

Lecture 11: 28 February, 2022

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Data Mining and Machine Learning
January–May 2022

Limitations of classification models

Recall

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

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?

|| Not useful if
variance is low

Dealing with bias

- A biased model always makes mistakes

Training Data

- 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, \dots, M_n on inputs D_1, D_2, \dots, D_n
 - A weak classifier is any classifier that has error rate strictly below 50%

Boosting

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 - A weak classifier is any classifier that has error rate strictly below 50%
- Each D_i is a weighted variant of original training data D
 - Initially all weights equal, D_1 $D = \{x_1, \dots, x_n\}$ $\frac{1}{N}$
 - Going from D_i to D_{i+1} : increase weights where M_i makes mistakes on D_i
 - M_{i+1} will compensate for errors of M_i

Boosting

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- Also, each model M_i gets a weight α_i based on its accuracy on D_i

Boosting

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 - A weak classifier is any classifier that has error rate strictly below 50%
- Each D_i is a weighted variant of original training data D
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 - Going from D_i to D_{i+1} : increase weights where M_i makes mistakes on D_i
 - M_{i+1} will compensate for errors of M_i
- Also, each model M_i gets a weight α_i based on its accuracy on D_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

Handwritten notes and diagram:

$\sum_i M_i(x)$

Counts +1 vs -1
+ve - Yes
-ve - No

↑ weighted vote

Yes	- +1
No	- -1

The boosting algorithm — Adaboost

- Initially, all data items have equal weight

AdaBoost($D, Y, \text{BaseLearner}, k$)

- Initialize $D_1(w_i) \leftarrow 1/n$ for all i ;
- for** $t = 1$ to k **do**
- $f_t \leftarrow \text{BaseLearner}(D_t)$;
- $e_t \leftarrow \sum_{i: f_t(D_t(\mathbf{x}_i)) \neq y_i} D_t(w_i)$;
- if** $e_t > 1/2$ **then**
- $k \leftarrow k - 1$;
- exit-loop
- else**
- $\beta_t \leftarrow e_t / (1 - e_t)$;
- $D_{t+1}(w_i) \leftarrow D_t(w_i) \times \begin{cases} \beta_t & \text{if } f_t(D_t(\mathbf{x}_i)) = y_i, \\ 1 & \text{otherwise} \end{cases}$;
- $D_{t+1}(w_i) \leftarrow \frac{D_{t+1}(w_i)}{\sum_{i=1}^n D_{t+1}(w_i)}$

The boosting algorithm — Adaboost

- Initially, all data items have equal weight
- Build a new model and compute its weighted error

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The boosting algorithm — Adaboost

- Initially, all data items have equal weight
- Build a new model and compute its weighted error
- Discard if error rate is above 50%

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The boosting algorithm — Adaboost

- 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

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- $f_t \leftarrow \text{BaseLearner}(D_t)$;
- $e_t \leftarrow \sum_{i: f_t(D_t(x_i)) \neq y_i} D_t(w_i)$;
 e_t small
- if** $e_t > 1/2$ **then**
- $k \leftarrow k - 1$;
- exit-loop
- else**
- $\beta_t \leftarrow e_t / (1 - e_t)$;
 $1 - e_t$ large
- $D_{t+1}(w_i) \leftarrow D_t(w_i) \times \begin{cases} \beta_t & \text{if } f_t(D_t(x_i)) = y_i, \\ 1 & \text{otherwise} \end{cases}$;
 $\frac{e_t}{1 - e_t}$ small
- $D_{t+1}(w_i) \leftarrow \frac{D_{t+1}(w_i)}{\sum_{i=1}^n D_{t+1}(w_i)}$;
 $-\beta_t < 1$

The boosting algorithm — Adaboost

- 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

$$\beta_1 = \frac{0.25}{1 - 0.25} = \frac{1}{3} \quad e_t = 0.25$$

AdaBoost($D, Y, \text{BaseLearner}, k$)

1. Initialize $D_1(w_i) \leftarrow 1/n$ for all i ;

2. **for** $t = 1$ to k **do**

3. $f_t \leftarrow \text{BaseLearner}(D_t)$;

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

10. $D_{t+1}(w_i) \leftarrow D_t(w_i) \times \begin{cases} \beta_t & \text{if } f_t(D_t(x_i)) = y_i \\ 1 & \text{otherwise} \end{cases}$

11. $D_{t+1}(w_i) \leftarrow \frac{D_{t+1}(w_i)}{\sum_{i=1}^n D_{t+1}(w_i)}$

$e_t \leq 1/2$

$e_t = 1/2 \quad e_t = 0.49$

$\beta_t = \frac{1}{1 - \frac{1}{2}} = 1$

$\frac{0.49}{0.51}$

The boosting algorithm — Adaboost

- 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

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

(Note: $\log \frac{1}{\beta_t}$ is circled in red in the original image, with a handwritten α_t next to it.)

AdaBoost($D, Y, \text{BaseLearner}, k$)

- Initialize $D_1(w_i) \leftarrow 1/n$ for all i ;
- for** $t = 1$ to k **do**
- $f_t \leftarrow \text{BaseLearner}(D_t)$; *e_t small*
- $e_t \leftarrow \sum_{i: f_t(D_t(x_i)) \neq y_i} D_t(w_i)$; *$\Rightarrow \beta_t$ small good*
- if** $e_t > 1/2$ **then**
- $k \leftarrow k - 1$;
- exit-loop
- else**
- $\beta_t \leftarrow e_t / (1 - e_t)$; *$\frac{1}{\beta_t}$*
- $D_{t+1}(w_i) \leftarrow D_t(w_i) \times \begin{cases} \beta_t & \text{if } f_t(D_t(x_i)) = y_i, \\ 1 & \text{otherwise} \end{cases}$; *β_t should be large when f_t is small*
- $D_{t+1}(w_i) \leftarrow \frac{D_{t+1}(w_i)}{\sum_{i=1}^n D_{t+1}(w_i)}$

The boosting algorithm — Adaboost

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- Initially all data items have equal weight, select M_1 as model with lowest error rate among N candidates

The boosting algorithm — Adaboost

- Each M_j could be a different type of model
- Can we pick best n out of N weak classifiers?
- Initially all data items have equal weight, select M_1 as model with lowest error rate among N candidates
- Inductively, assume we have selected M_1, \dots, M_j , with model weights $\alpha_1, \dots, \alpha_j$, and dataset is updated with new weights as D_{j+1}

The boosting algorithm — Adaboost

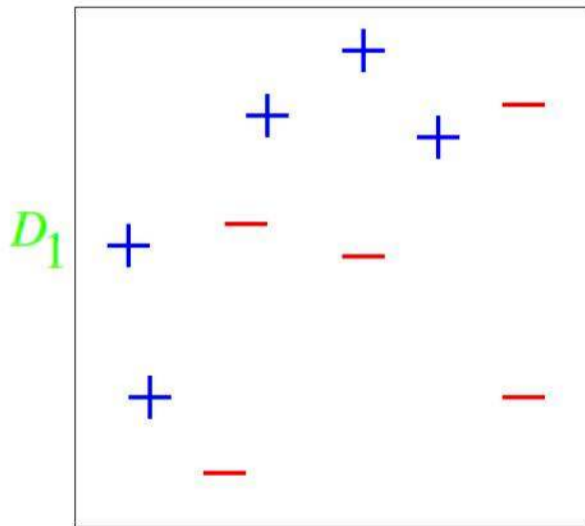
- Each M_j could be a different type of model
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 - Pick model with lowest error rate on D_{j+1} as M_{j+1}
 - Calculate α_{j+1} based on error rate of M_{j+1}
 - Reweight all training data based on error rate of M_{j+1}

The boosting algorithm — Adaboost

- Each M_j could be a different type of model
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 - Pick model with lowest error rate on D_{j+1} as M_{j+1}
 - Calculate α_{j+1} based on error rate of M_{j+1}
 - 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 α

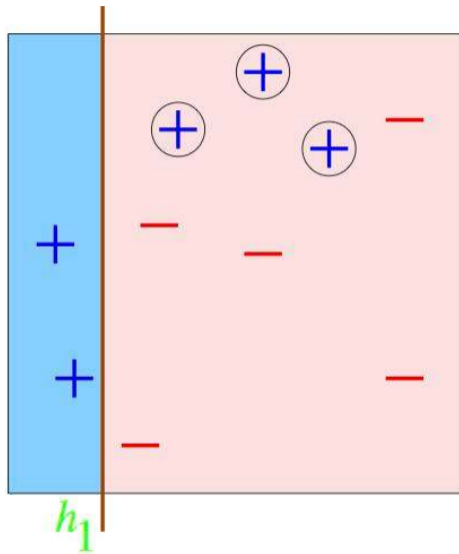
Boosting: An example

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



Boosting: An example

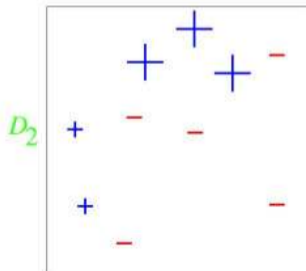
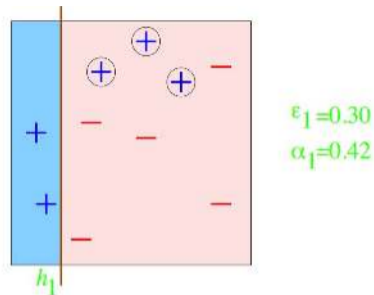
- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line



ϵ_1
 α_1

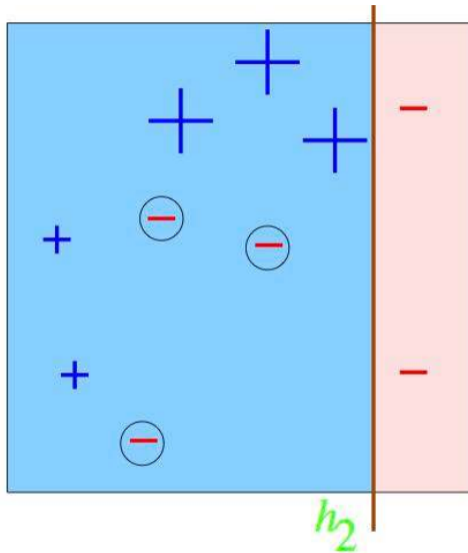
Boosting: An example

- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line
 - Increase weight of misclassified inputs



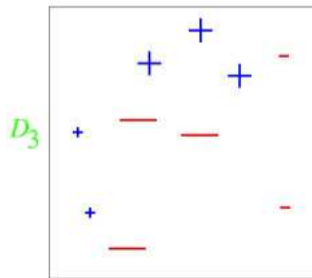
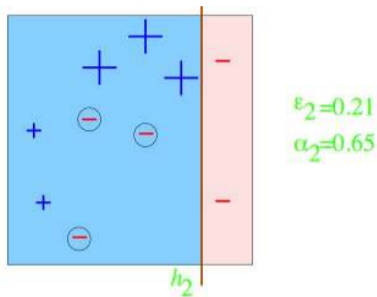
Boosting: An example

- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line
 - Increase weight of misclassified inputs
- Second separator: vertical line



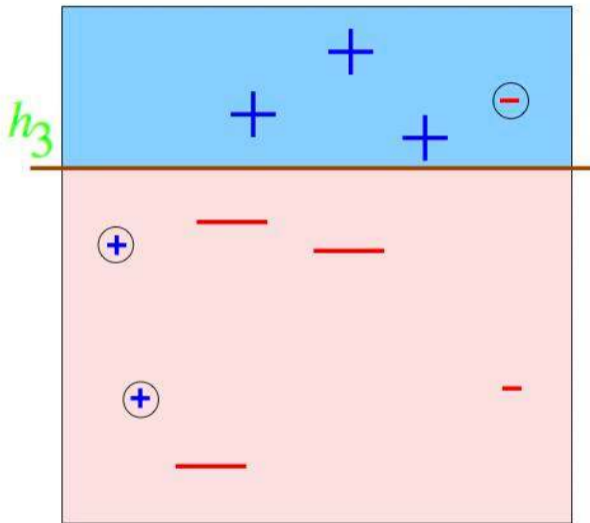
Boosting: An example

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- Second separator: vertical line
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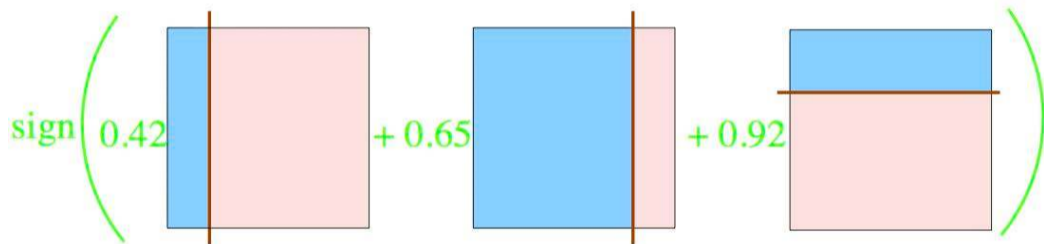
Boosting: An example

- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line
 - Increase weight of misclassified inputs
- Second separator: vertical line
 - Increase weight of misclassified inputs
- Third separator: horizontal line



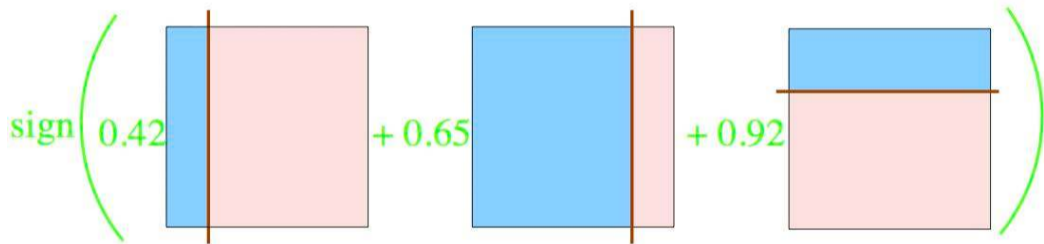
Boosting: An example

- Final classifier is weighted sum of three weak classifiers



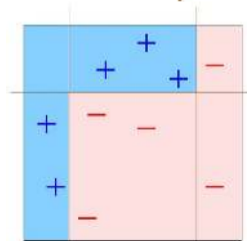
Boosting: An example

- Final classifier is weighted sum of three weak classifiers



- Pictorially

$$\alpha_j = f(e_j) \quad b_1, b_2, \dots, b_n$$
$$[\alpha_1, \alpha_2, \dots, \alpha_n]$$



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 $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$
- Fit a model $F(x)$ to minimize square loss

Gradient Boosting for Regression

- Training data $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$
- Fit a model $F(x)$ to minimize square loss
- The model F we build is good, but not perfect
 - $y_1 = 0.9, F(x_1) = 0.8$
 - $y_2 = 1.3, F(x_2) = 1.4$
 - ...

Gradient Boosting for Regression

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

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- What should h look like?

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- For each x_i , want $F(x_i) + h(x_i) = y_i$

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- What should h look like?
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- $h(x_i) = y_i - F(x_i)$

Gradient Boosting for Regression

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

Gradient Boosting for Regression

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- What should h look like?
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- $h(x_i) = y_i - F(x_i)$
- Fit a new model h (typically a regression tree) to the residuals $y_i - F(x_i)$
- If $F + h$ is not satisfactory, build another model h' to fit residuals $y_i - [F(x_i) + h(x_i)]$

$$\underbrace{y_i - [F(x_i) + h(x_i)]}_{F'(x_i)}$$

Gradient Boosting for Regression

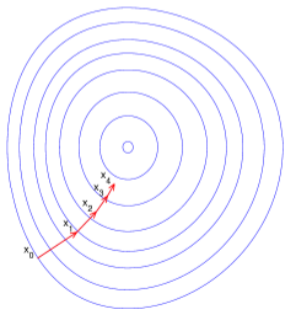
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- Why should this work?

Residuals and gradients

Gradient descent

- Move parameters against the gradient with respect to loss function

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

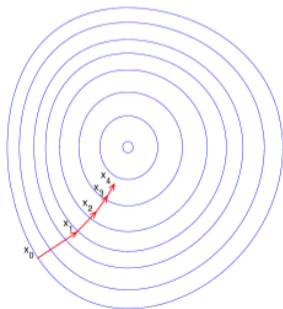


Residuals and gradients

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:

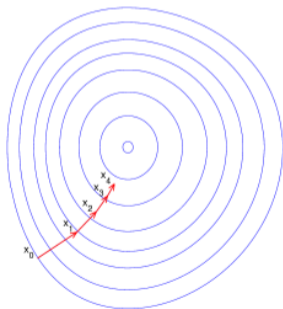
$$L(y, F(x)) = \underbrace{(y - F(x))}_{\text{residual}}^2 / 2$$

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:

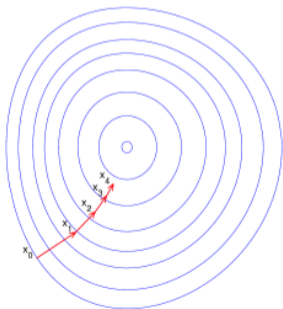
$$J = \sum_i L(y_i, F(x_i))$$

Residuals and gradients

Gradient descent

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- Individual loss:

$$L(y, F(x)) = (y - F(x))^2 / 2$$

- Minimize overall loss:

$$J = \sum_i L(y_i, F(x_i))$$

- $\frac{\partial J}{\partial F(x_i)} = \underline{F(x_i) - y}$

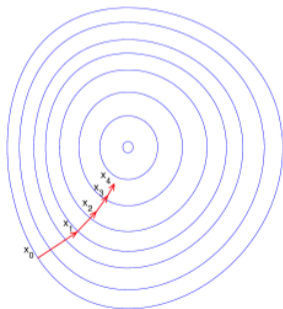
$$\frac{2(y - F(x_i))}{2} = y - F(x_i)$$

Residuals and gradients

Gradient descent

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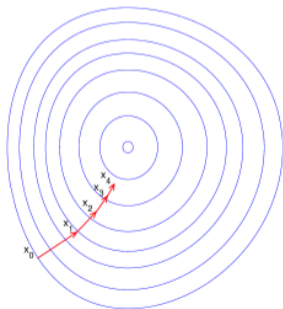
- Individual loss:
 $L(y, F(x)) = (y - F(x))^2 / 2$
- Minimize overall loss:
 $J = \sum_i L(y_i, F(x_i))$
- $\frac{\partial J}{\partial F(x_i)} = F(x_i) - y$
- Residual $y_i - F(x_i)$ is negative gradient

Residuals and gradients

Gradient descent

- Move parameters against the gradient with respect to loss function

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



- Individual loss:

$$L(y, F(x)) = (y - F(x))^2 / 2$$

- Minimize overall loss:

$$J = \sum_i L(y_i, F(x_i))$$

- $\frac{\partial J}{\partial F(x_i)} = F(x_i) - y$

- Residual $y_i - F(x_i)$ is negative gradient

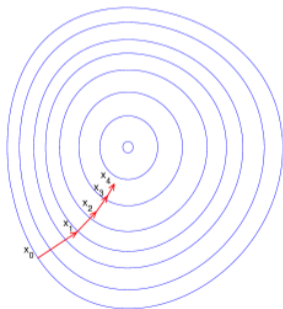
- Fitting h to residual is same as fitting h to negative gradient

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:

$$J = \sum_i L(y_i, F(x_i))$$

- $\frac{\partial J}{\partial F(x_i)} = F(x_i) - y$

- 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

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 - 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 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

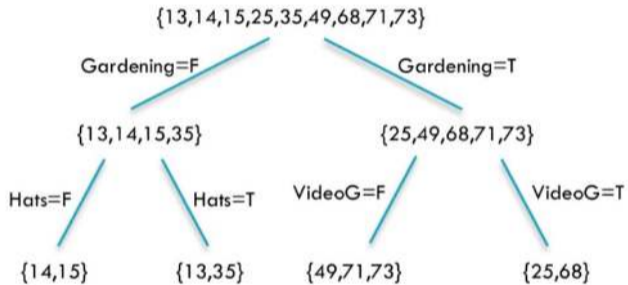
Person ID	Age	Likes Gardening	Plays Video Games	Likes Hats
1	13	FALSE	TRUE	TRUE
2	14	FALSE	TRUE	FALSE
3	15	FALSE	TRUE	FALSE
4	25	TRUE	TRUE	TRUE
5	35	FALSE	TRUE	TRUE
6	49	TRUE	FALSE	FALSE
7	68	TRUE	TRUE	TRUE
8	71	TRUE	FALSE	FALSE
9	73	TRUE	FALSE	TRUE

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

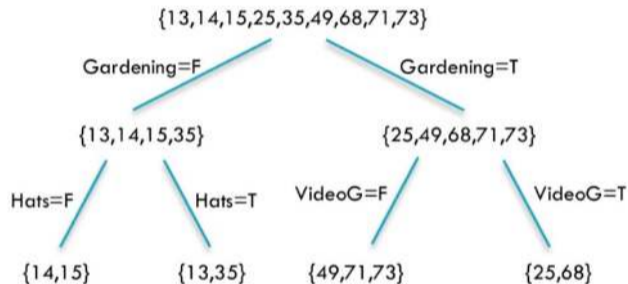
Regression Trees



Person ID	Age	Likes Gardening	Plays Video Games	Likes Hats
1	13	FALSE	TRUE	TRUE
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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

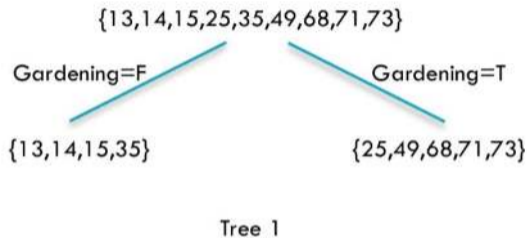
Regression Trees



Person ID	Age	Likes Gardening	Plays Video Games	Likes Hats
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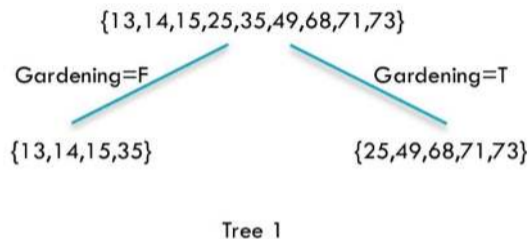
- **LikesHats** seems irrelevant, yet pops up
- Can we do better?

Residuals



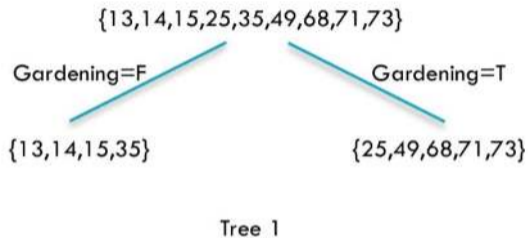
PersonID	Age	Tree1 Prediction	Tree1 Residual
1	13	19.25	-6.25
2	14	19.25	-5.25
3	15	19.25	-4.25
4	25	57.2	-32.2
5	35	19.25	15.75
6	49	57.2	-8.2
7	68	57.2	10.8
8	71	57.2	13.8
9	73	57.2	15.8

Residuals



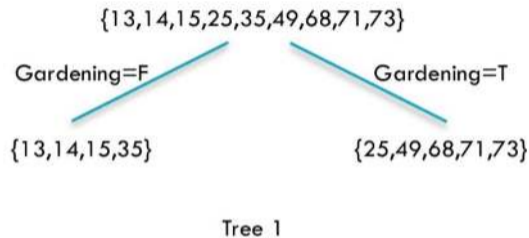
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Residuals



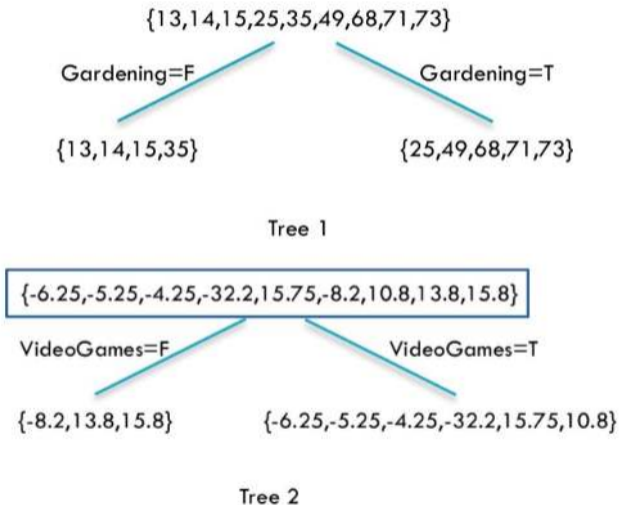
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Residuals



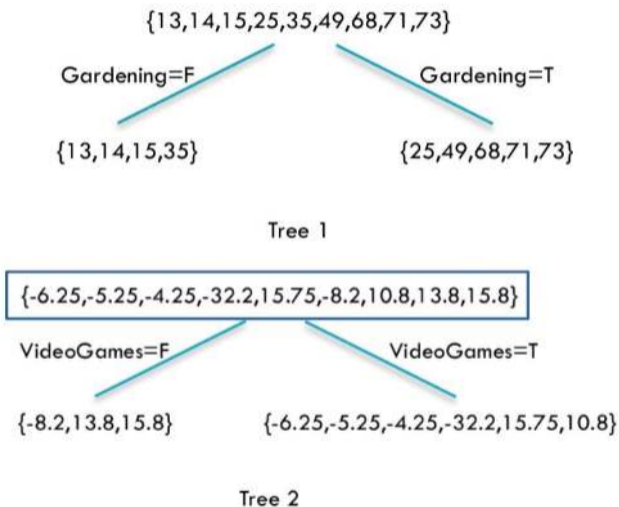
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Residuals



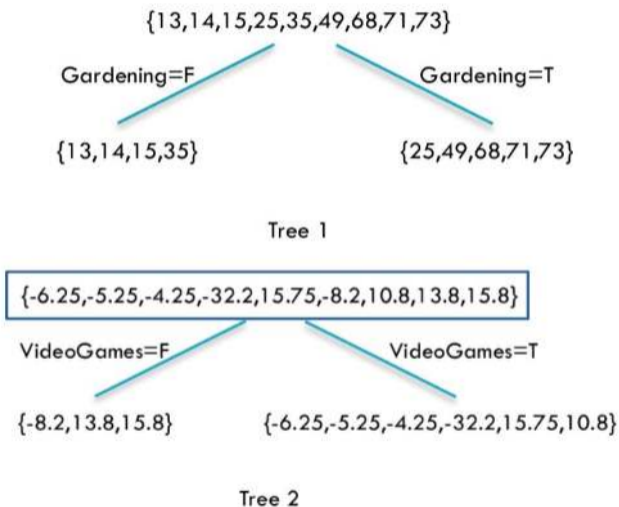
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Residuals



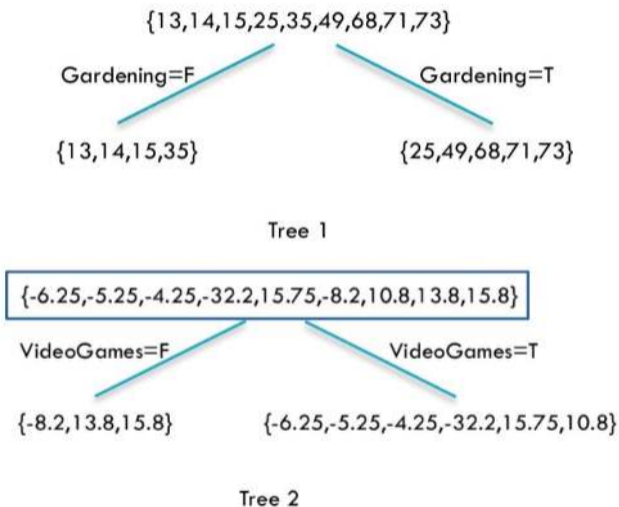
Person ID	Age	Tree1 Prediction	Tree1 Residual	Tree2 Prediction	Combined	Final Residual
1	13	19.25	-6.25	-3.567	15.68	-2.683
2	14	19.25	-5.25	-3.567	15.68	-1.683
3	15	19.25	-4.25	-3.567	15.68	-0.6833
4	25	57.2	-32.2	-3.567	53.63	-28.63
5	35	19.25	15.75	-3.567	15.68	+19.32
6	49	57.2	-8.2	7.133	64.33	-15.33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



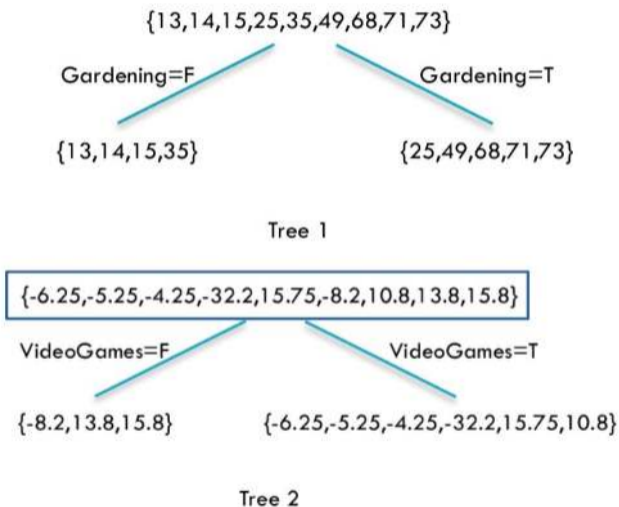
Person ID	Age	Tree1 Prediction	Tree1 Residual	Tree2 Prediction	Combined	Final Residual
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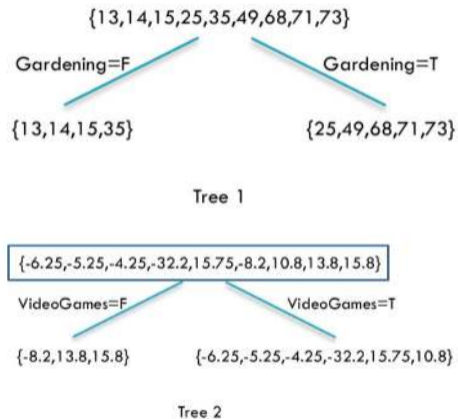
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6	49	57.2	-8.2	7.133	64.33	-15.33
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Gradient Boosting

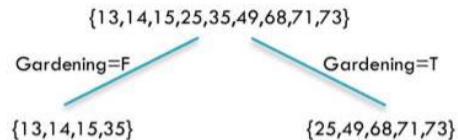
General Strategy



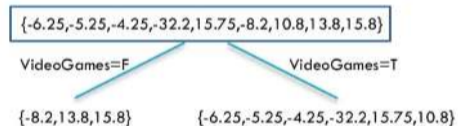
Gradient Boosting

General Strategy

- Build tree 1, F_1



Tree 1

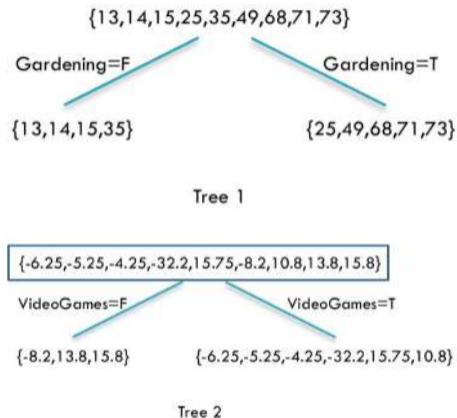


Tree 2

Gradient Boosting

General Strategy

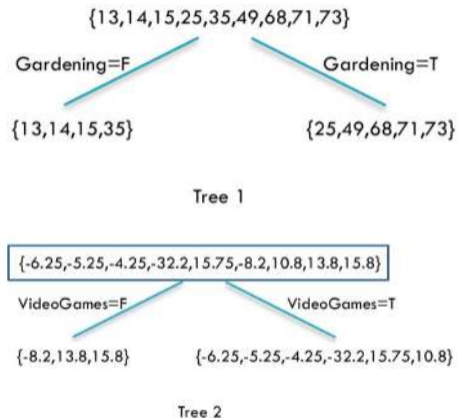
- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$



Gradient Boosting

General Strategy

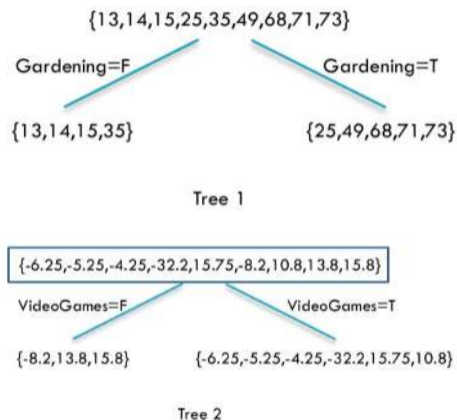
- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$
- Create a new model $F_2(x) = F_1(x) + h_1(x)$



Gradient Boosting

General Strategy

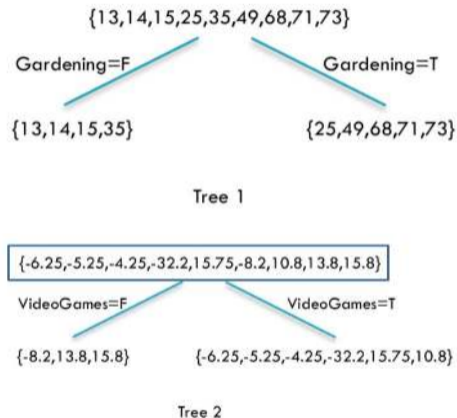
- Build tree 1, F_1
- Fit a model to residuals, $h_1(x) = y - F_1(x)$
- Create a new model $F_2(x) = F_1(x) + h_1(x)$
- Fit a model to residuals, $h_2(x) = y - F_2(x)$



Gradient Boosting

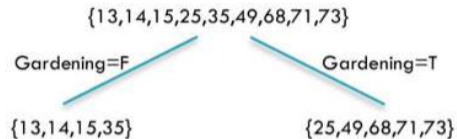
General Strategy

- 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 $F_3(x) = F_2(x) + h_2(x)$
- ...

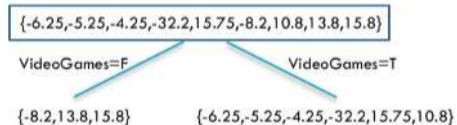


Hyper Parameters

Learning Rate



Tree 1

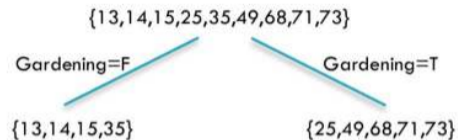


Tree 2

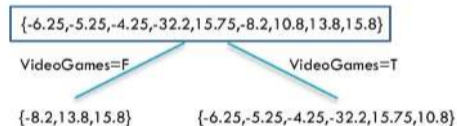
Hyper Parameters

Learning Rate

- h_j fits residuals of F_j



Tree 1

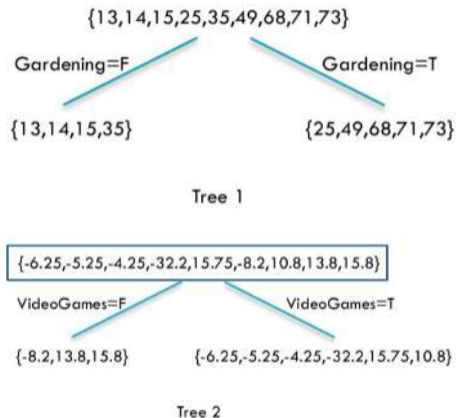


Tree 2

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

