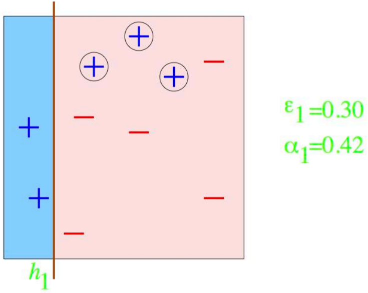


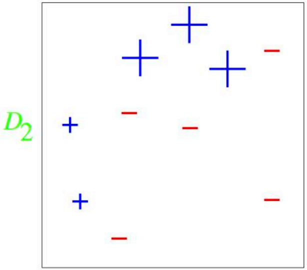

# Boosting: An example

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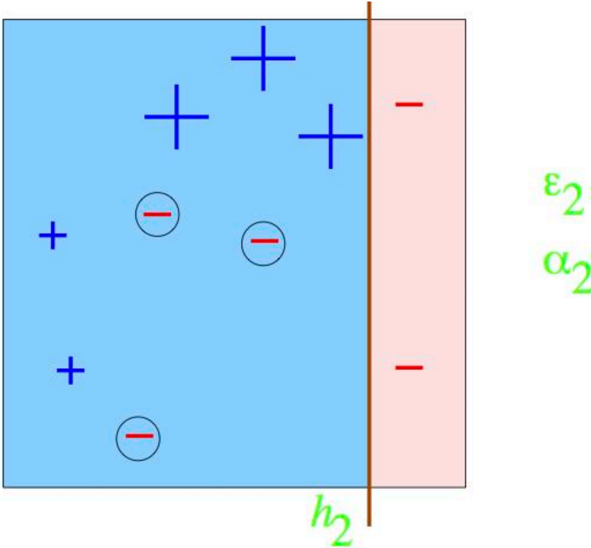
- Initial training data has equal weights
- First separator: vertical line
  - Increase weight of misclassified inputs
- Second separator: vertical line



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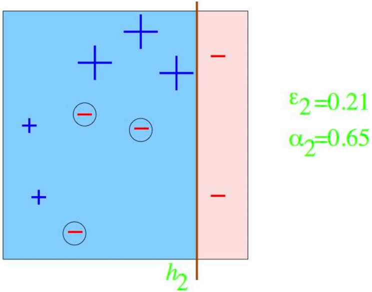


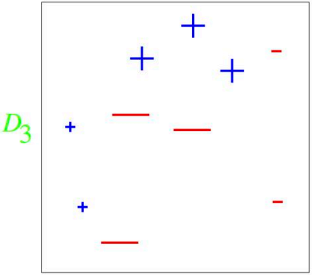

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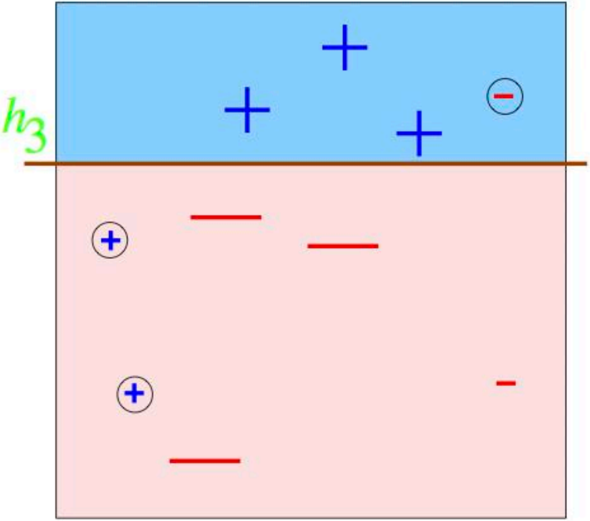
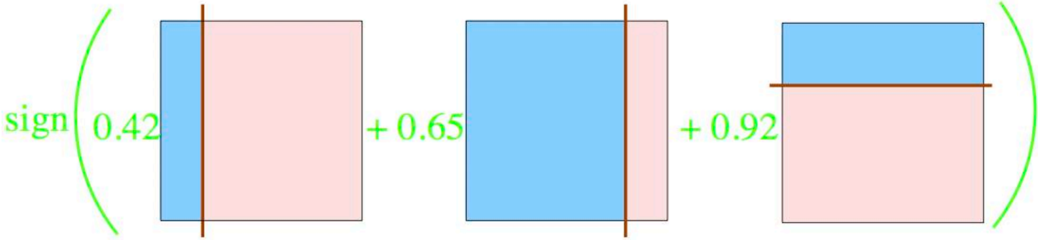
- Third separator: horizontal line



# Boosting: An example

- Final classifier is weighted sum of three weak classifiers



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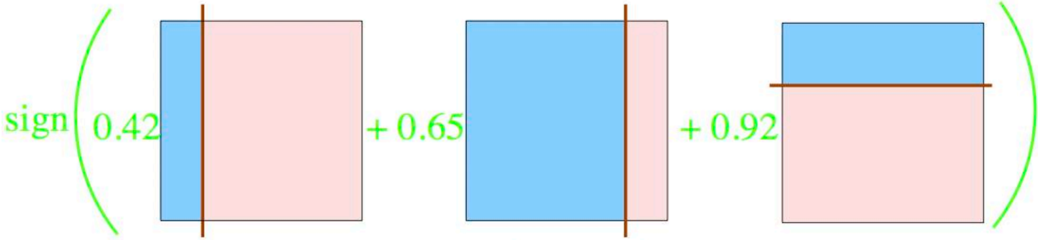
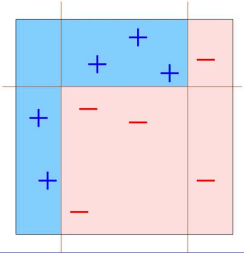



- Pictorially



# 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 $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
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  - $y_1 = 0.9$, $F(x_1) = 0.8$
  - $y_2 = 1.3$, $F(x_2) = 1.4$
  - ...

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- Add an additional model $h$, so that new prediction is $F(x) + h(x)$

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- $h(x_i) = y_i - F(x_i)$

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- $h(x_i) = y_i - F(x_i)$
- Fit a new model $h$ (typically a regression tree) to the residuals $y_i - F(x_i)$

h will fit $((x_1, y_1 - F(x_1)),$
$(x_2, y_2 - F(x_2)),$
$\vdots$
$(x_n, y_n - F(x_n)))$

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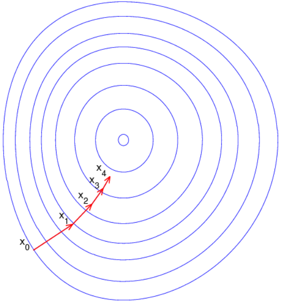
- Why should this work?

# Residuals and gradients

## Gradient descent

- Move parameters against the gradient with respect to loss function

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



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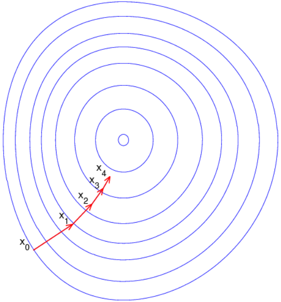


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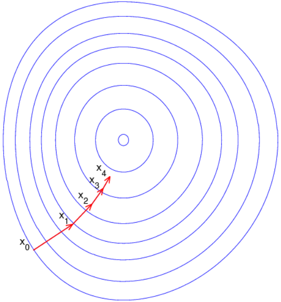


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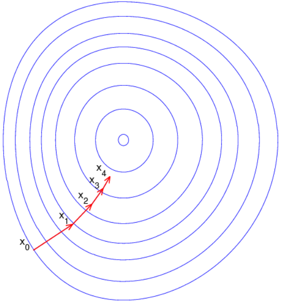


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- Minimize overall loss: $J = \sum_i L(y_i, F(x_i))$
- $\dfrac{\partial J}{\partial F(x_i)} = F(x_i) - y$

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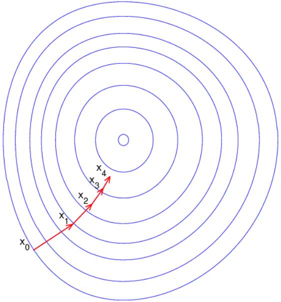
## Gradient descent

- Move parameters against the gradient with respect to loss function

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



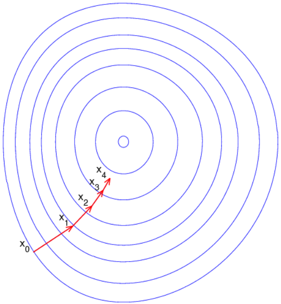

- Individual loss: $L(y, F(x)) = (y - F(x))^2/2$
- Minimize overall loss: $J = \sum_i L(y_i, F(x_i))$
- $\dfrac{\partial J}{\partial F(x_i)} = F(x_i) - y$
- Residual $y_i - F(x_i)$ is negative gradient

# Residuals and gradients

## Gradient descent

- Move parameters against the gradient with respect to loss function

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

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- Fitting $h$ to residual is same as fitting $h$ to negative gradient

# Residuals and gradients

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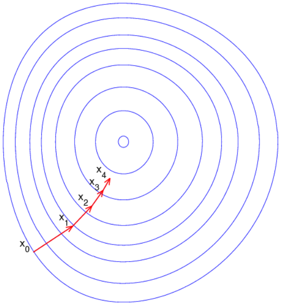


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- Residual $y_i - F(x_i)$ is negative gradient
- Fitting $h$ to residual is same as fitting $h$ to negative gradient
- Updating $F$ using residual is same as updating $F$ based on negative gradient

# 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 |

RANDOM

# 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 |
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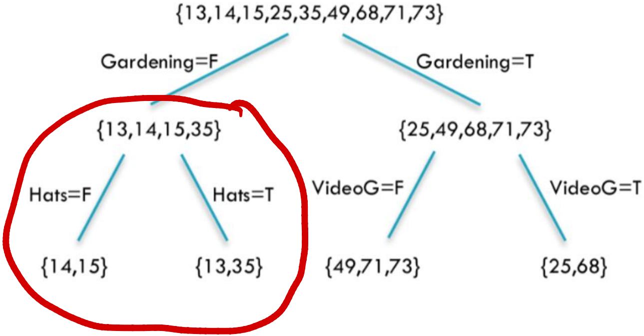
# Regression Trees




- **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 |
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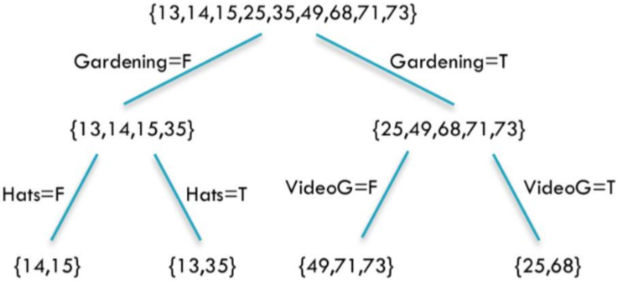
# Regression Trees




| Person ID | Age | Likes Gardening | Plays Video Games | Likes Hats |
|---|---|---|---|---|
| 1 | 13 | FALSE | TRUE | TRUE |
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| 3 | 15 | FALSE | TRUE | FALSE |
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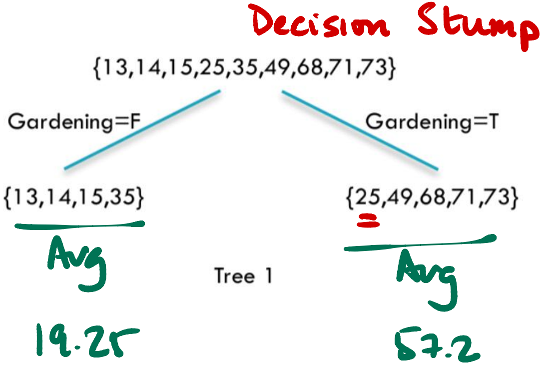
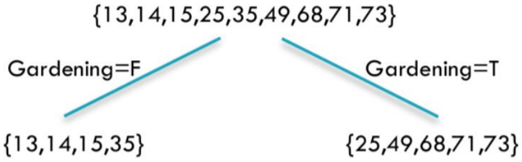
- **LikesHats** seems irrelevant, yet pops up
- Can we do better?

# 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

$y - F(x)$

| PersonID | Age | Tree1 Prediction | Tree1 Residual |
|---|---|---|---|
| 1 | 13 | 19.25 | -6.25 |
| 2 | 14 | 19.25 | -5.25 |
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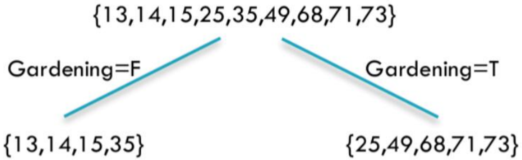


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| 1 | 13 | 19.25 | -6.25 |
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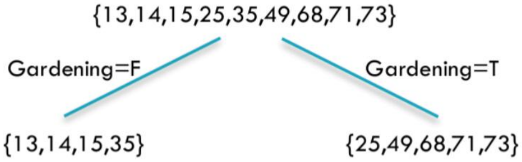


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|---|---|---|---|
| 1 | 13 | 19.25 | -6.25 |
| 2 | 14 | 19.25 | -5.25 |
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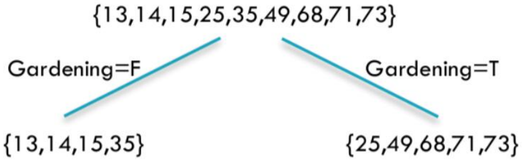


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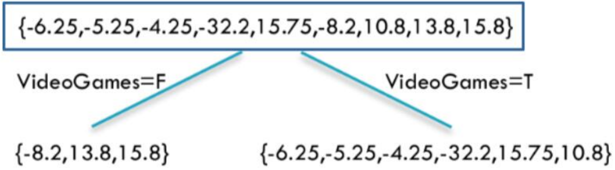
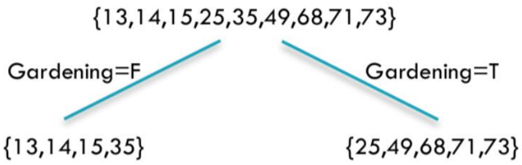


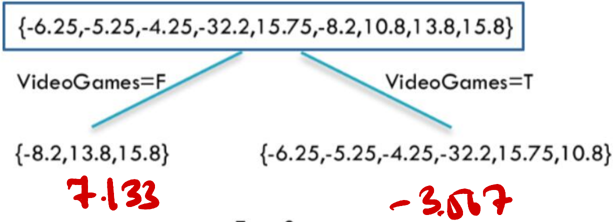

Tree 2

| 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



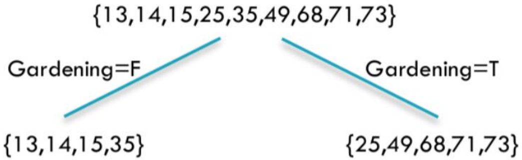

Tree 1




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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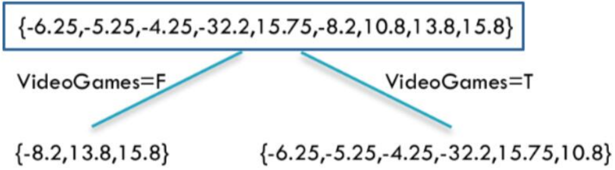


Tree 2

| 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 |
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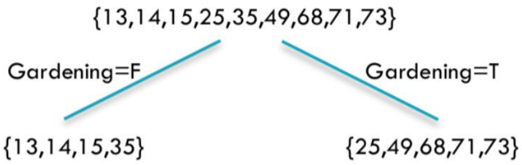


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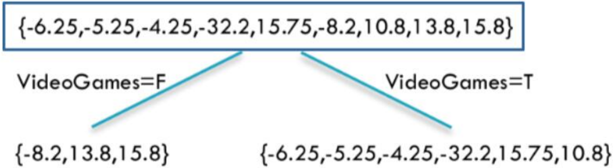


Tree 2

| 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 |
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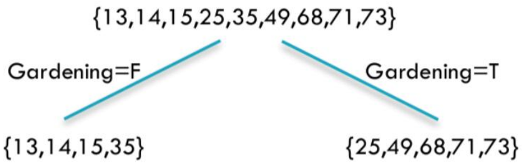


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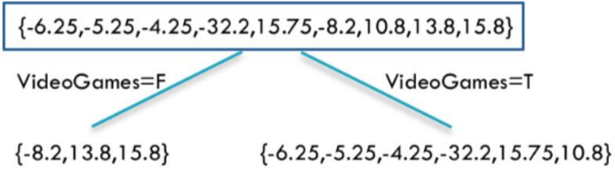


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| Person ID | Age | Tree1 Prediction | Tree1 Residual | Tree2 Prediction | Combined | Final Residual |
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| 1 | 13 | 19.25 | -6.25 | -3.567 | 15.68 | -2.683 |
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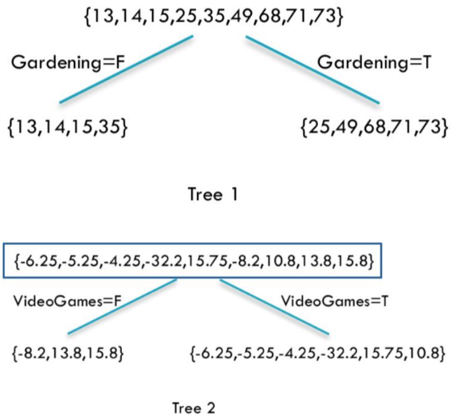
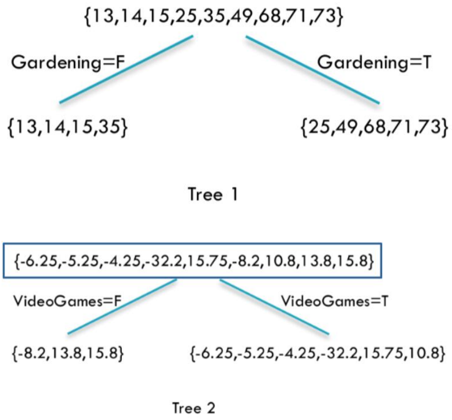
## General Strategy



## General Strategy

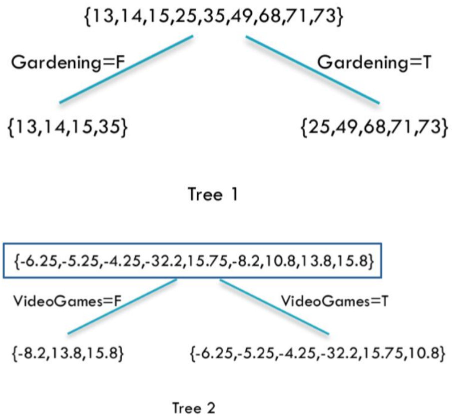
- Build tree 1, $F_1$



# Gradient Boosting

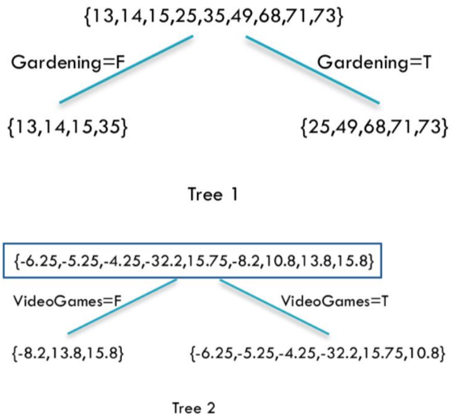
## General Strategy

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



## General Strategy

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



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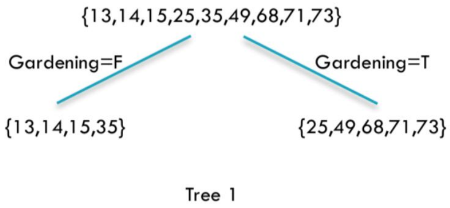
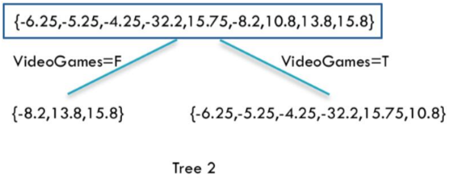
- Fit a model to residuals, $h_2(x) = y - F_2(x)$



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## General Strategy

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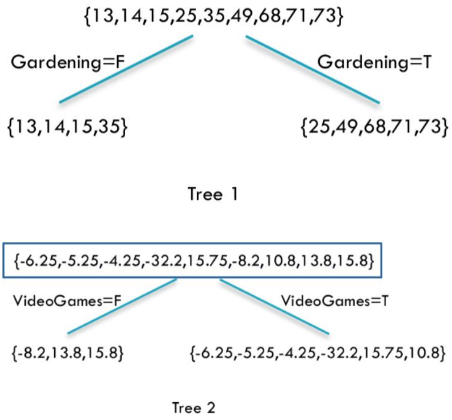
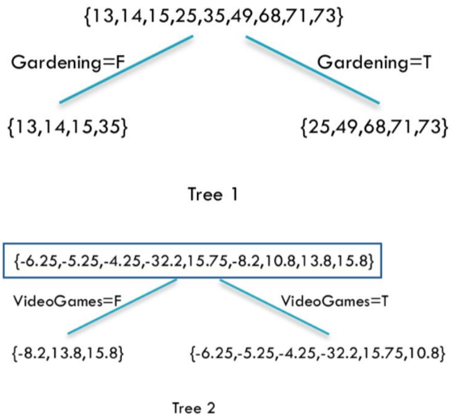
- Fit a model to residuals, $h_2(x) = y - F_2(x)$
- Create a new model $F_3(x) = F_2(x) + h_2(x)$
- ...



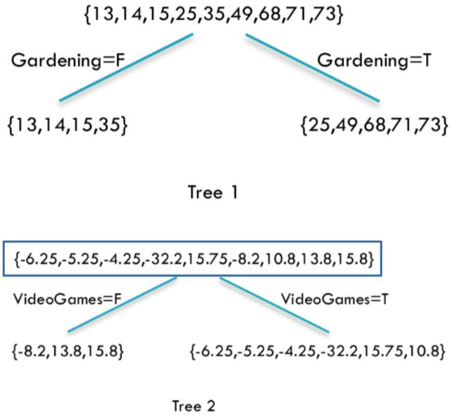
## Learning Rate



# Hyper Parameters

## Learning Rate

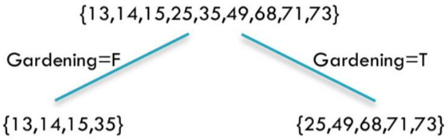
- $h_j$ fits residuals of $F_j$



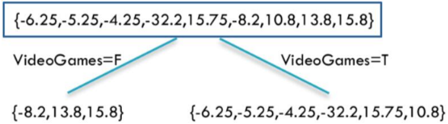
# Hyper Parameters

## 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




Tree 1




Tree 2

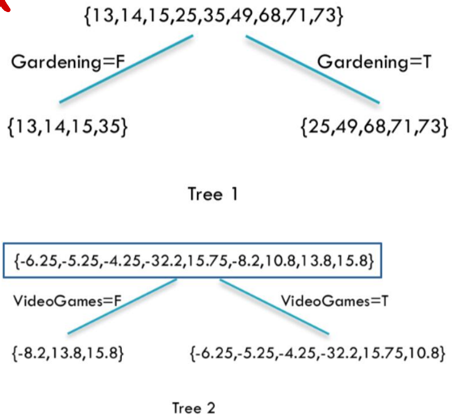
# Hyper Parameters

└ Model parameter that cannot be learned from data

## 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

Hyperparameter tuning



# Residuals and gradients

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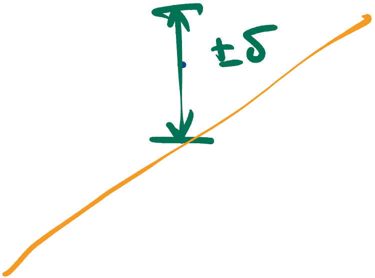
- More robust loss functions with outliers
  - Absolute loss $|y - f(x)|$
  - Huber loss

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



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

# Gradient Boosting for Classification

- Assume binary classification

0-1 loss

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

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- For each $x$, classifier produces scores $\langle s_0, s_1 \rangle$

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

$$\frac{e^{s_0}}{e^{s_0}+e^{s_1}} + \frac{e^{s_1}}{e^{s_0}+e^{s_1}} = 1$$

# Gradient Boosting for Classification

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xgboost

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- Fit regression trees to negative gradients to minimize cross entropy