# Lecture 12: 16 Feb, 2023 

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Data Mining and Machine Learning
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## Gradient Boosting

- AdaBoost uses weights on data-items 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 $\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)$
- Fit a model $F(x)$ to minimize square loss


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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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- Individual loss:

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L\left(y, F(x)=(y-F(x))^{2} / 2\right.
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- Minimize overall loss:

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J=\sum_{i} L\left(y_{i}, F\left(x_{i}\right)\right)
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- Fitting $h$ to residual is same as fitting $h$ to negative gradient


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- $\frac{\partial J}{\partial F\left(x_{i}\right)}=F\left(x_{i}\right)-y$
- Residual $y_{i}-F\left(x_{i}\right)$ 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


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

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

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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

$$
-g\left(x_{i}\right)=\frac{\partial L\left(y_{i}, F\left(x_{i}\right)\right)}{\partial F\left(x_{i}\right)}
$$

- Fit a regression tree $h$ to negative gradients $-g\left(x_{i}\right)$
- Update $F$ to $F+\rho h$
- $\rho$ is the learning rate


## Regression Trees

- Predict age based on given attributes

| Person <br> ID | Age | Likes <br> Garden <br> ing | Plays <br> Video <br> Games | Likes <br> 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 <br> ID | Age | Likes <br> Garden <br> ing | Plays <br> Video <br> Games | Likes <br> 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



■ LikesHats seems irrelevant, yet pops up

| Person <br> ID | Age | Likes <br> Garden <br> ing | Plays <br> Video <br> Games | Likes <br> 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



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

| Person <br> ID | Age | Likes <br> Garden <br> ing | Plays <br> Video <br> Games | Likes <br> 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

$\{13,14,15,35\}$
$\{25,49,68,71,73\}$

| PersonID Age | Tree1 <br> Prediction | Tree1 <br> 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

$\{13,14,15,35\}$
$\{25,49,68,71,73\}$

PersonID Age \begin{tabular}{ccc}
Tree1 <br>
Prediction

 

Tree1 <br>
Residual
\end{tabular}

|  |  |  |  |
| :---: | :---: | :---: | :---: |
|  | 13 | 19.25 | -6.25 |
| 2 | 14 | 19.25 | -5.25 |
| 3 | 15 | 19.25 | -4.25 |
| 4 | 25 | 57.2 | -32.2 |
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## Residuals



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| :---: | :---: | :---: | :---: |
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## Residuals



## Residuals

| $\{13,14,15,25,35,49,68,71,73\}$ | Per | $\begin{aligned} & \mathrm{A} \\ & \mathrm{~g} \\ & \mathbf{e} \end{aligned}$ | Tree 1 Predi ction | Tree1 Resi dual | Tree2 Predi ction | Co <br> mbi <br> ned | Final Resi dual |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| dening $=T$ | 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 |
| Tree 1 | 4 | 25 | 57.2 | -32.2 | -3.567 | 53.63 | -28.63 |
|  | 5 | 35 | 19.25 | 15.75 | -3.567 | 15.68 | +19.32 |
| $\{-6.25,-5.25,-4.25,-32.2,15.75,-8.2,10.8,13.8,15.8\}$ | 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 |

## Tree 2

## Residuals

| $\{13,14,15,25,35,49,68,71,73\}$ | $\begin{gathered} \text { Per } \\ \text { son } \\ \text { ID } \end{gathered}$ | $\begin{aligned} & \mathrm{A} \\ & \mathrm{~g} \\ & \mathrm{e} \end{aligned}$ | Tree1 Predi ction | Tree1 Resi dual | Tree2 Predi ction | $\begin{gathered} \text { Co } \\ \text { mbi } \\ \text { ned } \end{gathered}$ | Final Resi dual |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Gardening | 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 |
| Tree 1 | 4 | 25 | 57.2 | -32.2 | -3.567 | 53.63 | -28.63 |
| $\{-6.25,-5.25,-4.25,-32.2,15.75,-8.2,10.8,13.8,15.8\}$ | 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 |

Tree 2

## Residuals



Tree 2

## Residuals

| $\{13,14,15,25,35,49,68,71,73\}$ | Per son ID | $\begin{aligned} & \mathbf{A} \\ & \mathbf{g} \\ & \mathbf{e} \end{aligned}$ | Tree1 <br> Predi <br> ction | Tree 1 Resi dual | Tree2 <br> Predi <br> ction | Co <br> mbi <br> ned | Final <br> Resi <br> dual |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ning | 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 |
| Tree 1 | 4 | 25 | 57.2 | -32.2 | -3.567 | 53.63 | -28.63 |
|  | 5 | 35 | 19.25 | 15.75 | -3.567 | 15.68 | +19.32 |
| $\{-6.25,-5.25,-4.25,-32.2,15.75,-8.2,10.8,13.8,15.8\}$ | 6 | 49 | 57.2 | -8.2 | 7.133 | 64.33 | -15.33 |
| VideoGames=F$\{-8.2,13.8,15.8\}$ | 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 |

Tree 2

## Gradient Boosting

General Strategy


Tree 1


Tree 2

## 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, $h_{1}(x)=y-F_{1}(x)$


Tree 1


Tree 2

## Gradient Boosting

## General Strategy

■ Build tree 1, $F_{1}$
■ Fit a model to residuals, $h_{1}(x)=y-F_{1}(x)$
■ Create a new model $F_{2}(x)=F_{1}(x)+h_{1}(x)$


Tree 1


Tree 2

## Gradient Boosting

## General Strategy

■ Build tree 1, $F_{1}$
■ Fit a model to residuals, $h_{1}(x)=y-F_{1}(x)$
■ Create a new model $F_{2}(x)=F_{1}(x)+h_{1}(x)$

- Fit a model to residuals, $h_{2}(x)=y-F_{2}(x)$

$$
\{13,14,15,25,35,49,68,71,73\}
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Tree 1


Tree 2

## Gradient Boosting

## General Strategy

■ Build tree 1, $F_{1}$
■ Fit a model to residuals, $h_{1}(x)=y-F_{1}(x)$
■ 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 $F_{3}(x)=F_{2}(x)+h_{2}(x)$


Tree 1

Tree 2

## 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 $F_{j}$
- $F_{j+1}(x)=F_{J}(x)+L R \cdot h_{j}(x)$
- $L R$ controls contribution of residual
- $L R=1$ in our previous example


Tree 1


Tree 2

## Hyper Parameters

## Learning Rate

- $h_{j}$ fits residuals of $F_{j}$
- $F_{j+1}(x)=F_{J}(x)+L R \cdot h_{j}(x)$
- $L R$ controls contribution of residual
- $L R=1$ in our previous example

■ Ideally, choose $L R$ separately for each residual to minimize loss function

- Can apply different $L R$ to different leaves

$$
\{13,14,15,25,35,49,68,71,73\}
$$



Tree 1


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■ Fit regression trees to negative gradients to minimize cross entropy

