Foundations of Machine Learning (ECE 5984)

- Logistic Regression -

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Classification

Question	Answer "y"	
Is this email spam?	no	yes
Is the transaction fraudulent?	no	yes
Is the tumor malignant?	no	yes

y can only be one of two values

false true

0 1

useful for classification

"binary classification"

class = category

"negative class"

≠ "bad"

absence

"positive class"

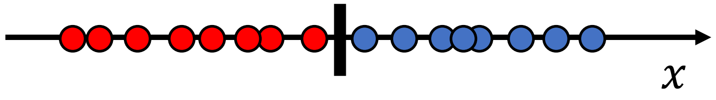
≠ "good"

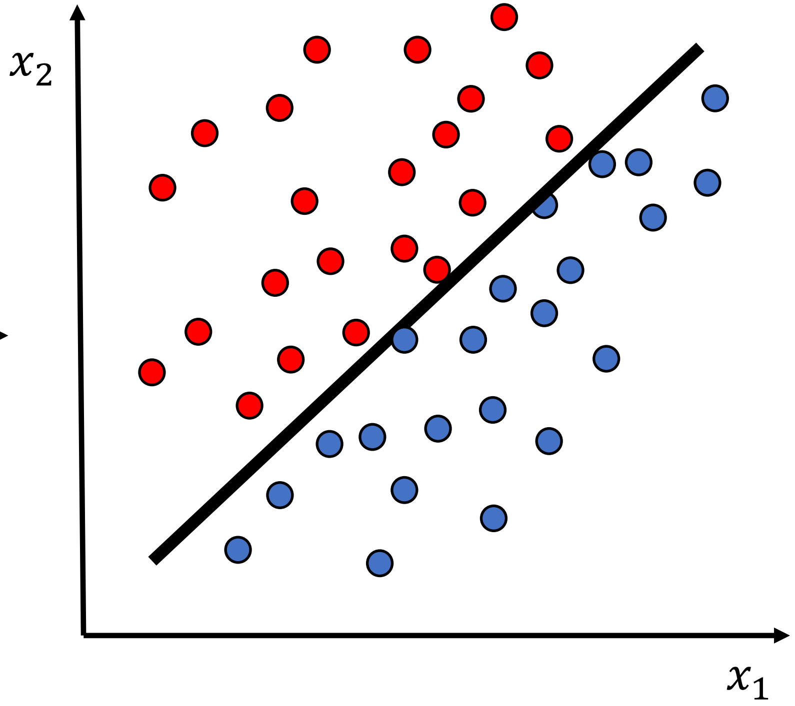
presence

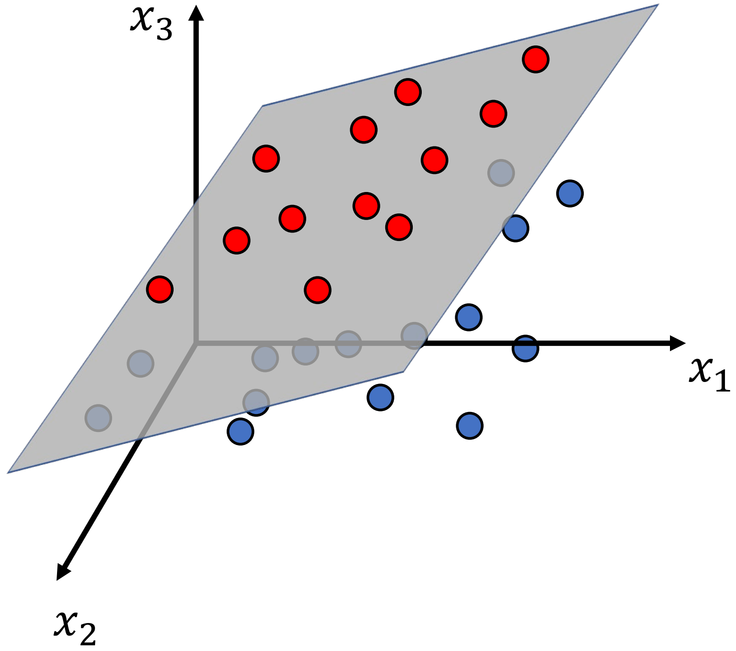
The Perceptron

Linear Classification

- Linear decision boundary







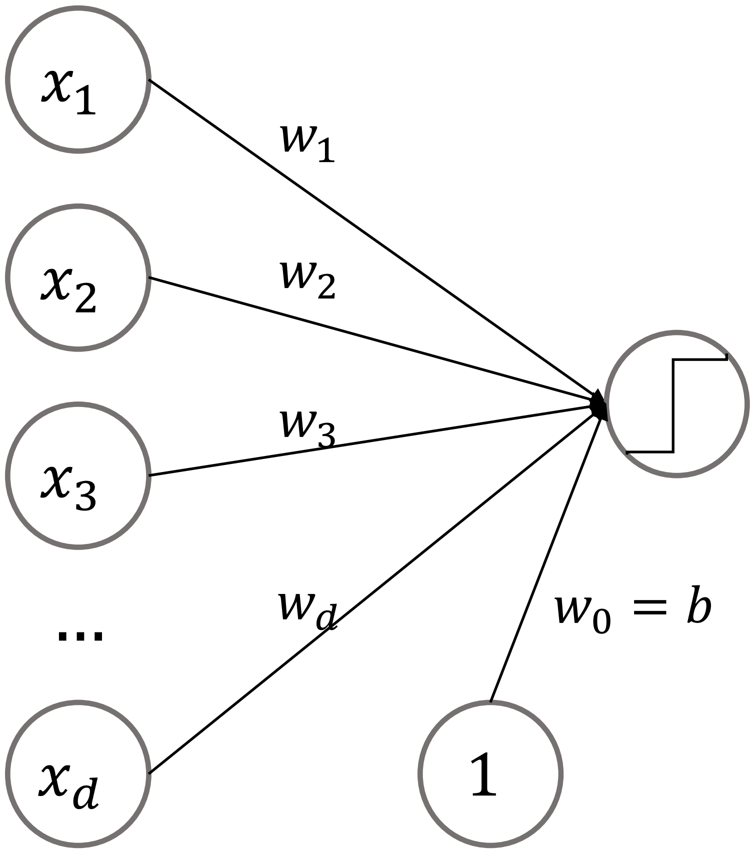
$x + b = 0$

$w_1 x_1 + w_2 x_2 + b = 0$

$w_1 x_1 + w_2 x_2 + w_3 x_3 + b = 0$

Rosenblatt's Perceptron

- A single perceptron as a linear decision boundary (hyperplane)

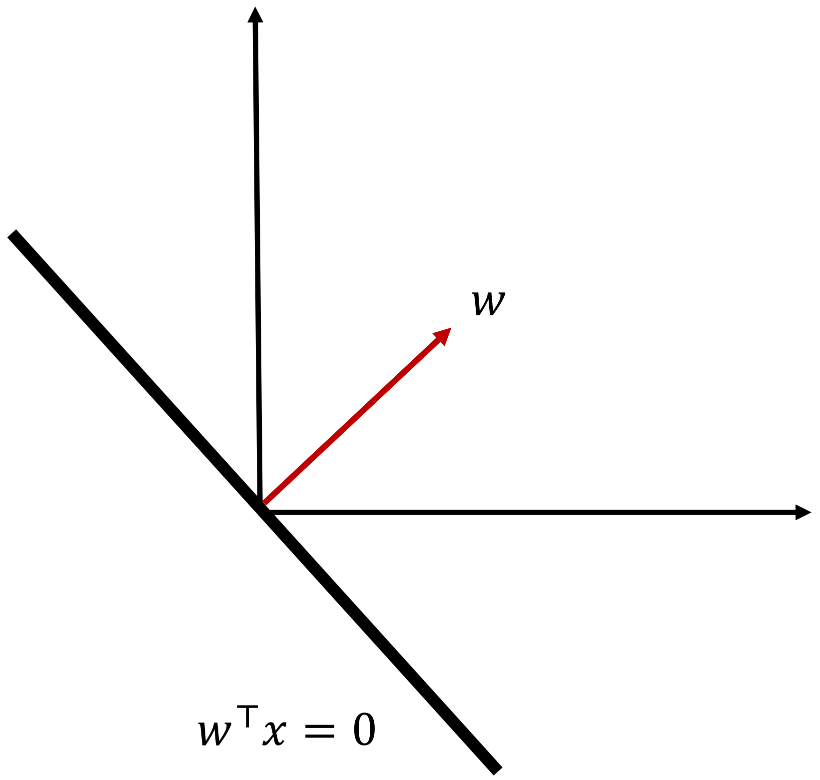


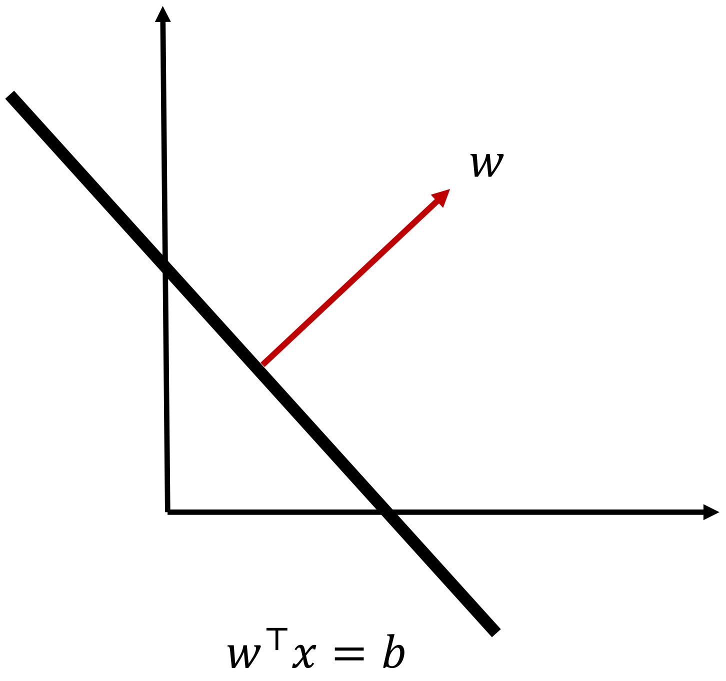
$$f(x) = \begin{cases} 1, & w^{\top}x \geq 0 \\ 0, & w^{\top}x < 0 \end{cases}$$

Rosenblatt, Psychological Review 1958

Perceptron

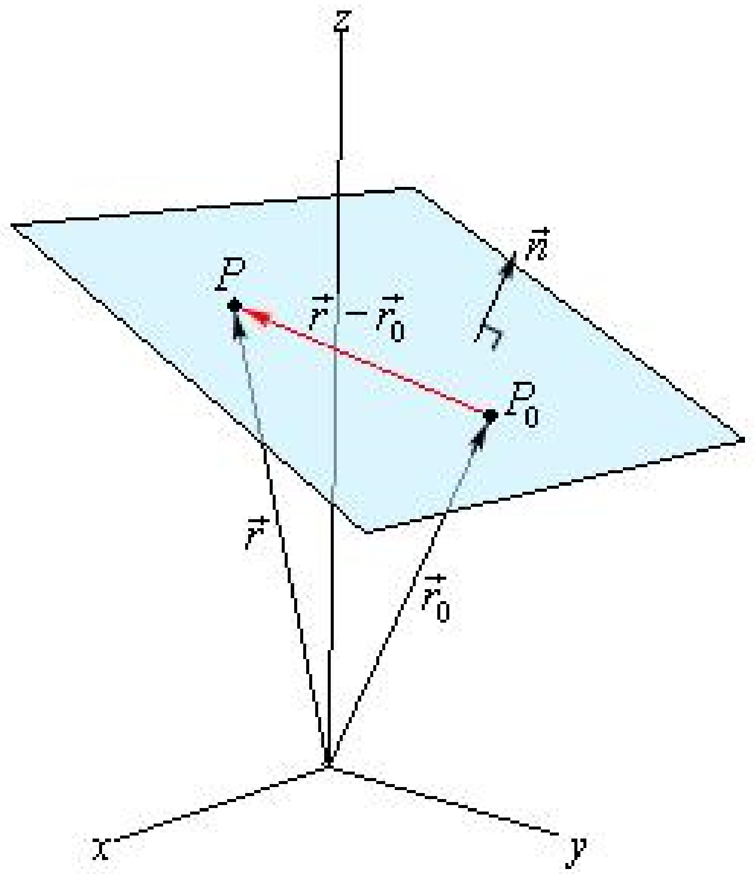
- Weight vector is orthogonal to the hyperplane





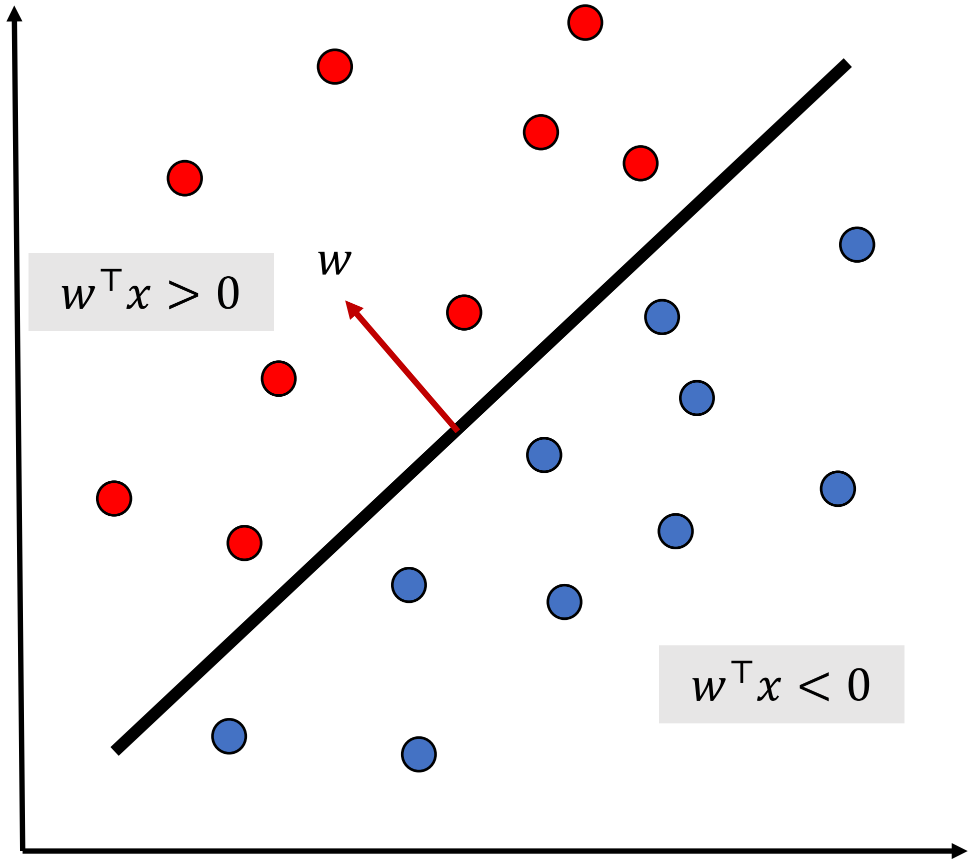
Perceptron

- Weight vector is orthogonal to the hyperplane



Perceptron

- Find a separating hyperplane

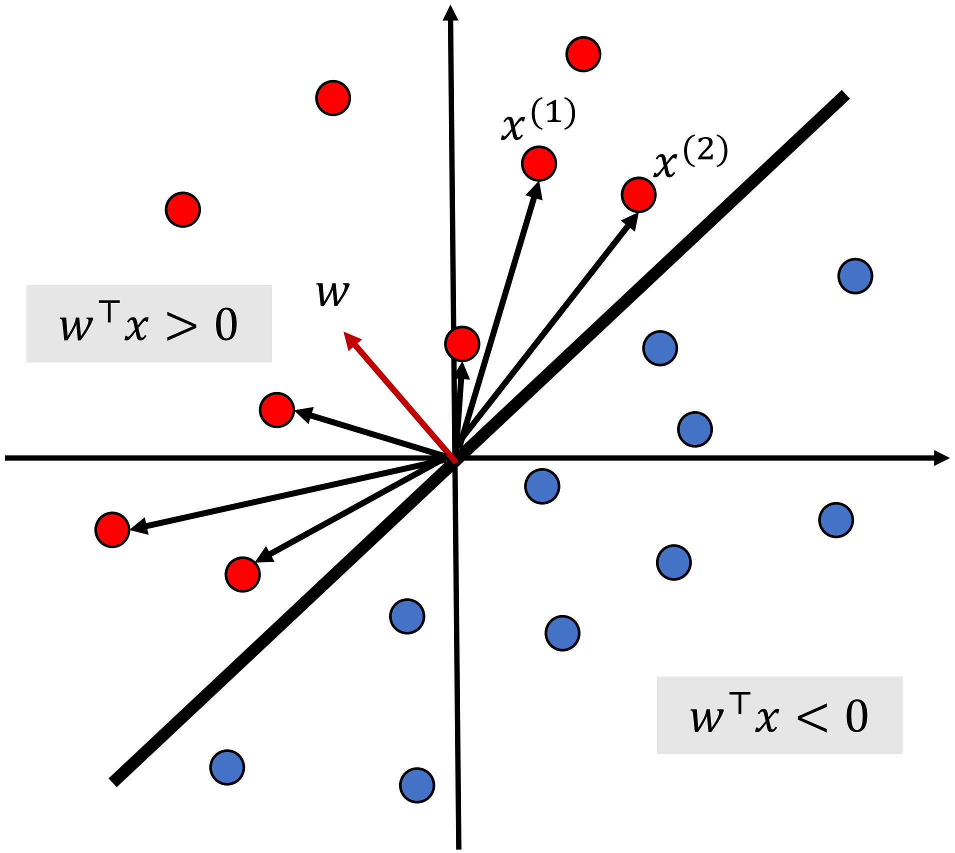


Perceptron

- Find a separating hyperplane

Angles between all positive examples $x^{(i)}$ and w should be less then ?? degree

Angles between all negative examples $x^{(i)}$ and w should be greater then ?? degree



Perceptron Learning Algorithm

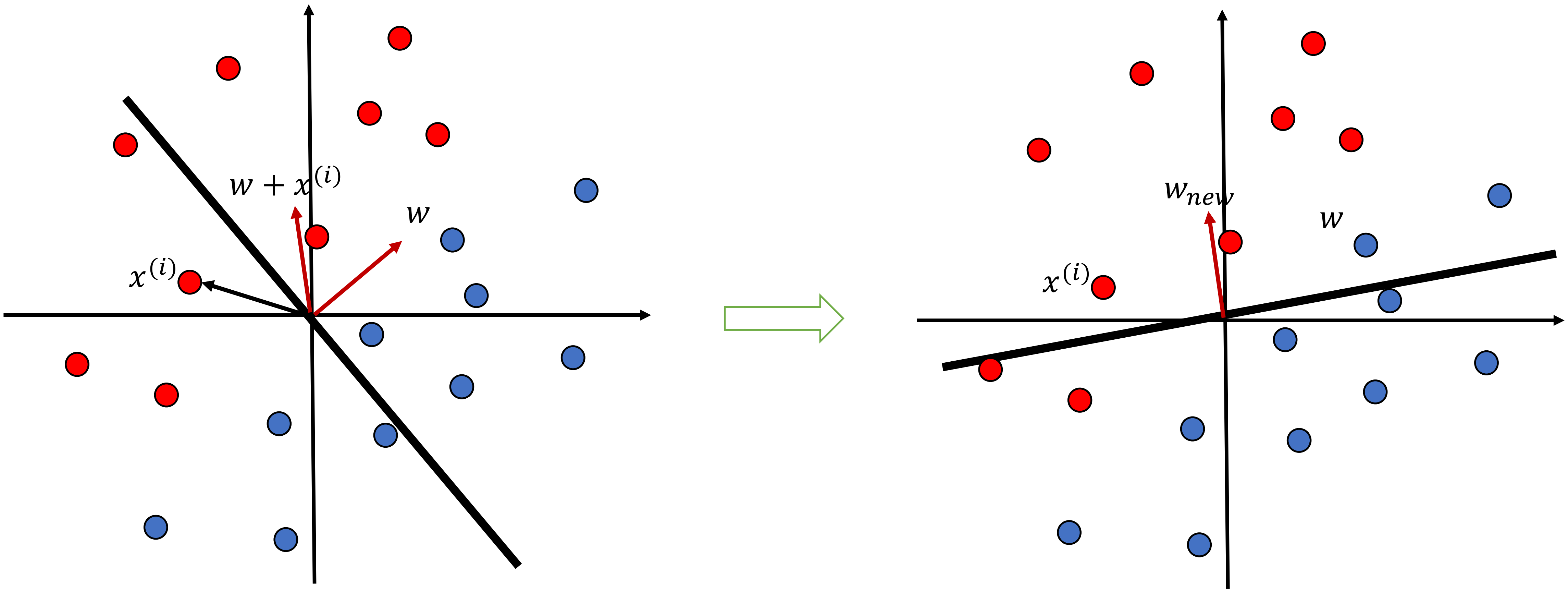
- Find the w vector that perfectly classify training examples

Algorithm: Perceptron Learning Algorithm

$P \leftarrow inputs \quad with \quad label \quad 1;$
$N \leftarrow inputs \quad with \quad label \quad 0;$
Initialize $\mathbf{w}$ randomly;
while !*convergence* **do**
  Pick random $\mathbf{x} \in P \cup N$;
  if $\mathbf{x} \in P \quad and \quad \mathbf{w}.\mathbf{x} < 0$ **then**
    $\boxed{\mathbf{w} = \mathbf{w} + \mathbf{x}\ ;}$
  end
  if $\mathbf{x} \in N \quad and \quad \mathbf{w}.\mathbf{x} \geq 0$ **then**
    $\boxed{\mathbf{w} = \mathbf{w} - \mathbf{x}\ ;}$
  end
end
//the algorithm converges when all the
inputs are classified correctly

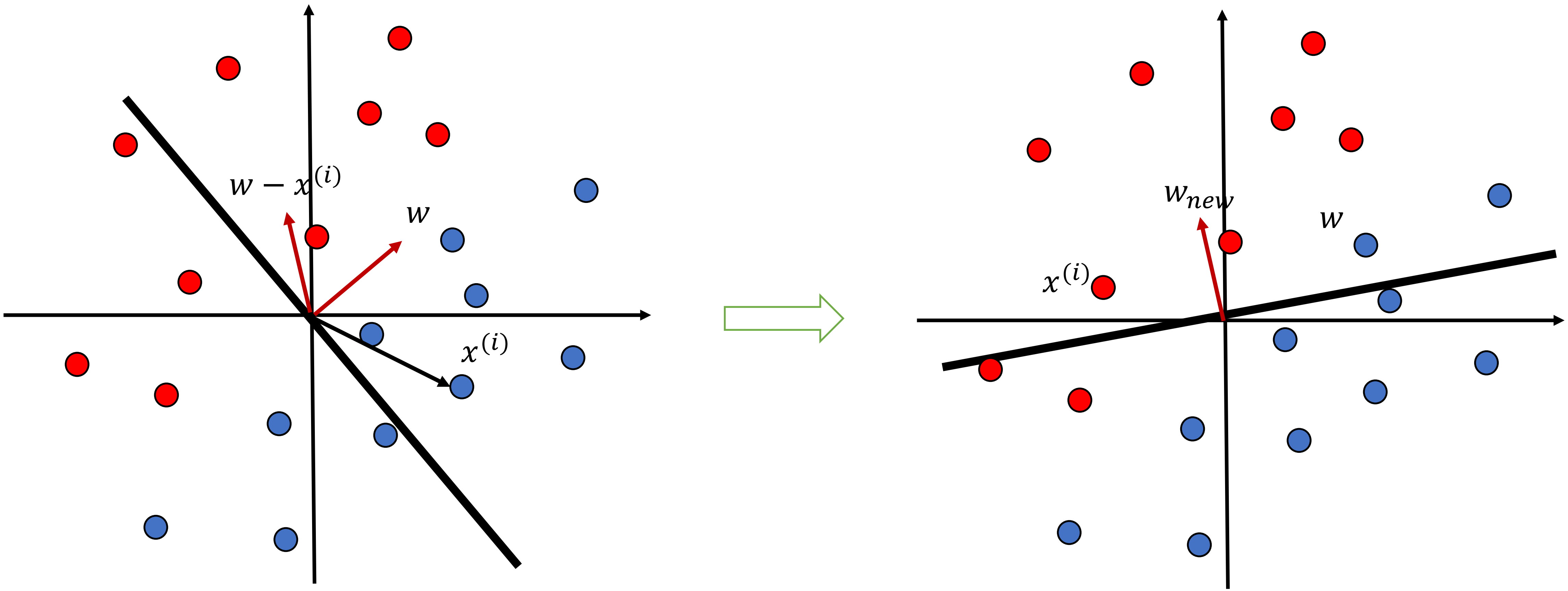
Perceptron Learning Algorithm

- Find a separating hyperplane



Perceptron Learning Algorithm

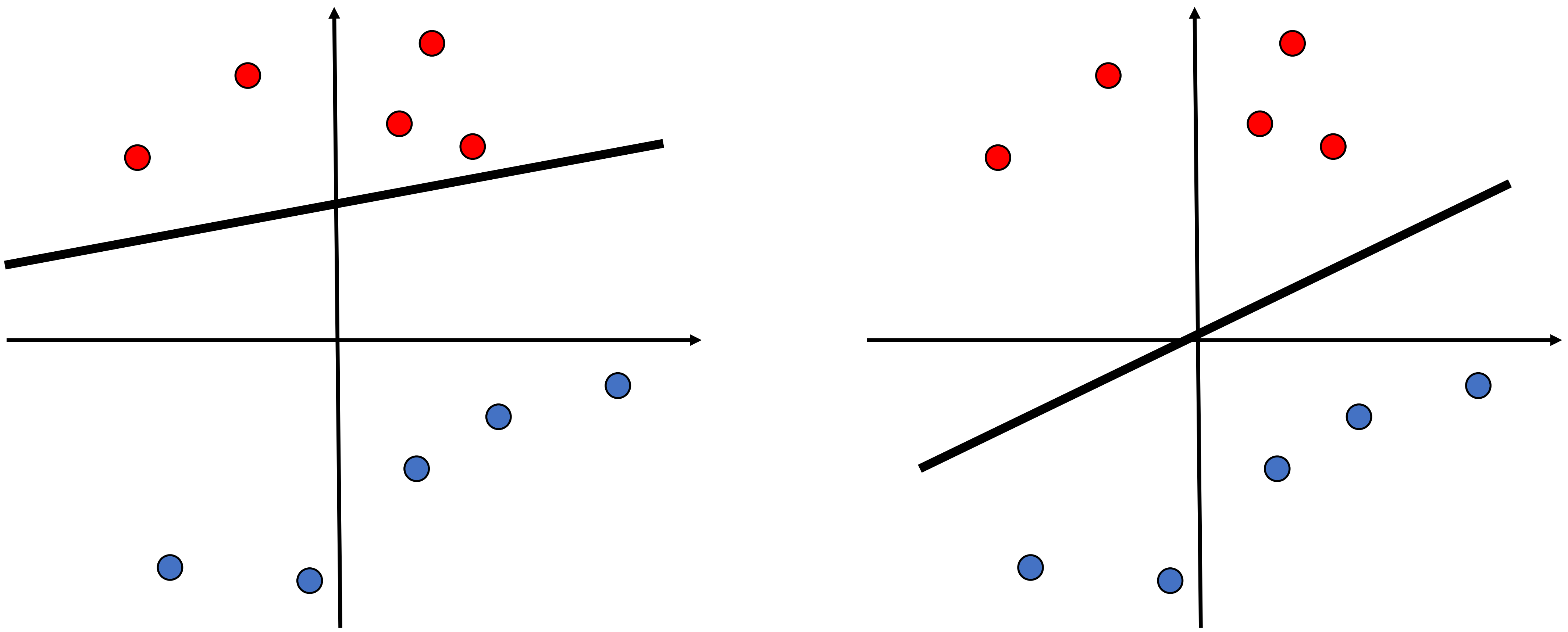
- Find a separating hyperplane



Logistic Regression

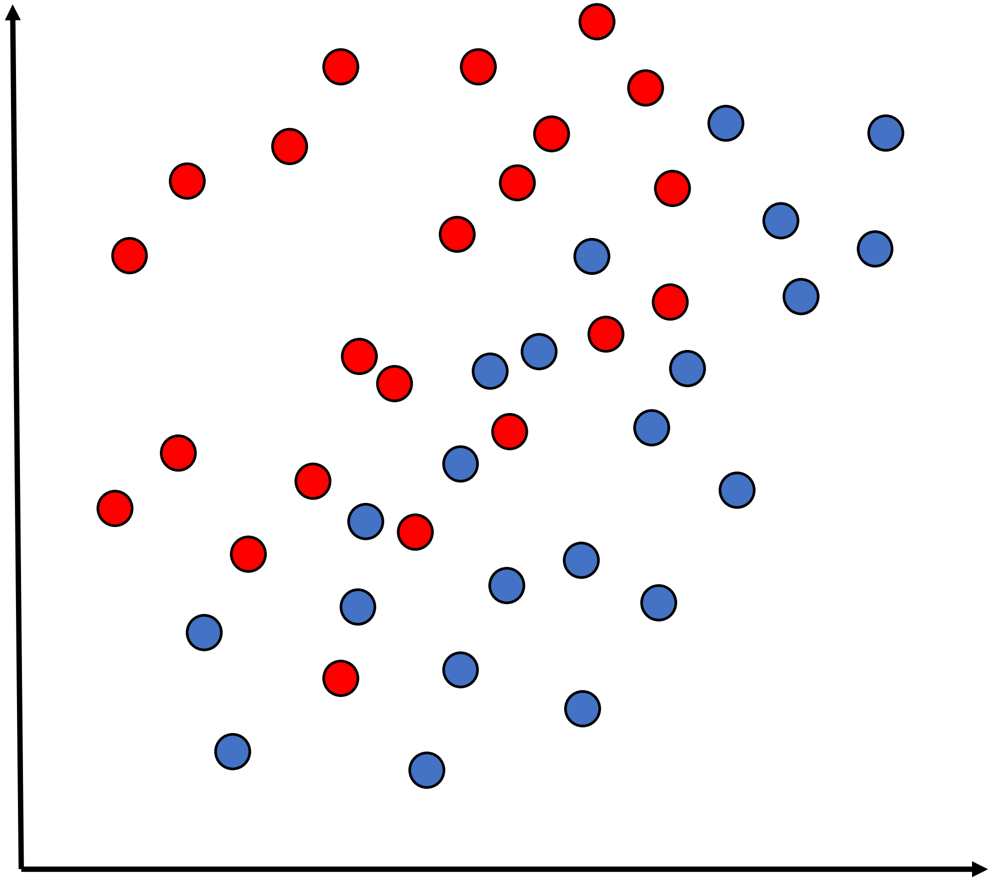
Problems of the Perceptron

- Which one is better?

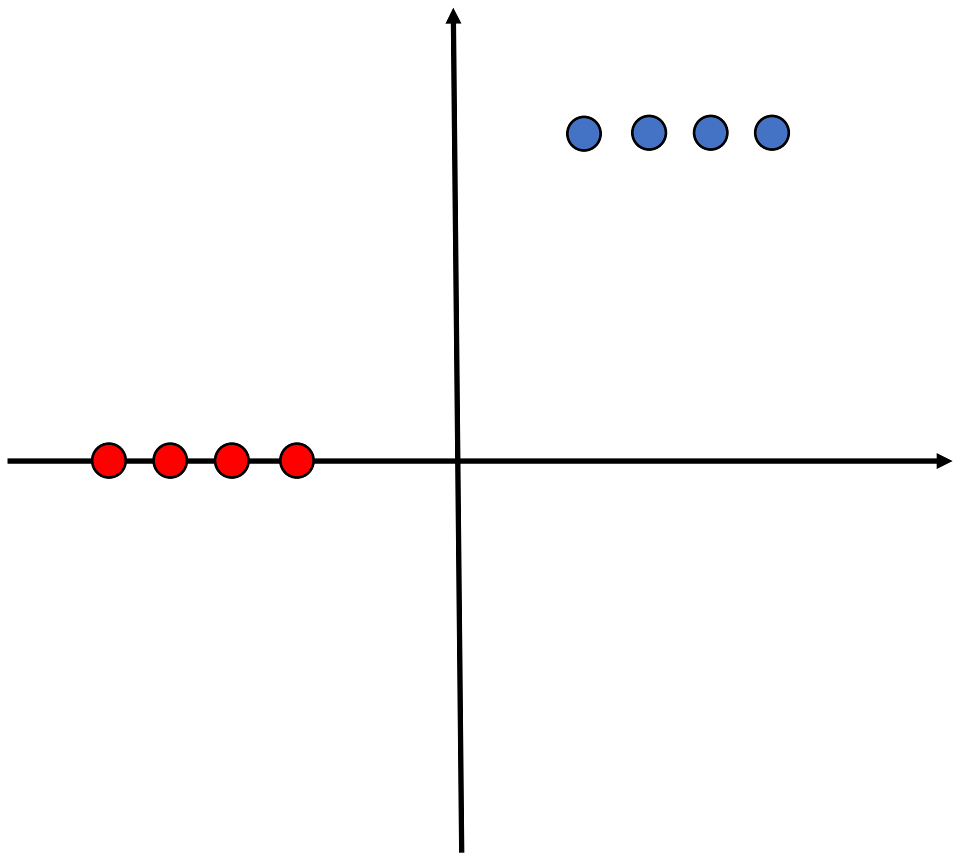


Problems of the Perceptron

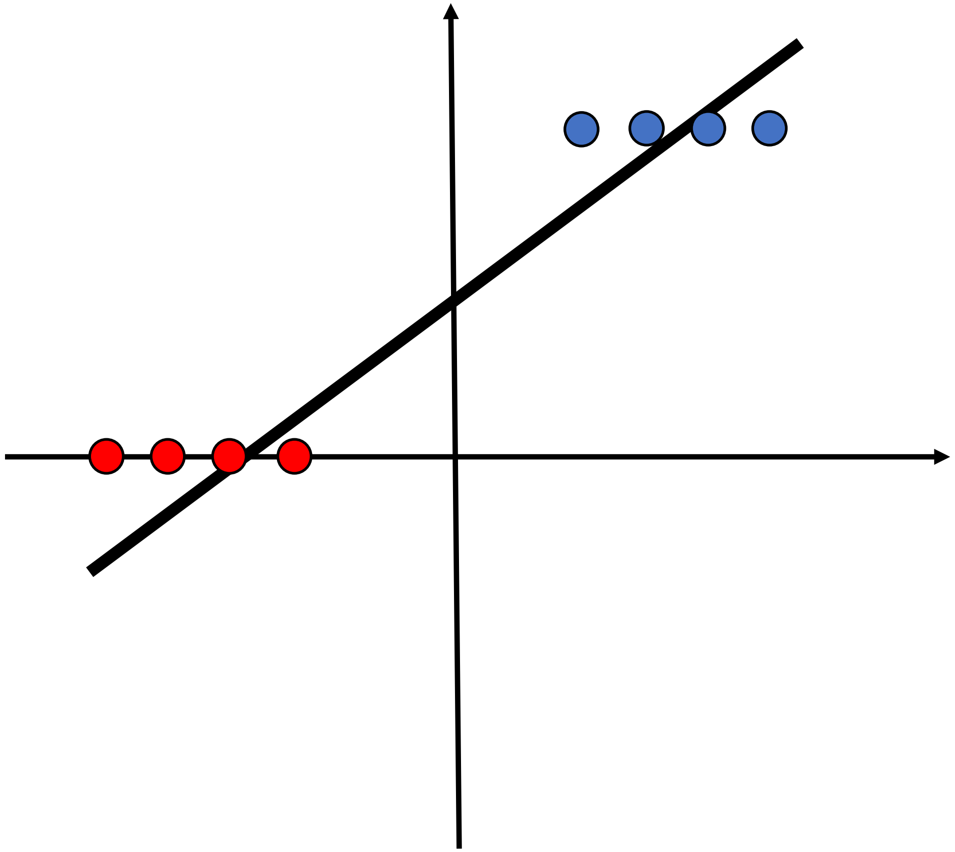
- What about not linearly separable cases?



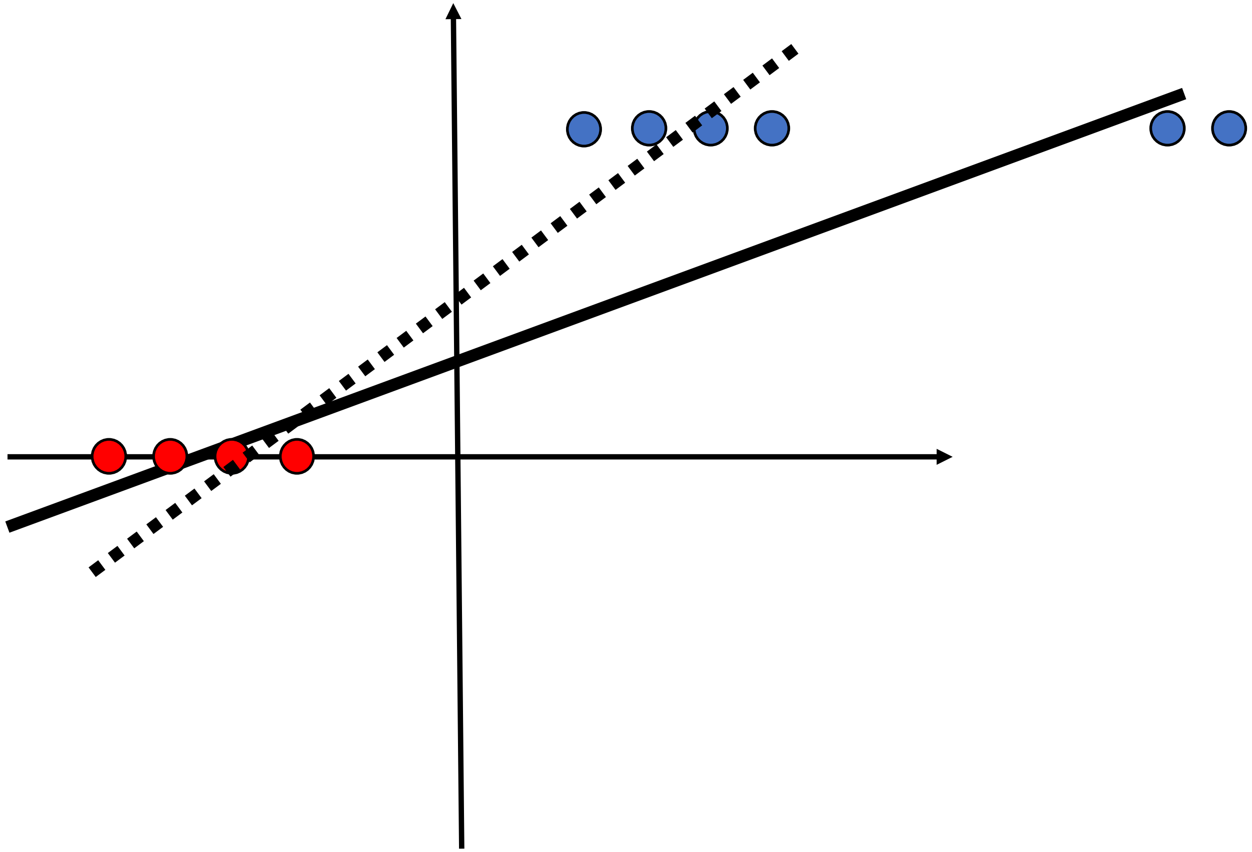
Classification w/ Linear Regression



Classification w/ Linear Regression

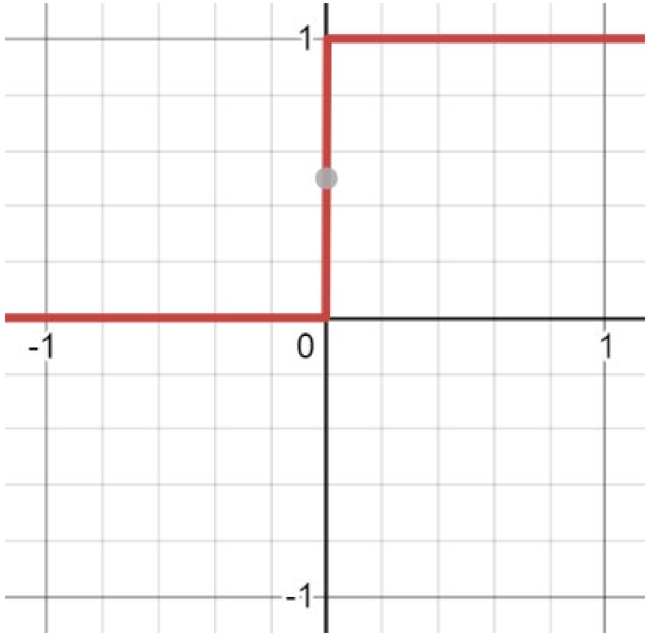


Classification w/ Linear Regression

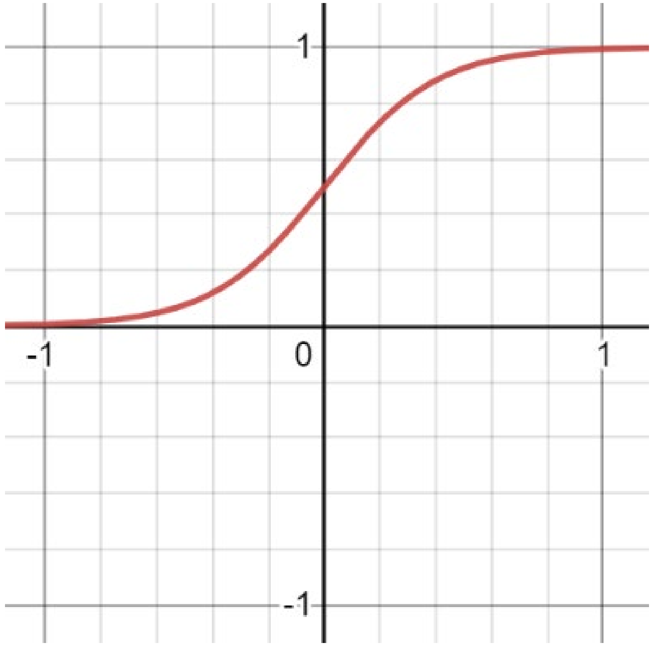


Logistic Function (aka Sigmoid)

- Squeezing the output of a 'linear equation' between 0 and 1



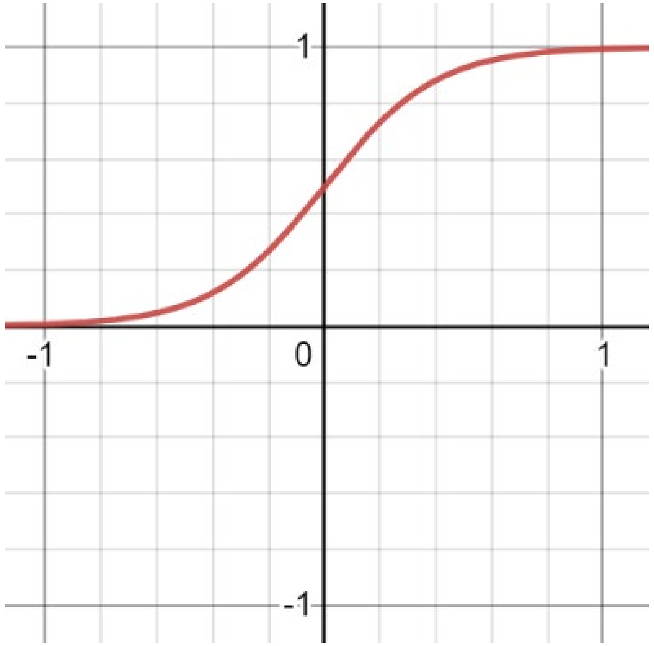
$$\text{step}(x) = \begin{cases} 1, & x \geq 0 \\ 0, & x < 0 \end{cases}$$



$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Logistic Function (aka Sigmoid)

- Squeezing the output of a ‘linear equation’ between 0 and 1



$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

$$z = w^{\top} x$$

$$f(x) = \frac{1}{1 + e^{-z}}$$

Logistic Regression

- $y = \sigma(w^\top x) = \frac{1}{1+e^{-w^\top x}}$

- Using the ‘logistic function’ to squeeze the output of a ‘linear equation’
  - $\sigma(w^\top x) \in [0,1]$ (w/ sigmoid)
  - $\mathrm{step}(w^\top x) \in \{0,1\}$ (thresholding)

- So, now it’s more like probability
  - $p(y = 1|x; w) = \sigma(w^\top x)$
  - $p(y = 0|x; w) = 1 - \sigma(w^\top x)$
  - $p(y = 0|x; w) = p(y = 1|x; w)$

MSE Loss for Logistic Regression

- Training set

	tumor size (cm) x_1	...	patient's age x_n	malignant? y
$i=1$	10		52	1
$\vdots$	2		73	0
	5		55	0
	12		49	1
$i=m$	...		...	...

MSE Loss for Logistic Regression

- Can we apply MSE loss function to logistic regression?

$$D = \{(x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)})\}$$
$$x^{(i)} \in \mathbb{R}^d, y^{(i)} \in \{0,1\}, w \in \mathbb{R}^d$$
$$X \in \mathbb{R}^{N \times d}, Y \in \{0,1\}^N$$

$$\mathrm{MSE}(w) = \frac{1}{2}\sum_{i=1}^{N}\left(y^{(i)} - \sigma(w^\top x^{(i)})\right)^2$$

Is it convex?

MSE Loss for Logistic Regression

- Convexity Check

Derivative of Sigmoid Function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

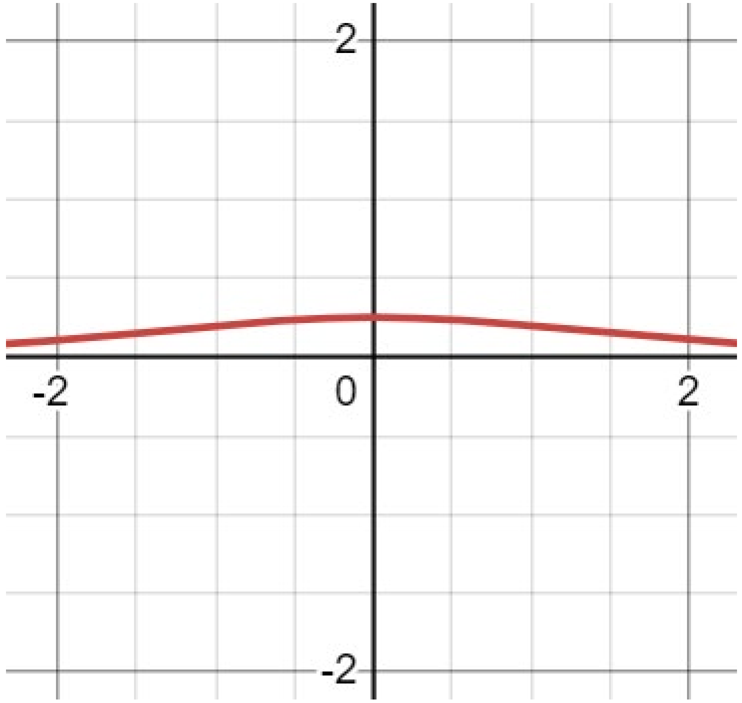
$$\frac{d\sigma(x)}{dx} =$$

Derivative of Sigmoid Function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1 + e^{-x})^2} = \frac{1}{(1 + e^{-x})} \frac{e^{-x}}{(1 + e^{-x})}$$

$$= \sigma(x)(1 - \sigma(x))$$



MSE Loss for Logistic Regression

- Convexity Check in 1D

$$\frac{\partial^2 L(w)}{\partial w^2} \geq 0$$

$$L(w) = \frac{1}{2}\sum_{i=1}^{N}\left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

$$\hat{y}^{(i)} = \sigma(wx^{(i)})$$

$$\frac{\partial L(w)}{\partial w} = \sum_{i=1}^{N} -\left(y^{(i)} - \hat{y}^{(i)}\right)\hat{y}^{(i)}\left(1 - \hat{y}^{(i)}\right)x^{(i)} = \sum_{i=1}^{N} -\left(y^{(i)}\hat{y}^{(i)} - y^{(i)}{\hat{y}^{(i)}}^2 - {\hat{y}^{(i)}}^2 + {\hat{y}^{(i)}}^3\right)x^{(i)}$$

$$\frac{\partial^2 L(w)}{\partial w^2} = \sum_{i=1}^{N} -\left(y^{(i)} - 2y^{(i)}\hat{y}^{(i)} - 2\hat{y}^{(i)} + 3{\hat{y}^{(i)}}^2\right)\underbrace{\hat{y}^{(i)}\left(1 - \hat{y}^{(i)}\right){x^{(i)}}^2}_{> 0}$$

MSE Loss for Logistic Regression

- Convexity Check in 1D

$$-3\hat{y}^{(i)^2} + 2\left(y^{(i)} + 1\right)\hat{y}^{(i)} - y^{(i)} \; ?$$

$$y^{(i)} \in \{0,1\}$$

if $y^{(i)} = 0$

$$-3\hat{y}^{(i)^2} + 2\hat{y}^{(i)} = -3\left(\hat{y}^{(i)} - \frac{2}{3}\right)\hat{y}^{(i)}$$

$$\hat{y}^{(i)} \in \left[0, \frac{2}{3}\right] \qquad \hat{y}^{(i)} \in \left[\frac{2}{3}, 1\right]$$

$$> 0 \qquad < 0$$

MSE Loss for Logistic Regression

- Convexity Check in 1D

$$-3{\hat{y}^{(i)}}^2 + 2\left(y^{(i)} + 1\right)\hat{y}^{(i)} - y^{(i)} \text{ ?}$$

$$y^{(i)} \in \{0,1\}$$

if $y^{(i)} = 1$

$$-3{\hat{y}^{(i)}}^2 + 4\hat{y}^{(i)} - 1 = -3\left(\hat{y}^{(i)} - \frac{1}{3}\right)\left(\hat{y}^{(i)} - 1\right)$$

$$\hat{y}^{(i)} \in \left[\frac{1}{3}, 1\right] \qquad \hat{y}^{(i)} \in \left[0, \frac{1}{3}\right]$$

$$> 0 \qquad < 0$$

MSE Loss for Logistic Regression

- Convexity Check in 2D

Log Loss

Log Loss (a.k.a Logistic Loss, Binary Cross Entropy)

$$D = \{(x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)})\}$$

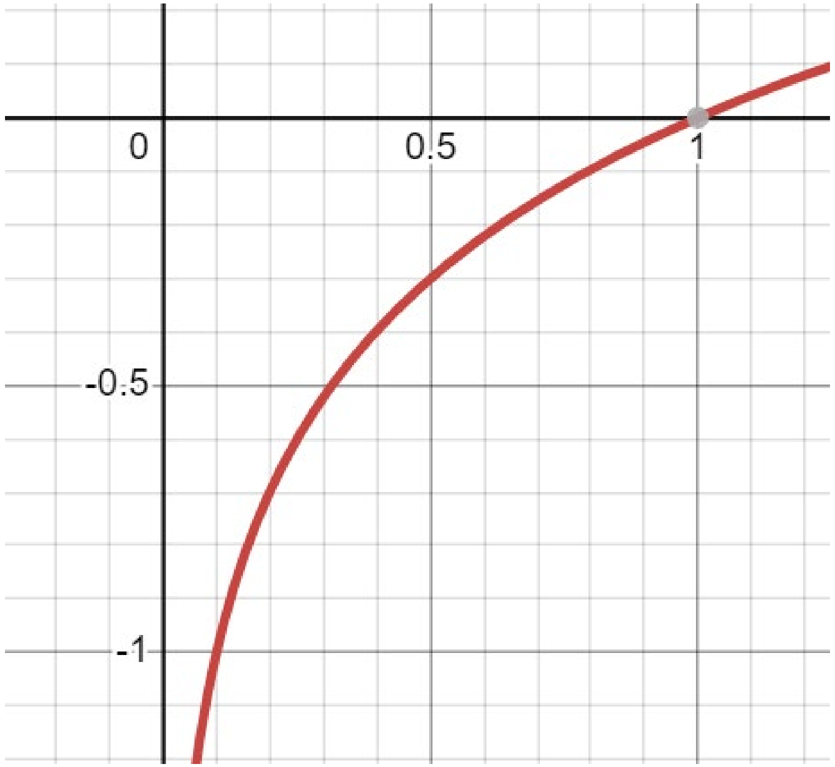
$$x^{(i)} \in \mathbb{R}^d, y^{(i)} \in \{0,1\}, w \in \mathbb{R}^d$$

$$\hat{y}^{(i)} = \sigma\left(w^\top x^{(i)}\right)$$

$$\mathrm{BCE}(w) = -\sum_{i=1}^{N} y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)$$

$$-\log(1-\hat{y}), \qquad y^{(i)} = 0$$

$$-\log(\hat{y}), \qquad y^{(i)} = 1$$

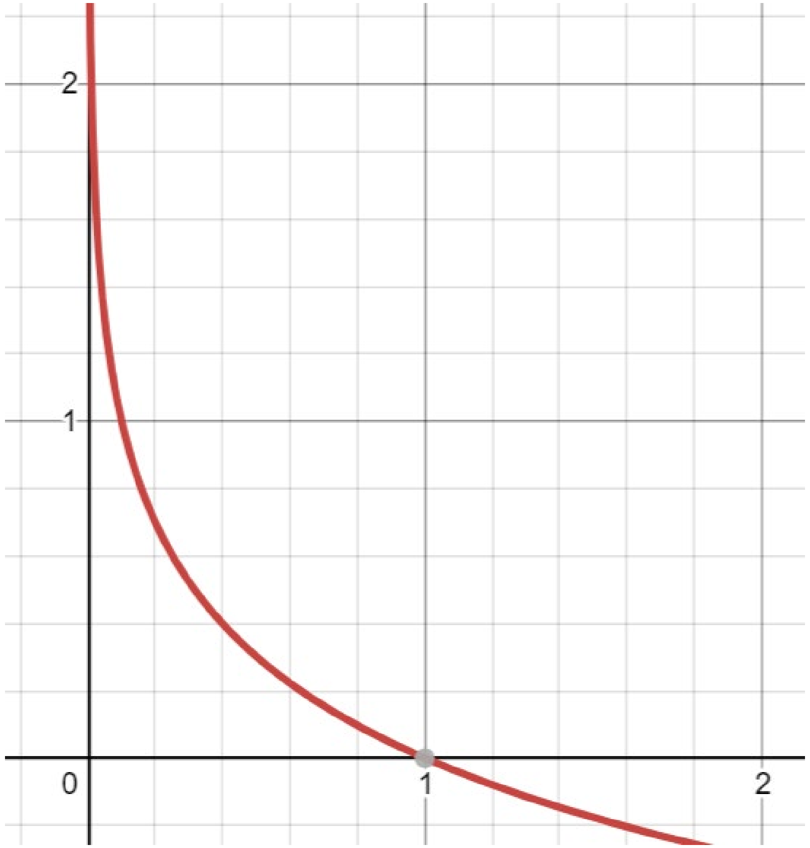


$\log(x)$

Log Loss (a.k.a Logistic Loss, Binary Cross Entropy)

if $y^{(i)} = 1$,

$-\log(\hat{y})$

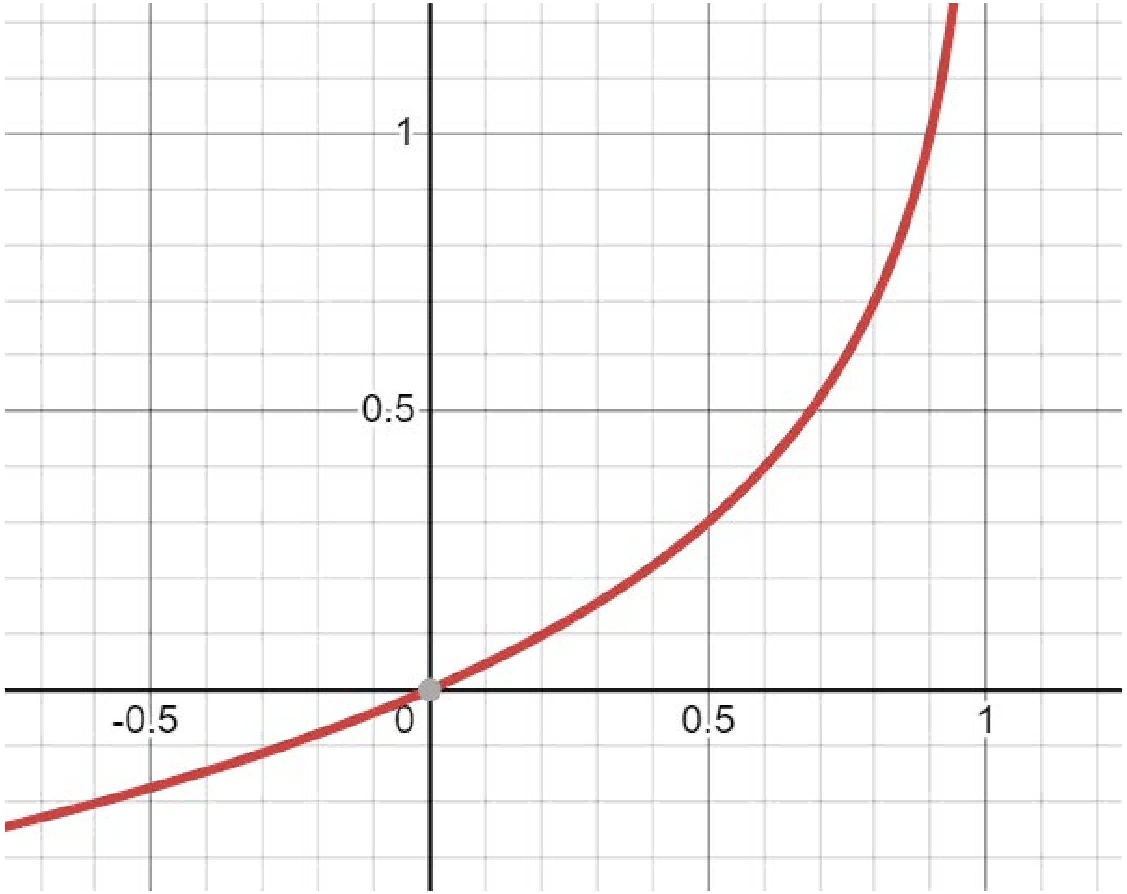


$-\log(\hat{y})$

Log Loss (a.k.a Logistic Loss, Binary Cross Entropy)

if $y^{(i)} = 0$,

$-\log(1 - \hat{y})$



$-\log(1 - \hat{y})$

Log Loss (a.k.a Logistic Loss, Binary Cross Entropy)

- Convexity Check in 1D

if $y^{(i)} = 1,$ $$L(w) = -\sum_{i=1}^{N} \log\left(\hat{y}^{(i)}\right)$$ $$\hat{y}^{(i)} = \sigma\left(wx^{(i)}\right)$$

$$\frac{\partial L(w)}{\partial w} =$$

$$\frac{\partial^2 L(w)}{\partial w^2} =$$

Log Loss (a.k.a Logistic Loss, Binary Cross Entropy)

- Convexity Check in 1D

if $y^{(i)} = 0,$

$$L(w) = -\sum_{i=1}^{N} \log\left(1 - \hat{y}^{(i)}\right)$$

$$\hat{y}^{(i)} = \sigma(wx^{(i)})$$

$$\frac{\partial L(w)}{\partial w} =$$

$$\frac{\partial^2 L(w)}{\partial w^2} =$$

Solving Logistic Regression

- Is it convex?
- Does it have a closed form solution?

Gradient Descent

$$\mathrm{BCE}(w) = -\sum_{i=1}^{N} y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)$$

$$\hat{y}^{(i)} = \sigma\left(w^\top x^{(i)}\right)$$

$$\frac{\partial \mathrm{BCE}(w)}{\partial w_j} =$$

Gradient Descent

$$\mathrm{BCE}(w) = -\sum_{i=1}^{N} y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)$$

$$\hat{y}^{(i)} = \sigma\left(w^{\top} x^{(i)}\right)$$

$$\frac{\partial \mathrm{BCE}(w)}{\partial w_j} = \sum_{i=1}^{N} \left(\hat{y}^{(i)} - y^{(i)}\right) x_j^{(i)}$$

$$w_j \coloneqq w_j - \alpha\left(\sum_{i=1}^{N} \left(\hat{y}^{(i)} - y^{(i)}\right) x_j^{(i)}\right)$$

(Gradient Descent)

Algorithm: Perceptron Learning Algorithm

$P \leftarrow$ *inputs with label* 1;
$N \leftarrow$ *inputs with label* 0;
Initialize $\mathbf{w}$ randomly;
while !*convergence* **do**
  Pick random $\mathbf{x} \in P \cup N$;
  if $\mathbf{x} \in P$ *and* $\mathbf{w.x} < 0$ **then**
    $\mathbf{w} = \mathbf{w} + \mathbf{x}$;
  end
  if $\mathbf{x} \in N$ *and* $\mathbf{w.x} \geq 0$ **then**
    $\mathbf{w} = \mathbf{w} - \mathbf{x}$;
  end
end
//the algorithm converges when all the inputs are classified correctly

Gradient Descent

$$\mathrm{BCE}(w) = -\sum_{i=1}^{N} y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)$$

$$\hat{y}^{(i)} = \sigma\left(w^{\top} x^{(i)}\right)$$

$$w \in \mathbb{R}^{d}$$

$$Y \in \mathbb{R}^{N}$$

$$X \in \mathbb{R}^{N \times d}$$

$$\frac{\partial \mathrm{BCE}(w)}{\partial w} = ?$$

Gradient Descent

$$\mathrm{BCE}(w) = -\sum_{i=1}^{N} y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)$$

$$\hat{y}^{(i)} = \sigma\left(w^{\top} x^{(i)}\right)$$

$$w \in \mathbb{R}^{d}$$

$$\frac{\partial \mathrm{BCE}(w)}{\partial w} = X^{\top}(\sigma(Xw) - Y)$$

$$Y \in \mathbb{R}^{N}$$

$$X \in \mathbb{R}^{N \times d}$$

$$w \coloneqq w - \alpha(X^{\top}(\sigma(Xw) - Y))$$

(Gradient Descent)

MLE

MLE for Logistic Regression

- Bernoulli distribution

parameter

$$p(x;p) = p^x(1-p)^{1-x}, \qquad x \in \{0,1\}$$

$$\begin{cases} x = 0, & 1-p \\ x = 1, & p \end{cases}$$

$$E[x] = p$$

$$\sum_{x\in\{0,1\}} xp(x) = 1 \cdot p + 0 \cdot (1-p) = p$$

MLE for Logistic Regression

- Finding the parameters that maximize 'conditional likelihood'

Assumption1: $p(y|x)$ is a Bernoulli distribution

Assumption2: I.I.D

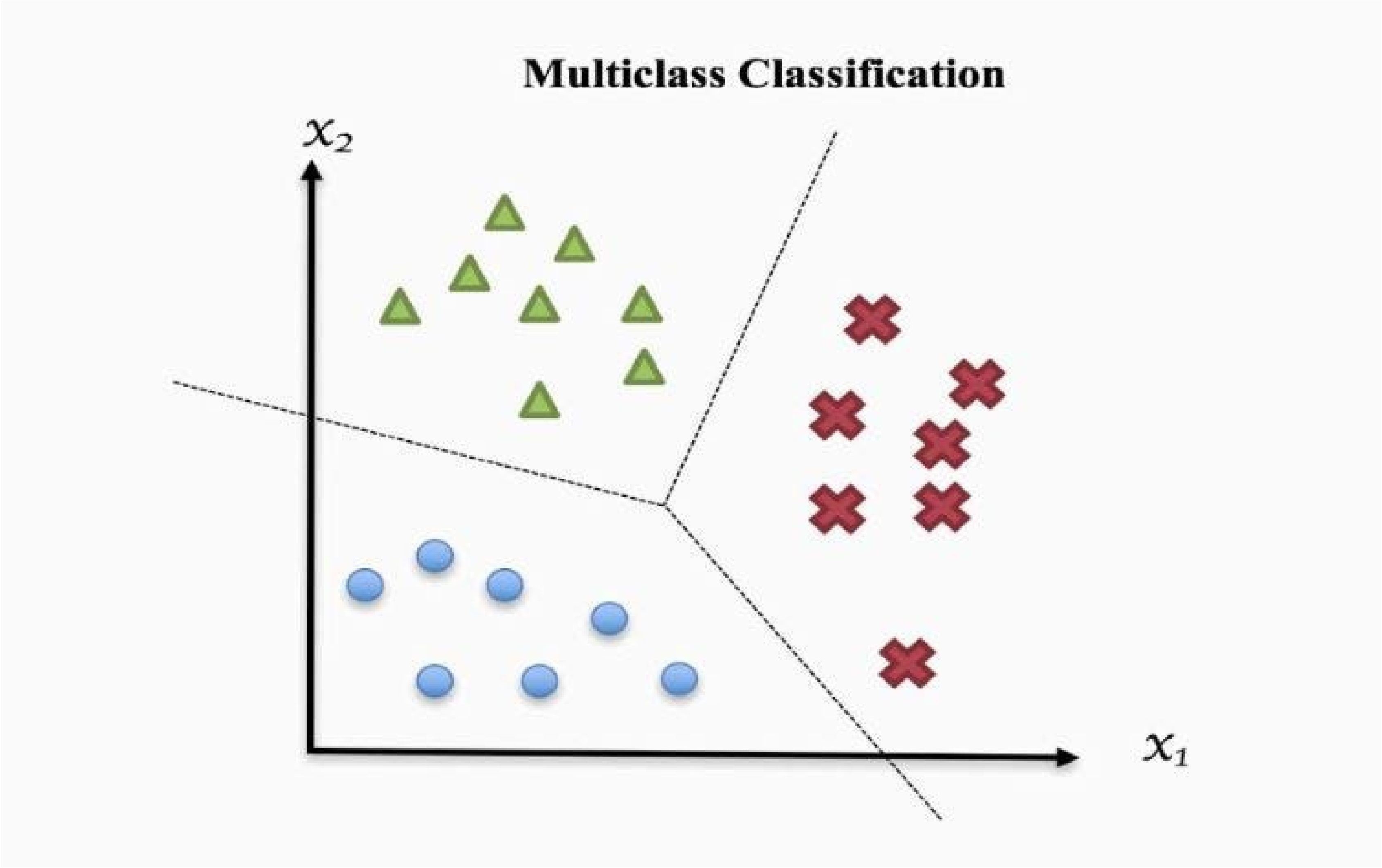
$$\log L(w) = \sum_{i=1}^{N} \log p(y^{(i)}|x^{(i)}; w) = \sum_{i=1}^{N} \log \sigma\left(w^\top x^{(i)}\right)^{y^{(i)}} \left(1 - \sigma\left(w^\top x^{(i)}\right)\right)^{1-y^{(i)}}$$

$$= \sum_{i=1}^{N} y^{(i)} \log \sigma\left(w^\top x^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \sigma\left(w^\top x^{(i)}\right)\right)$$

a.k.a Binary Cross Entropy (BCE) Loss

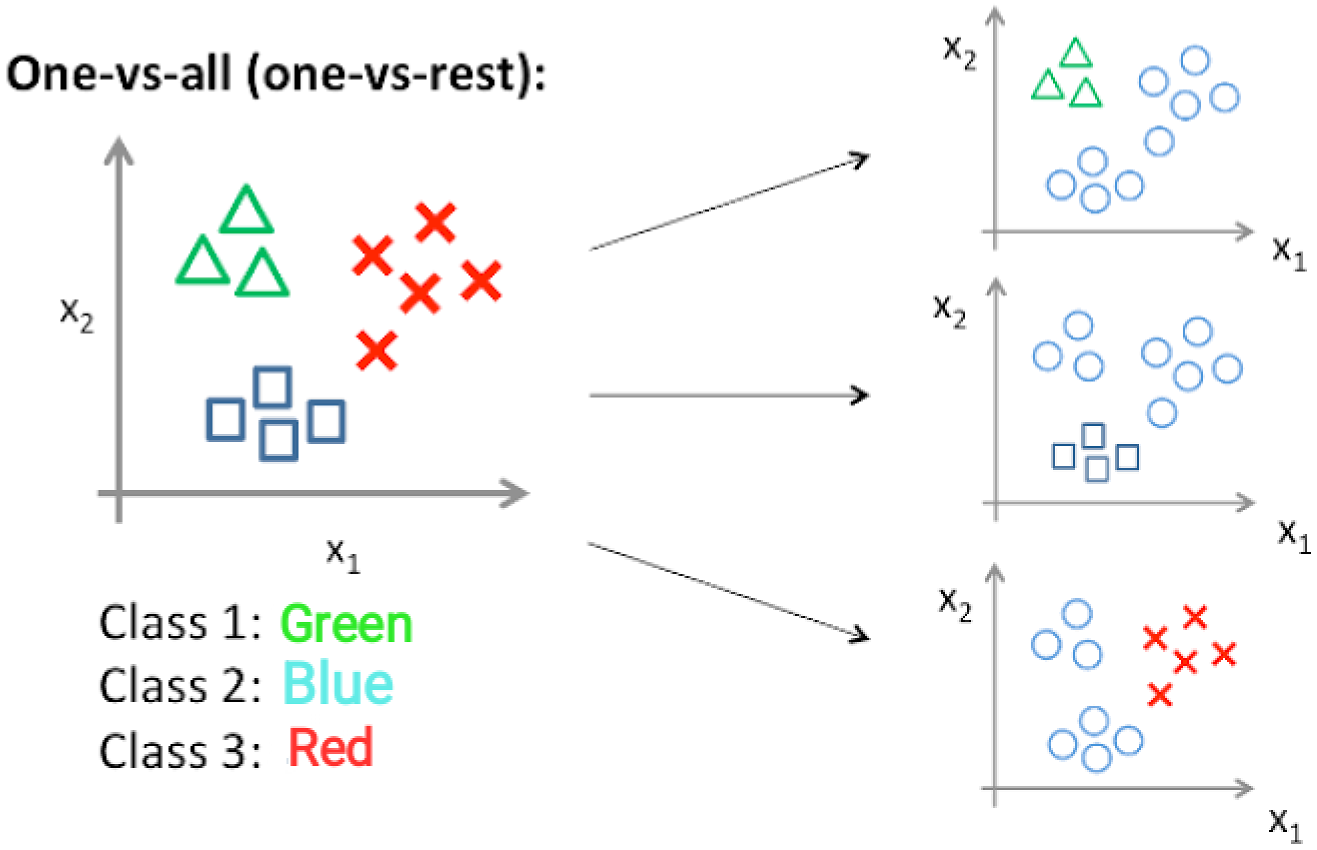
Multiclass Classification

Multiclass Classification



One vs. All for Multiclass Classification

- Sigmoid function and binary logistic regression



Softmax Function

- Sigmoid function and binary logistic regression

$$\sigma(x) = \frac{1}{1 + e^{-x}} \qquad y = \sigma(w^\top x)$$

Softmax Function

- 'Soft' 'Max' function
  - $[1,2,3,2,1] \rightarrow [0.0674, 0.183\ , 0.498, 0.183\ , 0.0674]$

$$\text{softmax: } \mathbb{R}^C \rightarrow [0,1]^C$$

$$||\text{softmax}||_1 = 1$$

$$\text{softmax}(z)_j = \frac{e^{z_j}}{\sum_{i=1}^{C} e^{z_i}}$$

$$\text{softmax}(z) = \begin{bmatrix} \frac{e^{z_1}}{\sum_{i=1}^{C} e^{z_i}} \\ \frac{e^{z_2}}{\sum_{i=1}^{C} e^{z_i}} \\ \vdots \\ \frac{e^{z_C}}{\sum_{i=1}^{C} e^{z_i}} \end{bmatrix} \in [0,1]^C$$

Multiclass Classification w/ Softmax Function

- Weight vectors for each class!

$$\hat{y}^{(i)} = \text{softmax}\left(Wx^{(i)}\right) \in \mathbb{R}^C \qquad W \in \mathbb{R}^{c\times d} \qquad w_k \in \mathbb{R}^d$$

$$p(y=0|x) =$$

Multiclass Classification w/ Softmax Function

- Weight vectors for each class!

$$\hat{y}^{(i)} = \mathrm{softmax}\left(W x^{(i)}\right) \in \mathbb{R}^{C} \qquad W \in \mathbb{R}^{c \times d} \qquad w_k \in \mathbb{R}^{d}$$

$$p(y = 0|x) = \frac{e^{w_0^\top x}}{e^{w_0^\top x} + e^{w_1^\top x} + e^{w_2^\top x}}$$

$$p(y = 1|x) = \frac{e^{w_1^\top x}}{e^{w_0^\top x} + e^{w_1^\top x} + e^{w_2^\top x}}$$

$$p(y = 2|x) = \frac{e^{w_2^\top x}}{e^{w_0^\top x} + e^{w_1^\top x} + e^{w_2^\top x}}$$

Multiclass Classification w/ Softmax Function

- When they 2 classes

$$p(y = 0|x) =$$

$$p(y = 1|x) =$$

Multiclass Classification w/ Softmax Function

- When they 2 classes

$$w^* = -(w_0 - w_1)$$

$$p(y=0|x) = \frac{e^{w_0^\top x}}{e^{w_0^\top x} + e^{w_1^\top x}} = \frac{e^{w_0^\top x}}{e^{w_0^\top x} + e^{w_1^\top x}} \frac{e^{-w_1^\top x}}{e^{-w_1^\top x}} = \frac{e^{(w_0 - w_1)^\top x}}{1 + e^{(w_0 - w_1)^\top x}} = \frac{e^{-w^{*\top} x}}{1 + e^{-w^{*\top} x}}$$

$$p(y=1|x) = \frac{e^{w_1^\top x}}{e^{w_0^\top x} + e^{w_1^\top x}} = \frac{e^{w_1^\top x}}{e^{w_0^\top x} + e^{w_1^\top x}} \frac{e^{-w_1^\top x}}{e^{-w_1^\top x}} = \frac{1}{1 + e^{-w^{*\top} x}}$$

$$1 - \frac{1}{1 + e^{-w^{*\top} x}} = \frac{e^{-w^{*\top} x}}{1 + e^{-w^{*\top} x}}$$

Categorical Distribution

- Categorical distribution can be used to model a random variable X that takes values in {1, …, C}

$$p(x;\phi) = \phi^x(1-\phi)^{1-x}$$

Bernoulli distribution

$$p(x = i) = \phi_i \qquad \phi_{1,\dots,}\phi_{C-1}$$

$$\sum_{i=1}^{C} \phi_i = 1 \qquad 1 - \sum_{i=1}^{C-1} \phi_i = \phi_C$$

$$p(x) = \prod_{i=1}^{C} \phi_i^{\mathbb{I}_i(x)} = \phi_1^{\mathbb{I}_1(x)} \phi_2^{\mathbb{I}_2(x)} \dots \phi_C^{\mathbb{I}_C(x)}$$

$$\mathbb{I}_i(x) = \begin{cases} 1 & \text{if } x == i \\ 0 & \text{otherwise} \end{cases}$$

MLE w/ categorical distribution

$$p(y|x) = \prod_{i=1}^{N} \prod_{j=1}^{C} \phi_j^{\mathbb{I}_j(y^{(i)})} \qquad y^{(i)} \in \{1, \ldots, C\}$$

$$\log p(y|x) =$$

MLE w/ categorical distribution

$$p(y|x) = \prod_{i=1}^{N} \prod_{j=1}^{C} \phi_j^{\mathbb{I}_j(y^{(i)})}$$

$$\log p(y|x) = \sum_{i=1}^{N} \log \prod_{j=1}^{C} \phi_j^{\mathbb{I}_j(y^{(i)})} = \sum_{i=1}^{N} \sum_{j=1}^{C} \log \phi_j^{\mathbb{I}_j(y^{(i)})} = \sum_{i=1}^{N} \sum_{j=1}^{C} \mathbb{I}_j(y^{(i)}) \log \phi_j$$

Cross Entropy Loss

- Cross Entropy Loss
  - BCE is a special case of CE (two classes)

$$\mathrm{CE}(w) = -\sum_{i=1}^{N}\sum_{c=1}^{C} y_c^{(i)} \log\left(\hat{y}_c{}^{(i)}\right)$$

$$\hat{y}^{(i)} = \mathrm{softmax}\left(Wx^{(i)}\right) \in \mathbb{R}^C \qquad W \in \mathbb{R}^{c\times d}$$

$$y^{(i)} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$ (one-hot vector) $\mathbb{I}_j(y^{(i)})$

$$\mathrm{BCE}(w) = -\sum_{i=1}^{N} y^{(i)} \log\left(\hat{y}^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - \hat{y}^{(i)}\right)$$

Derivative of the Softmax Function

$$y_j = \frac{e^{z_j}}{\sum_{i=1}^{C} e^{z_i}}$$

$$\frac{d}{dx}\left[\frac{f(x)}{g(x)}\right] = \frac{g(x)f'(x) - f(x)g'(x)}{\left(g(x)\right)^2}$$

1) $i \neq j$

$$\frac{\partial y_i}{\partial z_j} = \frac{\left(\sum_{k=1}^{C} e^{z_k}\right) \cdot 0 - e^{z_i} e^{z_j}}{\left(\sum_{k=1}^{C} e^{z_k}\right)^2} = -y_i y_j$$

2) $i = j$

$$\frac{\partial y_i}{\partial z_j} = \frac{\left(\sum_{k=1}^{C} e^{z_k}\right) \cdot e^{z_i} - e^{z_i} e^{z_i}}{\left(\sum_{k=1}^{C} e^{z_k}\right)^2} = y_i - y_i^2 = y_i(1 - y_i)$$

Derivative of the Softmax Function

$$y_j = \frac{e^{z_j}}{\sum_{i=1}^{C} e^{z_i}}$$

$$\frac{\partial y_i}{\partial z_j} = \begin{cases} y_i(1 - y_i), & i = j \\ -y_i y_j, & i \neq j \end{cases} = y_i\left(1\{i = j\} - y_j\right)$$

$$\frac{dy}{dz} = \begin{bmatrix} y_1(1 - y_1) & \cdots & -y_1 y_C \\ \vdots & \ddots & \vdots \\ -y_C y_1 & \cdots & y_C(1 - y_C) \end{bmatrix}$$

Cross-Entropy + Softmax

$$\log \mathrm{CE}(W) = -\sum_{i=1}^{C} y_i \log(\hat{y}_i) \qquad \hat{y}_i = \frac{e^{z_i}}{\sum_{j=1}^{C} e^{z_j}} \qquad z_c = W_c^{\top} x \qquad W_c \in \mathbb{R}^d \quad W \in \mathbb{R}^{c\times d}$$

$$\frac{\partial \hat{y}_i}{\partial z_j} = \begin{cases} \hat{y}_i(1-\hat{y}_i), & i = j \\ -\hat{y}_i\hat{y}_j, & i \neq j \end{cases}$$

$$\frac{\partial L}{\partial z_j} = -\frac{\partial}{\partial z_j}\sum_{i=1}^{C} y_i \log(\hat{y}_i) = -\sum_{i=1}^{C} y_i \frac{\partial \log(\hat{y}_i)}{\partial z_j} = -\sum_{i=1}^{C} \frac{y_i}{\hat{y}_i}\frac{\partial \hat{y}_i}{\partial z_j}$$

Cross-Entropy + Softmax

$$\log \mathrm{CE}(W) = -\sum_{i=1}^{C} y_i \log(\hat{y}_i) \qquad \hat{y}_i = \frac{e^{z_i}}{\sum_{j=1}^{C} e^{z_j}} \qquad z_c = W_c^{\top} x \qquad W_c \in \mathbb{R}^d \quad W \in \mathbb{R}^{c\times d}$$

$$\frac{\partial \hat{y}_i}{\partial z_j} = \begin{cases} \hat{y}_i(1-\hat{y}_i), & i = j \\ -\hat{y}_i\hat{y}_j, & i \neq j \end{cases}$$

$$\frac{\partial \mathrm{CE}(W)}{\partial z_j} = -\frac{\partial}{\partial z_j}\sum_{i=1}^{C} y_i \log(\hat{y}_i) = -\sum_{i=1}^{C} y_i \frac{\partial \log(\hat{y}_i)}{\partial z_j} = -\sum_{i=1}^{C} \frac{y_i}{\hat{y}_i}\frac{\partial \hat{y}_i}{\partial z_j}$$

$$= -\frac{y_j}{\hat{y}_j}\frac{\partial \hat{y}_j}{\partial z_j} - \sum_{i\neq j}^{C} \frac{y_i}{\hat{y}_i}\frac{\partial \hat{y}_i}{\partial z_j} = -\frac{y_j}{\hat{y}_j}\hat{y}_j\left(1-\hat{y}_j\right) + \sum_{i\neq j}^{C} \frac{y_i}{\hat{y}_i}\hat{y}_i\hat{y}_j$$

$$= -y_j + y_j\hat{y}_j + \sum_{i\neq j}^{C} y_i\hat{y}_j = -y_j + \hat{y}_j\sum_{i=1}^{C} y_i = \boldsymbol{\hat{y}_j - y_j}$$

$$\boxed{\frac{dL}{dz} = \hat{y} - y}$$

Gradient Descent

$$\frac{\partial}{\partial W_{c,j}} \mathrm{CE}(W) = \frac{\partial \mathrm{CE}(W)}{\partial z} \frac{\partial z}{\partial W_{c,j}} = \sum_{i=1}^{N} \left(\hat{y}^{(i)} - y^{(i)}\right) x_j^{(i)}$$

$$W_{c,j} \coloneqq W_{c,j} - \alpha \left(\sum_{i=1}^{N} \left(\hat{y}^{(i)} - y^{(i)}\right) x_j^{(i)} \right)$$

(Gradient Descent)

Gradient Descent

$$\frac{\partial}{\partial W_{c,j}}\mathrm{CE}(W) = \frac{\partial \mathrm{CE}(W)}{\partial z}\frac{\partial z}{\partial W_{c,j}} = \sum_{i=1}^{N}\left(\hat{y}^{(i)} - y^{(i)}\right)x_j^{(i)}$$

$$\frac{\partial}{\partial W}\mathrm{CE}(W) = \frac{\partial \mathrm{CE}(W)}{\partial z}\frac{\partial z}{\partial W_{c,j}} = (\mathrm{softmax}(WX) - Y)X^\top$$

$$W \in \mathbb{R}^{c\times d}$$

$$Y \in \mathbb{R}^{c\times N}$$

$$X \in \mathbb{R}^{d\times N}$$

$$\boxed{W \coloneqq W - \alpha(\mathrm{softmax}(WX) - Y)X^\top}$$

(Gradient Descent)