

# Lecture 12: 17 May, 2021

Madhavan Mukund

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

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

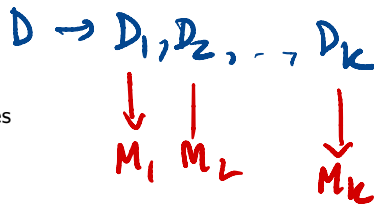
# Limitations of classification models

## 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?

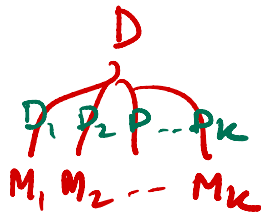


# Dealing with bias

- A biased model always makes mistakes
  - 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%

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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,  $D_1$   $\frac{1}{N}$  if  $|D|=N$
  - 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  $M_i$

$$d_j \in D$$

$w_j$  - weights

$$\sum w_j = 1$$

Decision Stump

Single node decision tree

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  - $M_{i+1}$  will compensate for errors of  $M_i$
- Also, each model  $M_i$  gets a weight  $\alpha_i$  based on its accuracy on  $D_i$

$$M_1, M_2, \dots, M_k$$

$$\alpha_1, \alpha_2, \dots, \alpha_k$$

- used each model got an equal vote

Weighted vote



# Boosting

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  - $M_{i+1}$  will compensate for errors of  $M_i$
- Also, each model  $M_i$  gets a weight  $\alpha_i$  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

$$-(\alpha_1 + \alpha_2 - \alpha_i)$$

$$\sum \alpha_i$$
$$M_i(x) = 0 \text{ or } -1$$

$$\sum_{i=1}^n \alpha_i M_i(x)$$
$$+1, -1$$
$$\sum \alpha_i$$
$$M_i(x) = 1$$

# 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
- $f_t \leftarrow \text{BaseLearner}(D_t)$ ;
- $e_t \leftarrow \sum_{i: f_t(D_t(\mathbf{x}_i)) \neq y_i} D_t(w_i)$ ;  $e_t = 0.1$   $\beta_t = \frac{0.1}{0.9}$
- if  $e_t > 1/2$  then
- $k \leftarrow k - 1$ ;  $e_t \leq 1/2 = 0.4$
- exit-loop
- else
- $\beta_t \leftarrow e_t / (1 - e_t)$ ;  $\beta_t = \frac{\leq 1/2}{1 - (\leq 1/2)} = \frac{0.4}{0.6}$
- $D_{t+1}(w_i) \leftarrow \underline{D_t(w_i)} \times \begin{cases} \underline{\beta_t} & \text{if } f_t(D_t(\mathbf{x}_i)) = y_i \\ 1 & \text{otherwise} \end{cases}$ ;
- $D_{t+1}(w_i) \leftarrow \frac{D_{t+1}(w_i)}{\sum_{i=1}^n D_{t+1}(w_i)}$  **Normalize**

# The boosting algorithm — Adaboost

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

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- Damping factor — reduce weight of correct inputs

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# The boosting algorithm — Adaboost

- Initially, all data items have equal weight
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- Reweight data items and normalize

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# The boosting algorithm — Adaboost

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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

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

*Handwritten notes:  $\alpha_t \sim \frac{1}{\beta_t}$ ,  $\alpha_t = \log \frac{1}{\beta_t}$ ,  $y \in \{0,1\}$*

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*Handwritten notes:  $e_t$  fraction of error*

*Handwritten notes:  $e_t$  small - good*

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  - Pick model with lowest error rate on  $D_{j+1}$  as  $M_{j+1}$
  - Calculate  $\alpha_{j+1}$  based on error rate of  $M_{j+1}$
  - Reweight all training data based on error rate of  $M_{j+1}$

Multiplicative  
updates

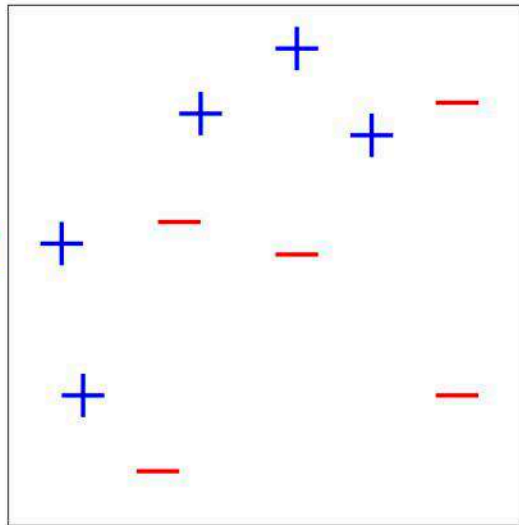
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- Note that same model  $M$  may be picked in multiple iterations, assigned different weights  $\alpha$

# Boosting: An example

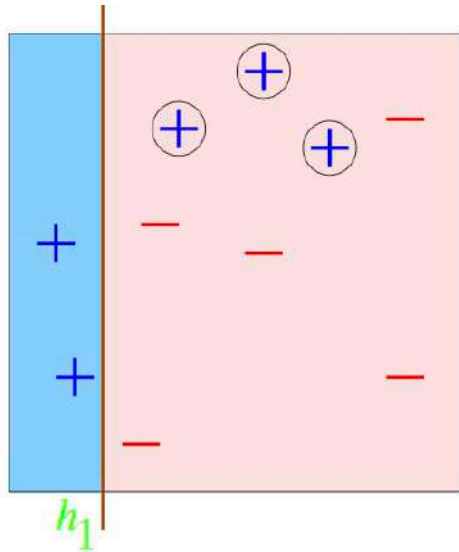
- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights

$D_1$



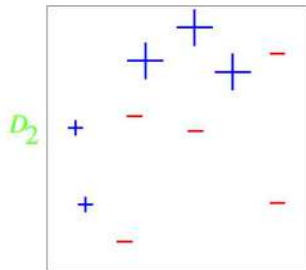
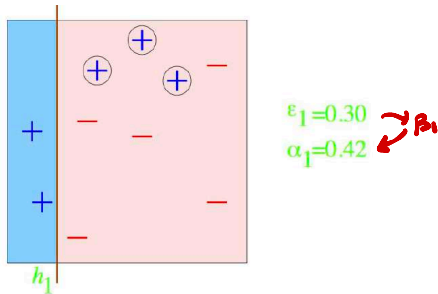
# Boosting: An example

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



# Boosting: An example

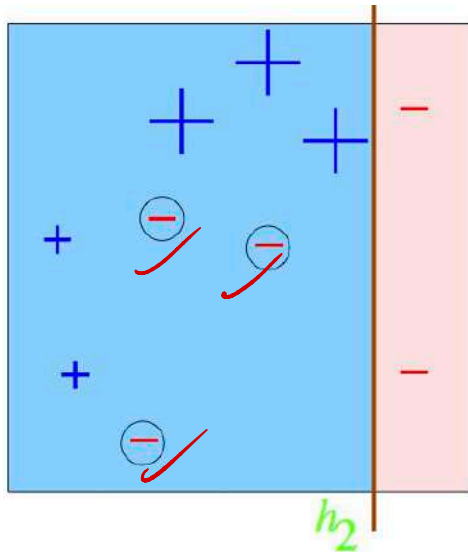
- Weak classifiers are horizontal and vertical lines
- Initial training data has equal weights
- First separator: vertical line
  - Increase weight of misclassified inputs





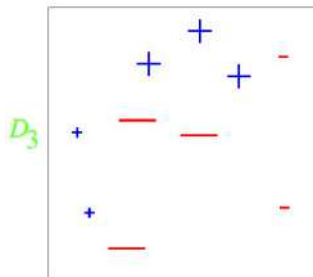
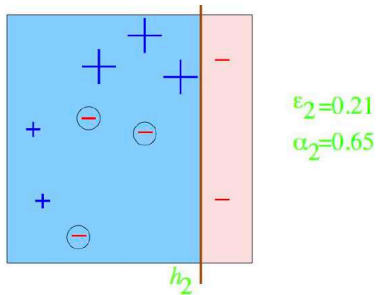
# Boosting: An example

- 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



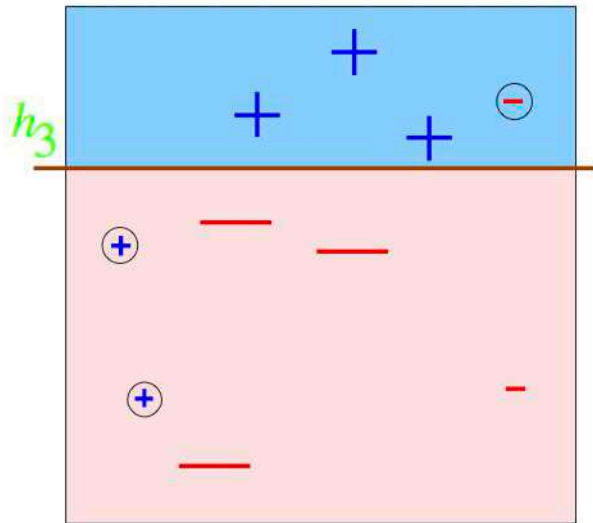
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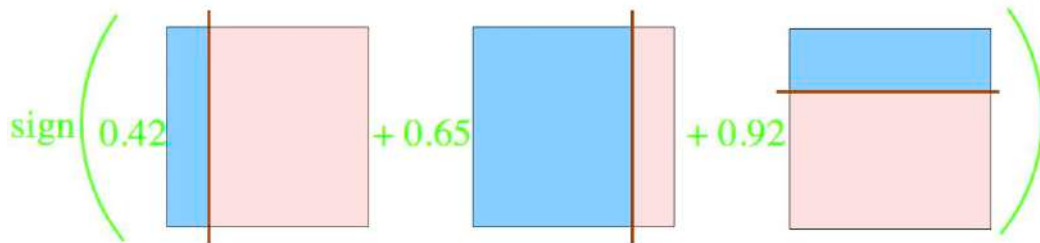
# Boosting: An example

- Weak classifiers are horizontal and vertical lines
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- First separator: vertical line
  - Increase weight of misclassified inputs
- Second separator: vertical line
  - Increase weight of misclassified inputs
- Third separator: horizontal line



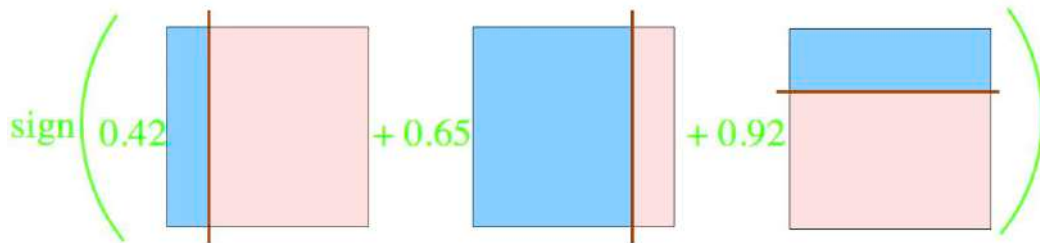
# Boosting: An example

- Final classifier is weighted sum of three weak classifiers

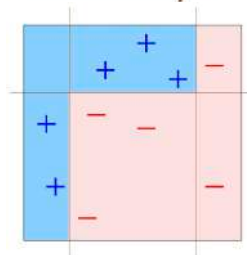


# Boosting: An example

- Final classifier is weighted sum of three weak classifiers



- Pictorially



# 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

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



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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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- If  $F + h$  is not satisfactory, build another model  $h'$  to fit residuals  $y_i - [F(x_i) + h(x_i)]$

# Gradient Boosting for Regression

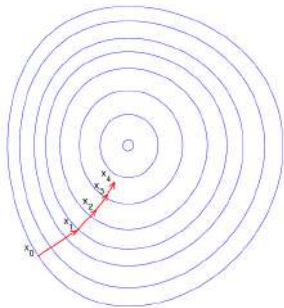
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- Why should this work?

# Residuals and gradients

## Gradient descent

- Move parameters against the gradient with respect to loss function

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



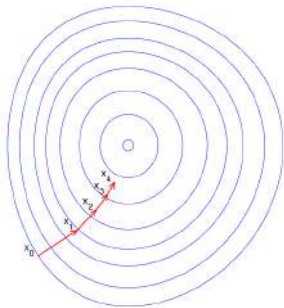


# Residuals and gradients

## 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:

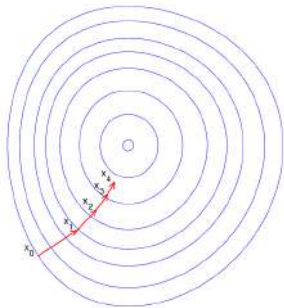
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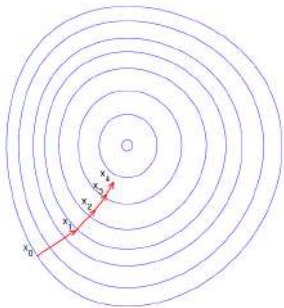
- Move parameters against the gradient with respect to loss function

$$\theta_0 + \theta_1 x_1 + \theta_2 x_2$$

↑

$$\theta_i \leftarrow \theta_i - \frac{\partial J}{\partial \theta_i} \text{ --- Loss fn}$$

$$\frac{\partial \text{Loss}}{\partial \theta_i}$$



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

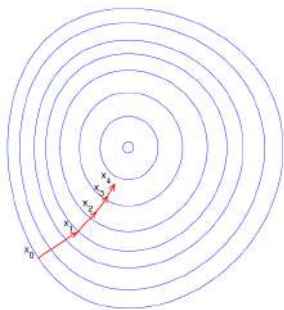
$$\frac{2 \cdot (y_i - F(x_i))}{2} = -1$$

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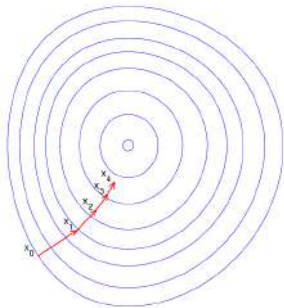
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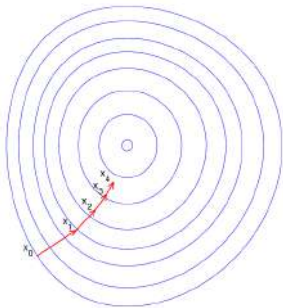
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# Residuals and gradients

## Gradient descent

- Move parameters against the gradient with respect to loss function

$$\theta_i \leftarrow \theta_i - \frac{\partial J}{\partial \theta_i} \quad \text{red } \delta$$



- Individual loss:

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

- Minimize overall loss:

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

$$F + \delta h$$

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

- 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

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

$$x_1 - y_1$$

$$x_2 - y_2$$

$$x_n - y_n$$

$$F$$

- 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

$$x_1 \rightarrow v_1$$

$$x_2 \rightarrow v_2$$

$$x_n \rightarrow v_n$$