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# Linear Classification

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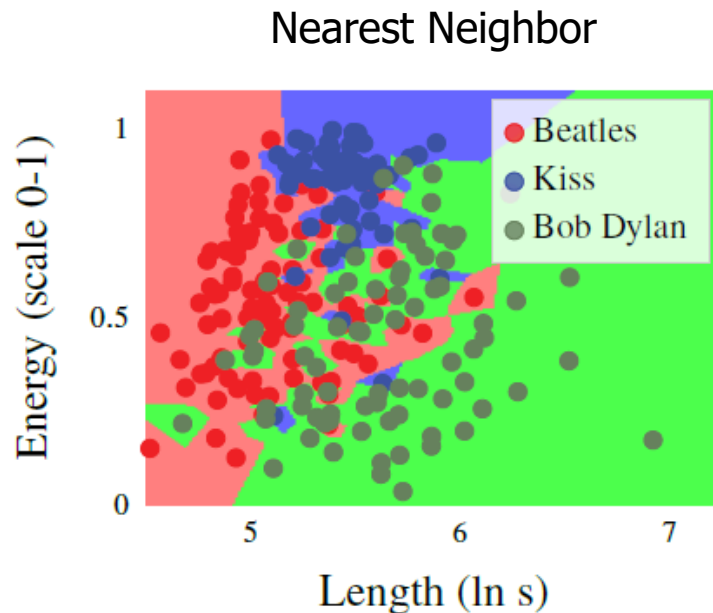
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Some figures are copied from the following books

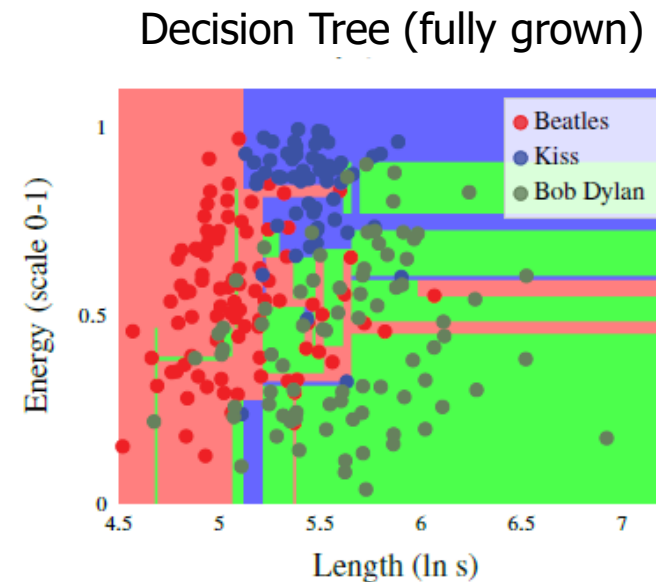
- **LWLS** - Andreas Lindholm, Niklas Wahlström, Fredrik Lindsten, Thomas B. Schön, *Machine Learning: A First Course for Engineers and Scientists*, Cambridge University Press, 2022.
- **Mitchell** - Tom M. Mitchell, *Machine Learning*, McGraw-Hill Education, 1997.

# Classification Boundary

- Classification: given training examples  $\{(x^{(i)}, y^{(i)})\}_{i=1}^N$ , learn  $f: x \mapsto y$ , where  $y$  is categorical
- If  $x$  is numerical and has  $d$  attributes, then it is a  $d$ -dimension vector



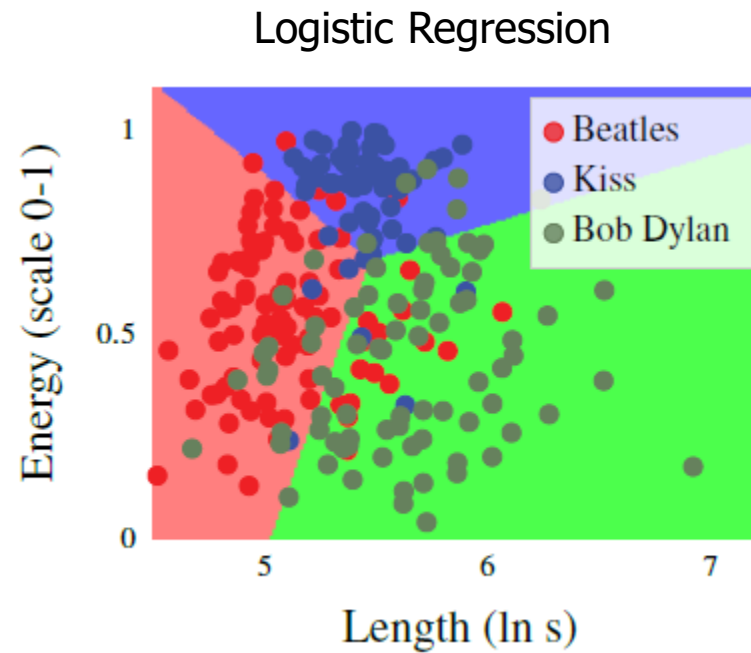
(Fig. 2.5(a) in LWLS)



(Fig. 2.11(a) in LWLS)

# Linear Classification Boundary

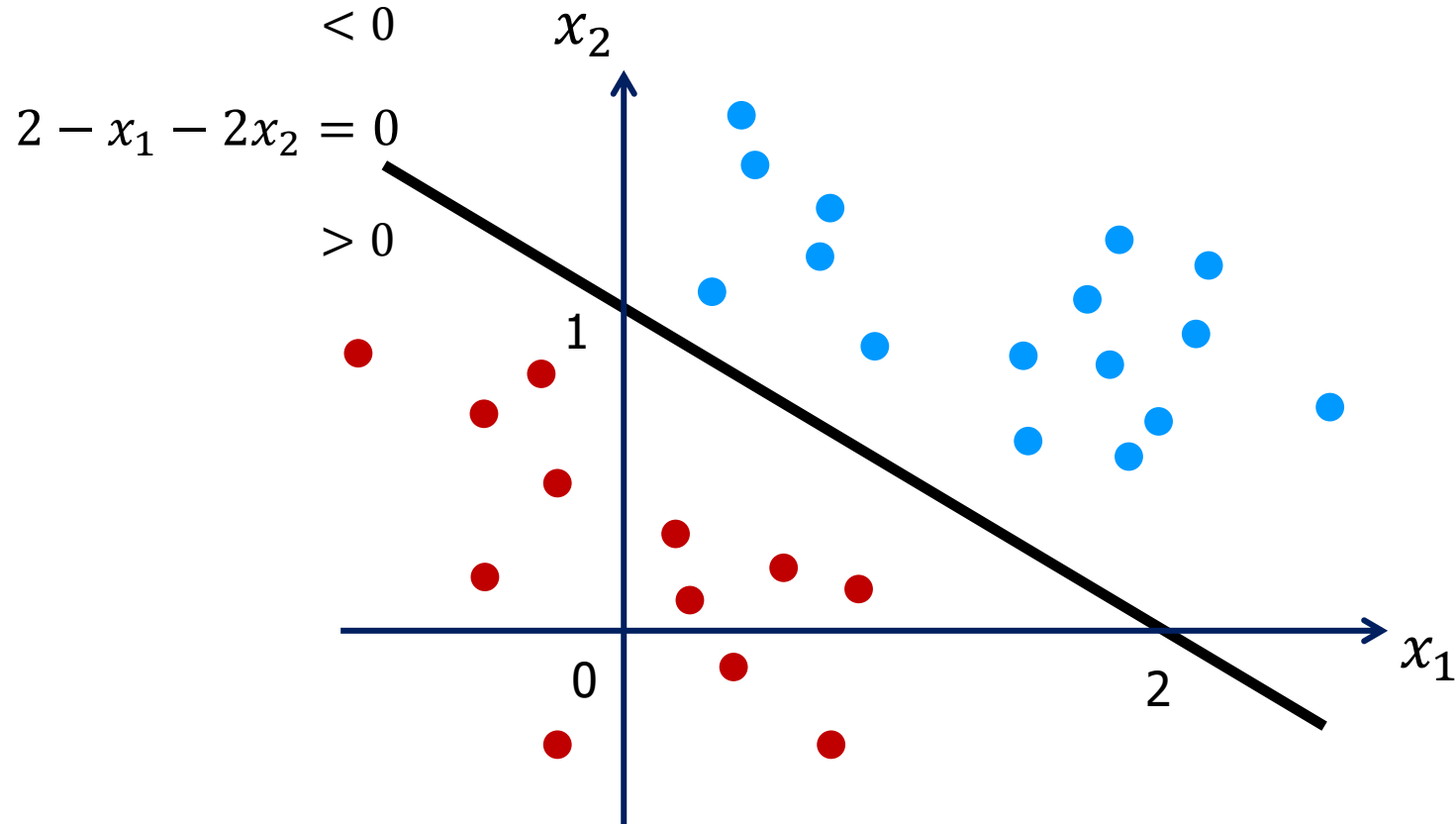
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(Fig. 3.6 in LWLS)

Note: Logistic regression is in fact a [classification](#) method, not a [regression](#) method

# Let's draw a linear boundary



- A linear boundary is a **hyperplane**, represented as a linear equation
$$w_0 + w_1x_1 + w_2x_2 + \dots + w_dx_d = 0$$
- It separates the space into two half spaces

# Linear Boundary

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- A linear boundary is a linear equation:

$$w_0 + w_1x_1 + w_2x_2 + \dots + w_dx_d = 0$$

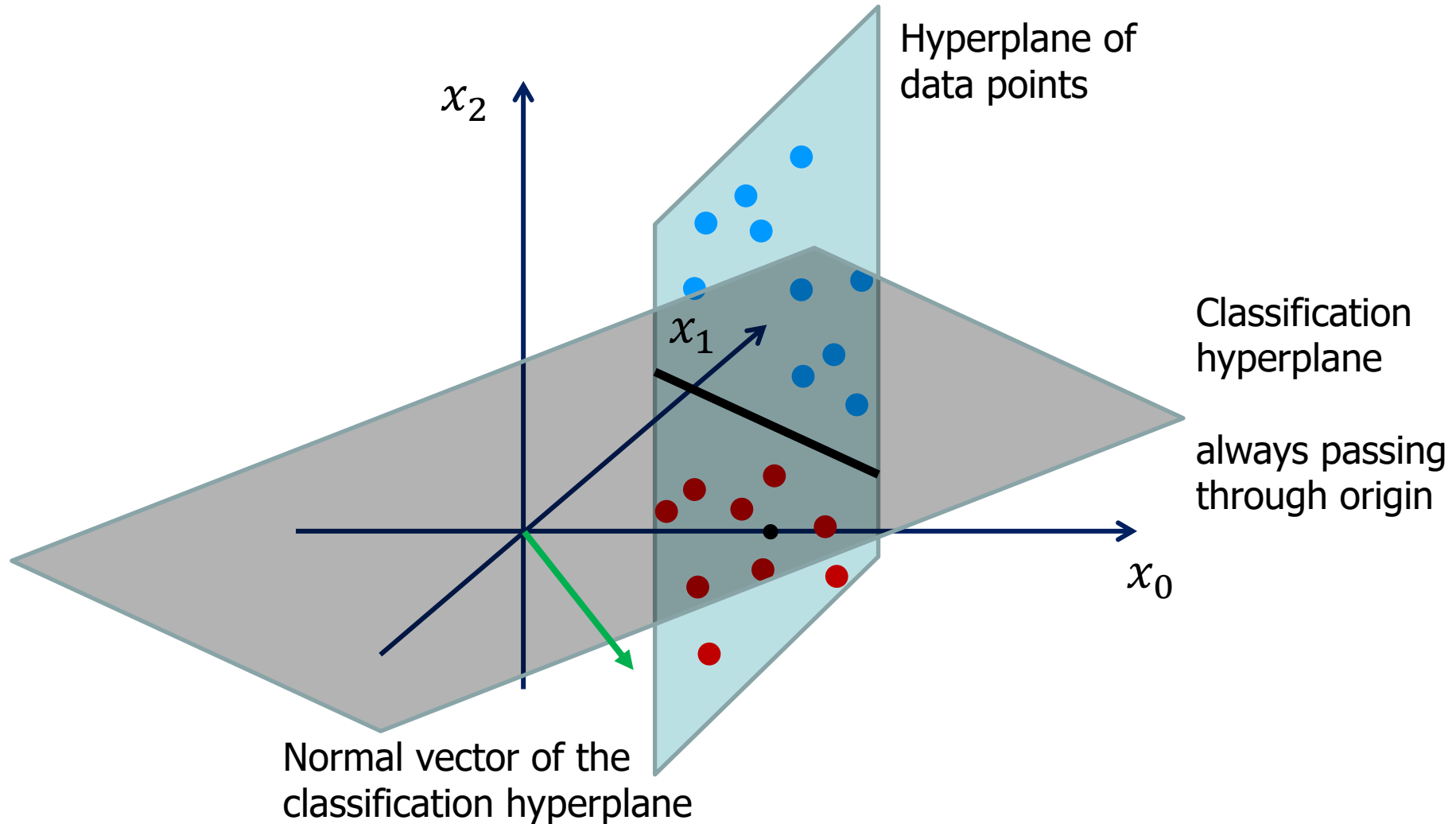
$$[w_0 \quad w_1 \quad \dots \quad w_d] \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix} = 0, \text{ or } \mathbf{w}^T \begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix} = 0$$

- $\mathbf{w}$  is the weight vector
- $\begin{bmatrix} 1 \\ \mathbf{x} \end{bmatrix}$  is the **extended** feature vector ( $d + 1$  dimensional)
- **For convenience, we will view  $\mathbf{x}$  as the extended feature vector**

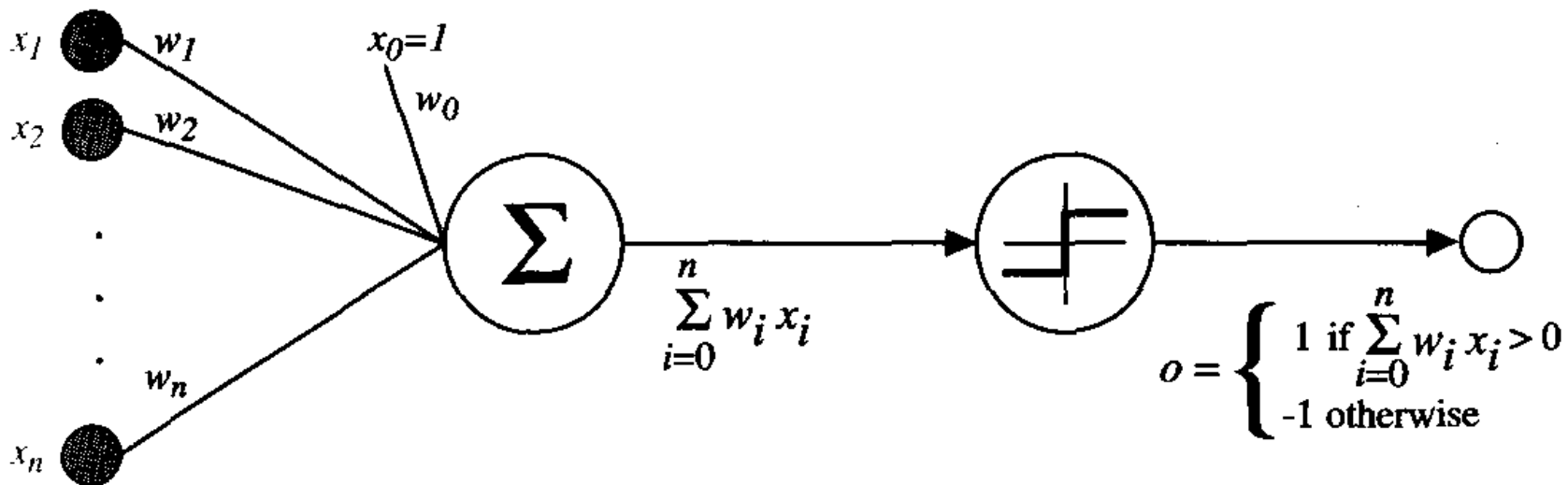
$$\mathbf{x} = (x_0, x_1, \dots, x_d)^T \text{ where } x_0 = 1$$

- So  $\mathbf{w}^T \mathbf{x} = 0$  on the boundary (hyperplane),  $\mathbf{w}$  is the normal vector
- $\mathbf{w}^T \mathbf{x} > 0$  on one side and  $\mathbf{w}^T \mathbf{x} < 0$  on the other side

# Geometry of the Extended Space



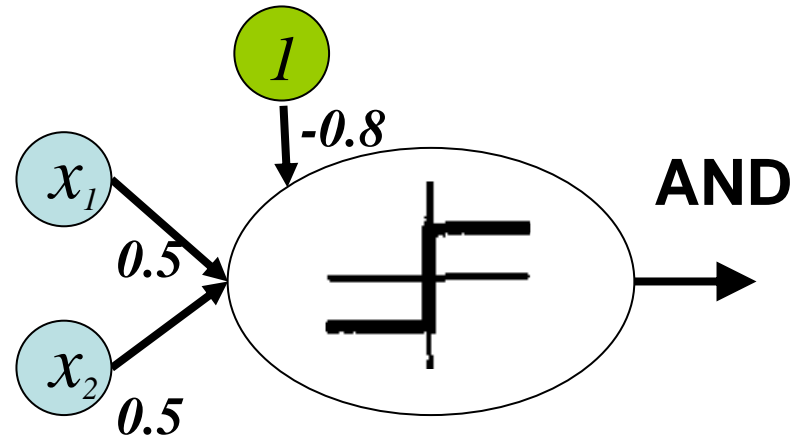
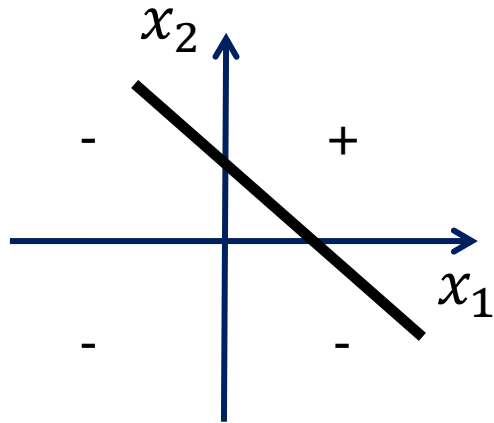
# Perceptron



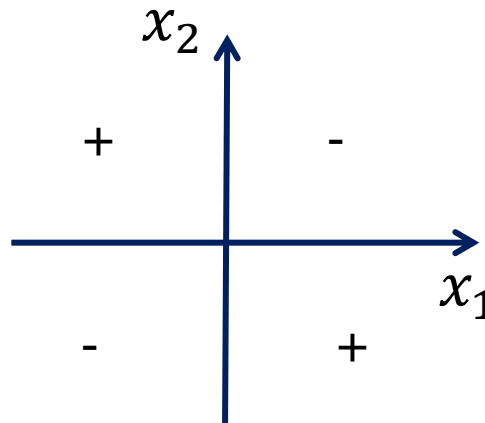
- Perceptron is a function that maps  $\mathbf{x}$  to either 1 or -1  
$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x})$$
- This is a **linear binary classifier** where one side of the classification boundary is 1 and the other side is -1

# Perceptron's Representation Power

- Basic logic operations: AND, OR, NOT
  - They are all **linearly separable**



- How about XOR?
  - Not linearly separable





# How to Learn a Perceptron?

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- Perceptron is a function mapping  $x$  to either 1 or -1

$$f(x) = \text{sign}(w^T x)$$

- How to learn this function, i.e., the weights  $w$ ?
- One idea is to start from an **initial** vector  $w$ , and then **iteratively** update its value **till some condition**
- This is an **optimization** procedure
  - Initialization: **Random?**
  - Iterative updates: **How?**
  - Termination condition: **What?**

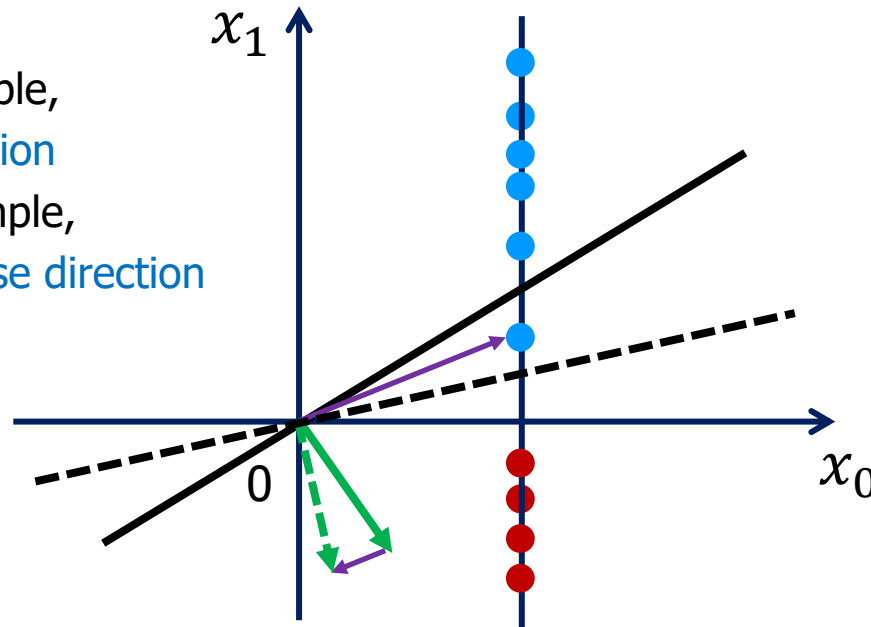
# Perceptron Update Rule

- Initialization: **Random**
- Iterative updates: **Update  $w$  for each misclassified training example**
- Termination condition: **Till all examples are correctly classified**
  - **Would not terminate** if training examples are not linearly separable

- Idea
  - For a misclassified **positive** example, update  $w$  along the example's **direction**
  - For a misclassified **negative** example, update  $w$  along the example's **reverse direction**

$$w \leftarrow w + \eta (y^{(i)} - f(x^{(i)})) x^{(i)}$$

Step size  $\eta > 0$ , usually small



- Always converges for linearly separable cases!

# How about non-linearly separable cases?

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- Linear classification may still be desirable even if it misclassifies some training examples
- The perceptron update rule does not work in this case!  
Why?
  - Each update considers **only one misclassified** training example.
- How about we consider **all misclassified** training example together for each update?
- One thought: perhaps update  $w$  to **reduce the number of misclassifications?**
  - Doesn't work because this quantity is **piecewise constant!**

# Perceptron Criterion Function

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- Minimize perceptron criterion function

$$E(\mathbf{w}) = \sum_{i \in \text{misclassified}} -\mathbf{w}^T \mathbf{x}^{(i)} \underbrace{\left( y^{(i)} - f(\mathbf{x}^{(i)}) \right)}$$

- Computer gradient w.r.t.  $\mathbf{w}$      2 (pos example) or -2 (neg example)

$$\nabla_{\mathbf{w}} E(\mathbf{w}) = \sum_{i \in \text{misclassified}} -\mathbf{x}^{(i)} \left( y^{(i)} - f(\mathbf{x}^{(i)}) \right)$$

- Update rule (via gradient descent)

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \sum_{i \in \text{misclassified}} \mathbf{x}^{(i)} \left( y^{(i)} - f(\mathbf{x}^{(i)}) \right)$$

- Terminate till classification error is acceptable

# Comparing the Two Update Rules

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- Perceptron update rule

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \left( y^{(i)} - f(\mathbf{x}^{(i)}) \right) \mathbf{x}^{(i)}, \quad \forall i \in \text{misclassified}$$

- Perceptron criterion function update rule

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \sum_{i \in \text{misclassified}} \mathbf{x}^{(i)} \left( y^{(i)} - f(\mathbf{x}^{(i)}) \right)$$

- The former can be viewed as a **stochastic approximation** of the true gradient of the perceptron criterion function
  - Also called **stochastic gradient descent**
- Using one example to approximate the gradient may be too stochastic. Let's use a few examples instead
  - **Batch processing:**

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \sum_{i \in \text{a subset of misclassified}} \mathbf{x}^{(i)} \left( y^{(i)} - f(\mathbf{x}^{(i)}) \right)$$

# Another Loss Function

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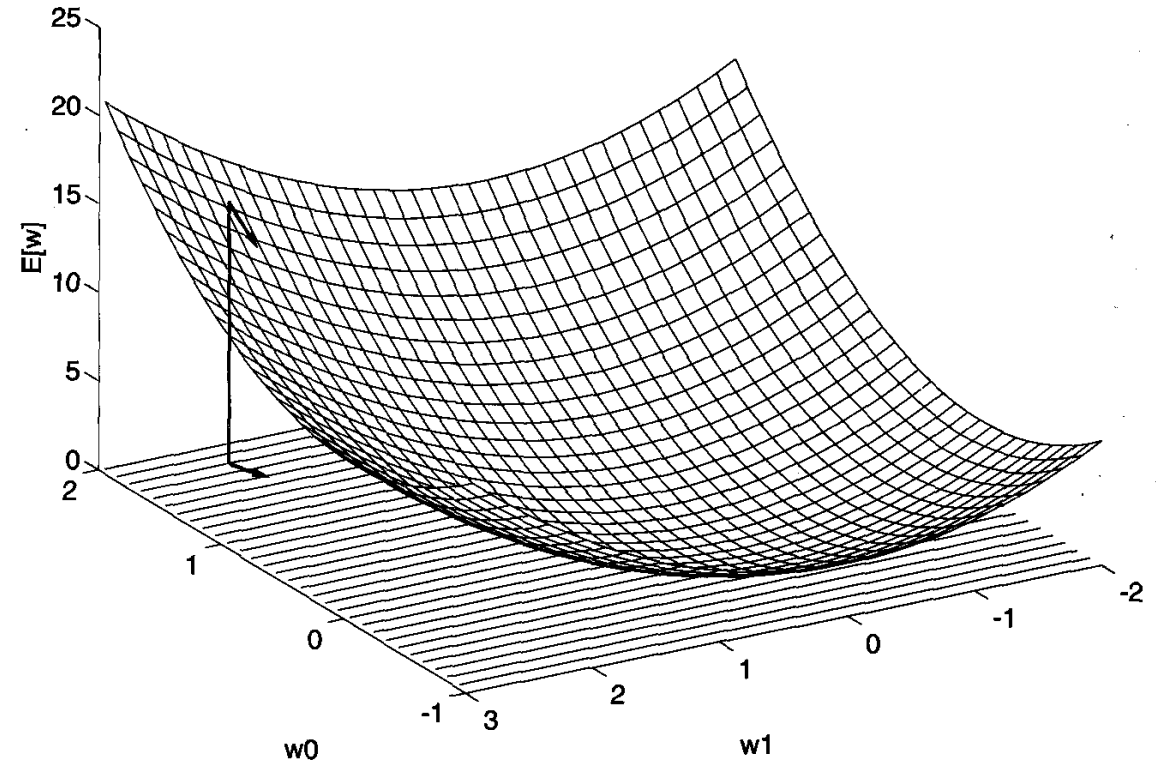
- For non-linearly separable cases, the perceptron criterion update rule may still not converge if the termination condition is not set appropriately
  - Because correctly classified examples may be misclassified after update!
- How about we define a loss function that considers **all training examples**, including the correctly classified ones?
- We hope  $\mathbf{w}^T \mathbf{x}$  is close to  $y$  for all training examples
- Let's use squared error (some definition divides it by  $N$ )

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2$$

# The Hypothesis Space

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2$$

- Quadratic function of  $\mathbf{w}$
- Convex!
- Global minimum  
(if it has a minimum)
  
- How to minimize  $E(\mathbf{w})$ ?



(Fig. 4.4 in Mitchell)

# Delta Rule

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- Also called the LMS (least-mean-square) rule, Widrow-Hoff rule)
- Minimize square error loss

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2$$

- Computer gradient w.r.t.  $\mathbf{w}$

$$\nabla_{\mathbf{w}} E(\mathbf{w}) = \sum_{i=1}^N -\mathbf{x}^{(i)} (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})$$

- Update rule (via gradient descent)

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \sum_{i=1}^N \mathbf{x}^{(i)} (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})$$

- Always converges, although may take a very long time



# Delta Rule's Stochastic Version

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- Similar to the perceptron update rule, we could approximate the true gradient of the squared error loss with the **stochastic gradient** computed from a **single training example**, then the update rule is:

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \mathbf{x}^{(i)} (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})$$

- We can also use a **batch** to have a better approximation

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \sum_{i \in \text{subset of training}} \mathbf{x}^{(i)} (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})$$

# Another Way to Minimize Squared Error

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$$\begin{aligned} E(\mathbf{w}) &= \frac{1}{2} \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2 \\ &= \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \end{aligned}$$

where  $\mathbf{X} \in \mathbb{R}^{N \times (d+1)}$  is the extended training data matrix,  $\mathbf{y} \in \{-1, 1\}^N$  is the label vector

- This is the approximation error (L2 norm) of the linear equation system

$$\mathbf{X}\mathbf{w} = \mathbf{y}$$

- This error is minimized by the **least-square solution**

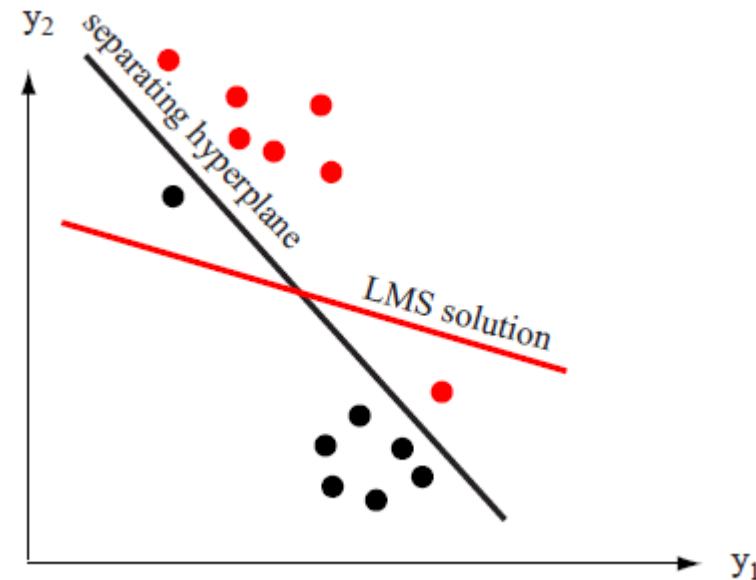
$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$



Pseudo-inverse of  $\mathbf{X}$

# Remarks on Squared Error Minimization

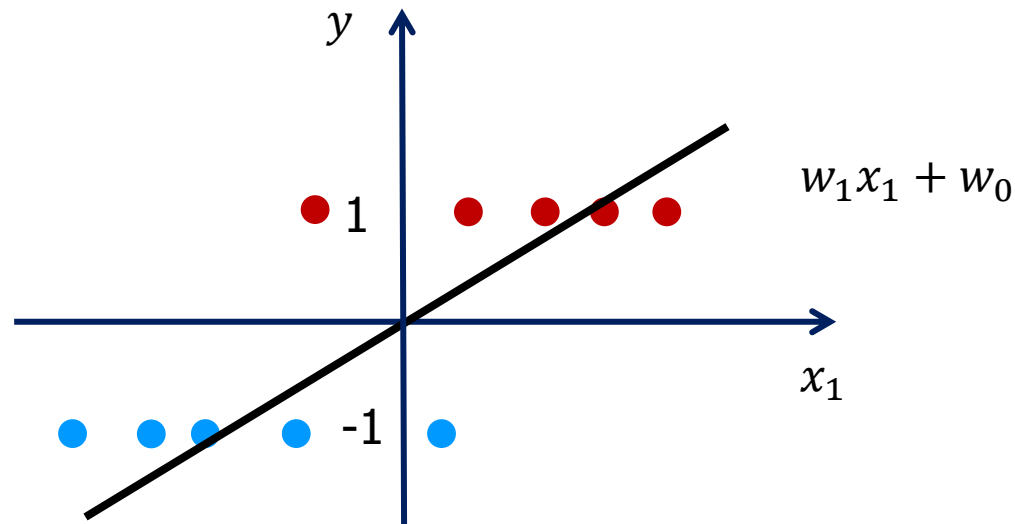
- Delta rule is preferred over the least-square solution, because
  - $X^T X$  may be singular
  - It avoids large matrix inverse
  - Automatically copes with some computational problems due to roundoff or truncation
- The solution  $w$  found by minimizing the squared error may not be optimal in terms of minimizing the classification error among all linear classification methods, even for linearly separable cases!



(Fig. 5.17 in Duda, Hart & Stork, Pattern Classification, 2001, Wiley)

# Geometric Interpretation of Squared Error

- Let's look at the 1d case

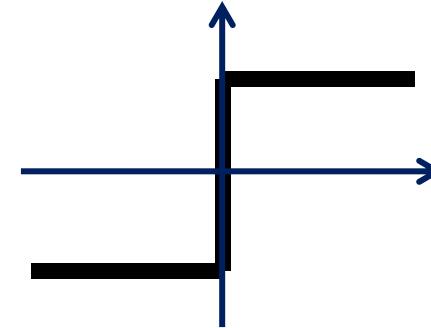


- $E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2$  is fitting the training data using linear regression with squared error
- **Correctly classified** examples (points far from origin) may have a significant contribution to this loss!

# Step Function → Smooth Function

- Perceptron

$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x})$$



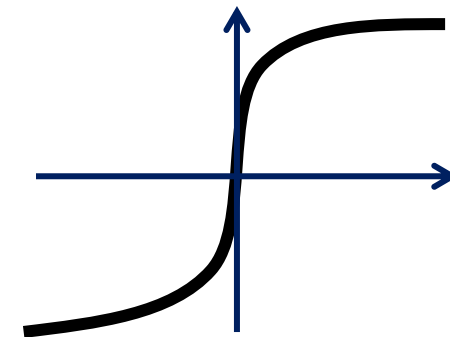
- Hyperbolic tangent activation

$$f(\mathbf{x}) = \tanh(\mathbf{w}^T \mathbf{x}) = \frac{1 - e^{-\mathbf{w}^T \mathbf{x}}}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$

- $\tanh()$  is a scaled **logistic sigmoid** function

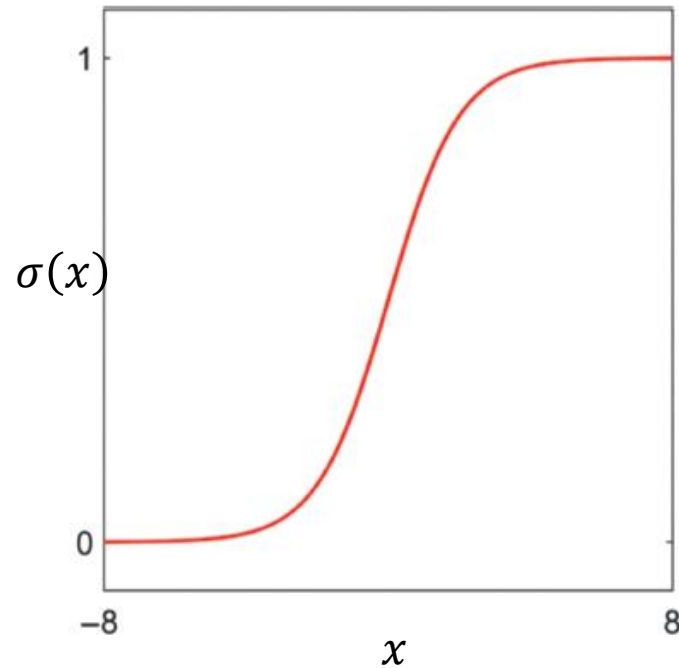
$$\tanh(x) = 2\sigma(x) - 1$$

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

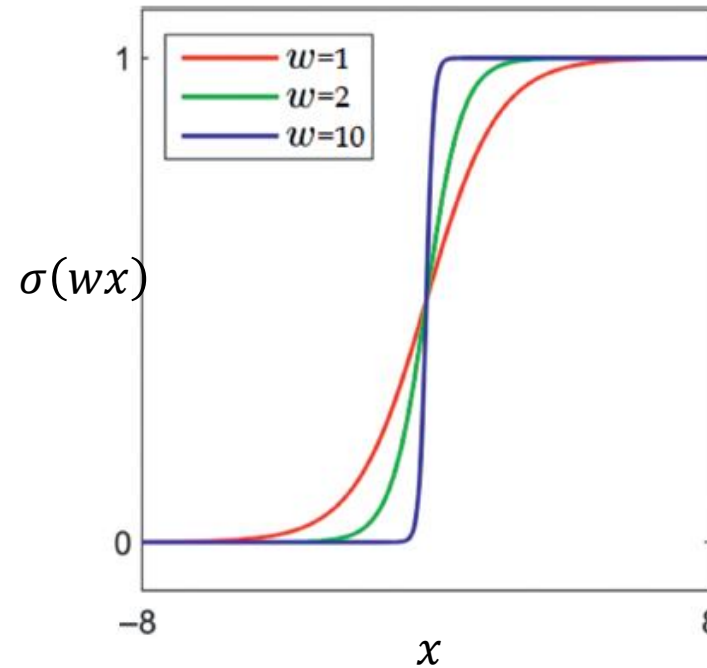


# Logistic Sigmoid Function

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



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



- As  $\|w\|$  increases, it approximates the step function more closely

# Logistic and Logit

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- Logistic function

$$y = \sigma(x) = \frac{1}{1 + e^{-x}}, x \in \mathbb{R}$$

- Logit function: the inverse function

$$x = \text{logit}(y) = \log\left(\frac{y}{1-y}\right), 0 < y < 1$$

- If  $y$  is viewed as probability of one class, then  $1 - y$  is the probability of the other class
  - Logit is then the log of their ratio, or **log of odds**
- The word “logistic” is related to “logic”, and “logarithmic”

# Logistic Regression with Squared Error

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- Minimize squared error loss

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^N (y^{(i)} - \tanh(\mathbf{w}^T \mathbf{x}^{(i)}))^2$$

- This is essentially **regression** with squared error using the  $\tanh(\cdot)$  function, which is a scaled **logistic** function; this is why it's called "logistic regression"
- This function is not convex w.r.t.  $\mathbf{w}$ , but we can still use gradient descent to find a local optimum

$$\nabla E(\mathbf{w}) = \sum_{i=1}^N \left( y^{(i)} - \frac{2}{1 + e^{-\mathbf{w}^T \mathbf{x}^{(i)}}} + 1 \right) \frac{2}{(1 + e^{-\mathbf{w}^T \mathbf{x}^{(i)}})^2} e^{-\mathbf{w}^T \mathbf{x}^{(i)}} (-\mathbf{x}^{(i)})$$

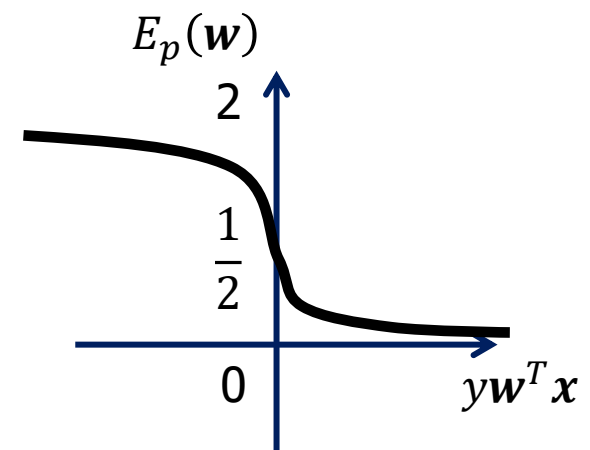


# Logistic Regression with Squared Error

- Let's look at the error for each example

$$\begin{aligned} E_p(\mathbf{w}) &= \frac{1}{2} (y - \tanh(\mathbf{w}^T \mathbf{x}))^2 \\ &= \frac{1}{2} \begin{cases} (1 - 2\sigma(\mathbf{w}^T \mathbf{x}) + 1)^2 & \text{if } y = +1 \\ (-1 - 2\sigma(\mathbf{w}^T \mathbf{x}) + 1)^2 & \text{if } y = -1 \end{cases} \\ &= 2 \begin{cases} \sigma^2(-\mathbf{w}^T \mathbf{x}) & \text{if } y = +1 \\ \sigma^2(\mathbf{w}^T \mathbf{x}) & \text{if } y = -1 \end{cases} \\ &= 2\sigma^2(-y\mathbf{w}^T \mathbf{x}) \end{aligned}$$

- Bigger loss if  $y$  and  $\mathbf{w}^T \mathbf{x}$  have different signs
  - But perhaps **not big enough** for very wrong  $\mathbf{w}^T \mathbf{x}$
- This is not convex for  $y\mathbf{w}^T \mathbf{x}$ 
  - So not convex for  $\mathbf{w}$

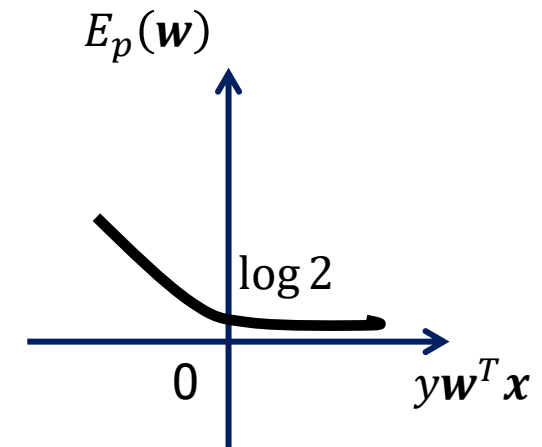


# Logistic Regression with Log Error

- Define point-wise **log error** cost

$$E_p(\mathbf{w}) = \begin{cases} -\log(\sigma(\mathbf{w}^T \mathbf{x})) & \text{if } y = +1 \\ -\log(\sigma(-\mathbf{w}^T \mathbf{x})) & \text{if } y = -1 \end{cases}$$
$$= -\log(\sigma(y\mathbf{w}^T \mathbf{x})) = \log(1 + e^{-y\mathbf{w}^T \mathbf{x}})$$

- **Much bigger** loss when  $y$  and  $\mathbf{w}^T \mathbf{x}$  have different signs
- This is convex for  $y\mathbf{w}^T \mathbf{x}$ 
  - So convex for  $w$



# Logistic Regression with Log Error

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- Sum all point-wise log error together → **Softmax Loss**

$$E(\mathbf{w}) = \sum_{i=1}^N \log \left( 1 + e^{-y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}} \right)$$

- This is a convex function of  $\mathbf{w}$  !
- Compute gradient w.r.t.  $\mathbf{w}$ , then take gradient descent

$$\nabla E(\mathbf{w}) = - \sum_{i=1}^N \frac{e^{-y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}}}{1 + e^{-y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}}} y^{(i)} \mathbf{x}^{(i)}$$

- Or compute Hessian and then use Newton's method

$$\nabla^2 E(\mathbf{w}) = \sum_{i=1}^N \sigma(y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}) \left( \mathbf{1} - \sigma(y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}) \right) \mathbf{x}^{(i)} \mathbf{x}^{(i)T}$$

# Why Called Softmax?

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- Without loss of generality, assume  $a < b$

$$\begin{aligned}\max\{a, b\} &= b \\ &= a + (b - a) = \log e^a + \log e^{b-a} \\ &< \log e^a + \log(1 + e^{b-a}) \\ &= \log(e^a + e^b) \\ &\doteq \textit{softmax}\{a, b\}\end{aligned}$$

- Single-sample log error cost

$$\begin{aligned}\log\left(1 + e^{-y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)}}\right) &= \log\left(e^0 + e^{-y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)}}\right) \\ &= \textit{softmax}\{0, -y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)}\}\end{aligned}$$

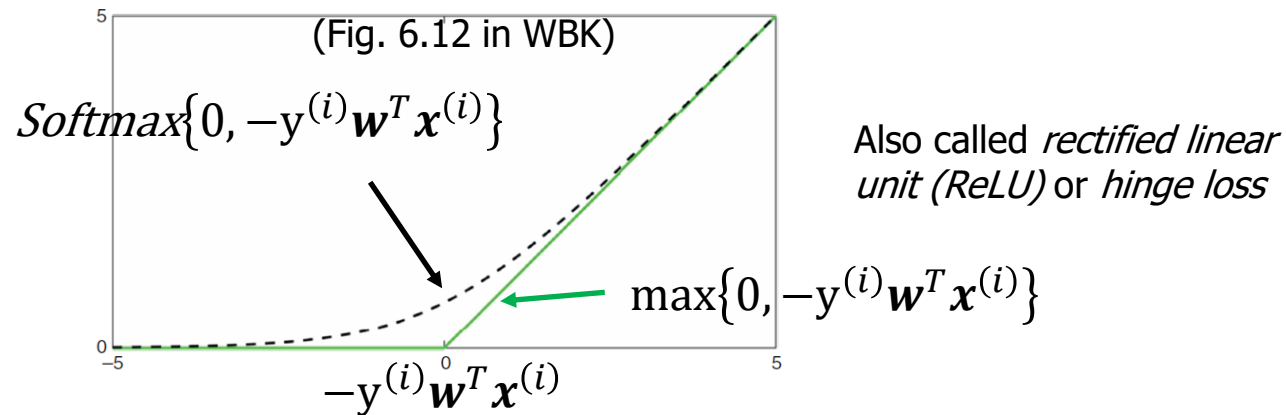
- The log error cost is thus the softmax between 0 and  $-y^{(i)}\mathbf{w}^T\mathbf{x}^{(i)}$

# Softmax vs. Max

- Remember perceptron criterion function

$$\begin{aligned} E(\mathbf{w}) &= \sum_{i \in \text{misclassified}} -\mathbf{w}^T \mathbf{x}^{(i)} (y^{(i)} - f(\mathbf{x}^{(i)})) \\ &= \sum_{i \in \text{misclassified}} -2y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)} > 0 \end{aligned}$$

- For correctly classified examples, the loss is 0
- Therefore, its single-sample loss is  $\max\{0, -2y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}\}$ 
  - If we neglect the scale 2, then it's  $\max\{0, -y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}\}$



# Comparing Four Losses

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- Perceptron criterion function (perceptron update rule)

$$E(\mathbf{w}) = \sum_{i \in \text{misclassified}} -\mathbf{w}^T \mathbf{x}^{(i)} (y^{(i)} - f(\mathbf{x}^{(i)})) = \sum_{i=1}^N \max\{0, -2y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}\}$$

- Perceptron squared error (delta rule)

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^N (y^{(i)} - \mathbf{w}^T \mathbf{x}^{(i)})^2 = \frac{1}{2} \sum_{i=1}^N (1 - y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)})^2$$

- Logistic regression with squared error

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^N (y^{(i)} - \tanh(\mathbf{w}^T \mathbf{x}^{(i)}))^2 = 2 \sum_{i=1}^N \left( \frac{e^{-y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}}}{1 + e^{-y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}}} \right)^2$$

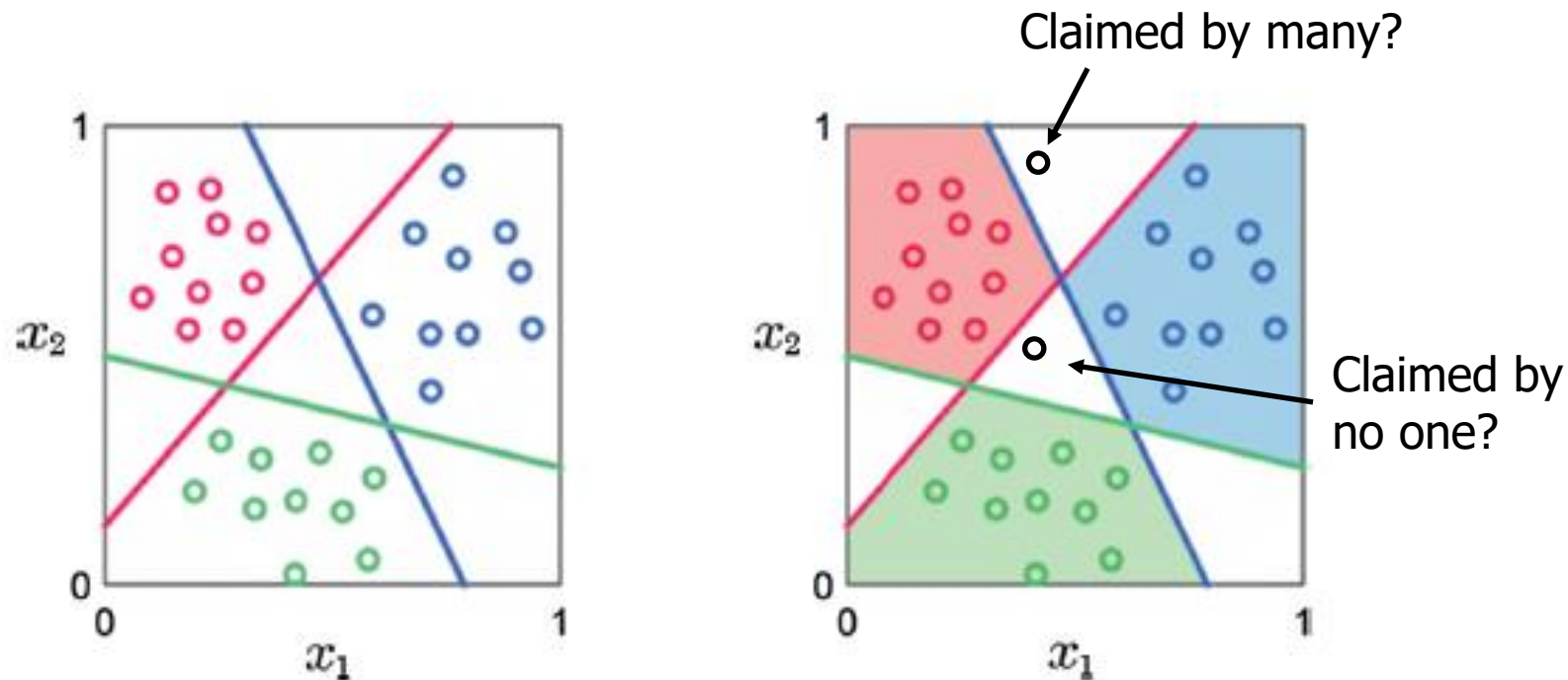
- Logistic regression with log error

$$E(\mathbf{w}) = \sum_{i=1}^N \log(1 + e^{-y^{(i)} \mathbf{w}^T \mathbf{x}^{(i)}})$$

- Let's [draw](#) them on whiteboard!

# Multi-Class Classification

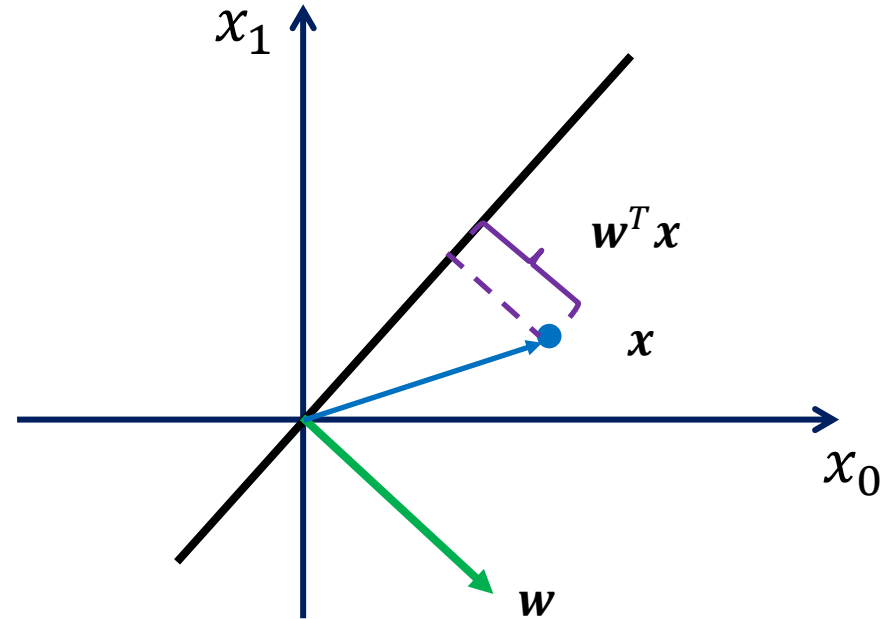
- How do we generalize binary linear classification to multiple (e.g.,  $C$ ) classes?
- First idea: train  $C$  one-versus-all classifiers



(Figs. 7.2 and 7.3 of WBK)

# Distance from Classification Boundary

- If  $x$  is on the positive side
  - Distance is  $\frac{w^T x}{\|w\|_2}$
- If  $x$  is on the negative side
  - Distance is  $-\frac{w^T x}{\|w\|_2}$
- If we assume  $w$  is **normalized** as  $\|w\|_2 = 1$ , then the **signed distance** is simply  $w^T x$
- This normalization can be achieved by regularization

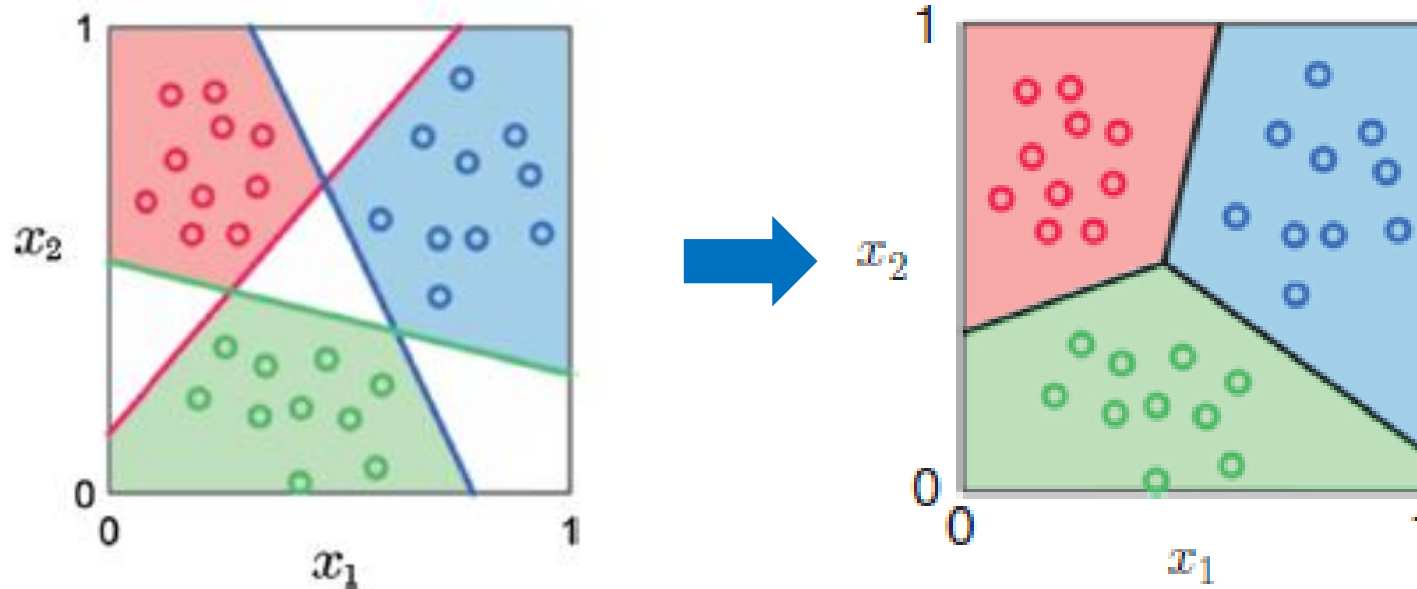




# Fusing all OvA Classifiers Together

- Output the class whose OvA classification boundary has the largest signed distance to the example

$$\hat{y} = \arg \max_{j=0, \dots, C-1} \mathbf{w}_j^T \mathbf{x}, \quad \text{s. t. } \|\mathbf{w}\|_2 = 1$$



# Multi-Class Perceptron

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- We hope that the signed distance between each training example and the binary classification boundary of its **target class** is the largest
- If it's not, then this example is likely **misclassified**

- Based on this idea, we can define a loss function

$$\begin{aligned} E(\mathbf{w}_0, \dots, \mathbf{w}_{C-1}) &= \sum_{i=1}^N \left\{ \left( \max_{j=0, \dots, C-1} \mathbf{w}_j^T \mathbf{x}^{(i)} \right) - \mathbf{w}_{y^{(i)}}^T \mathbf{x}^{(i)} \right\} \\ &= \sum_{i=1}^N \left\{ \max_{\substack{j=0, \dots, C-1 \\ j \neq y^{(i)}}} \left( 0, \left( \mathbf{w}_j - \mathbf{w}_{y^{(i)}} \right)^T \mathbf{x}^{(i)} \right) \right\} \end{aligned}$$

- This is similar to the **binary Perceptron Criterion Function**, convex but has non-differentiable points

# Max $\rightarrow$ Softmax

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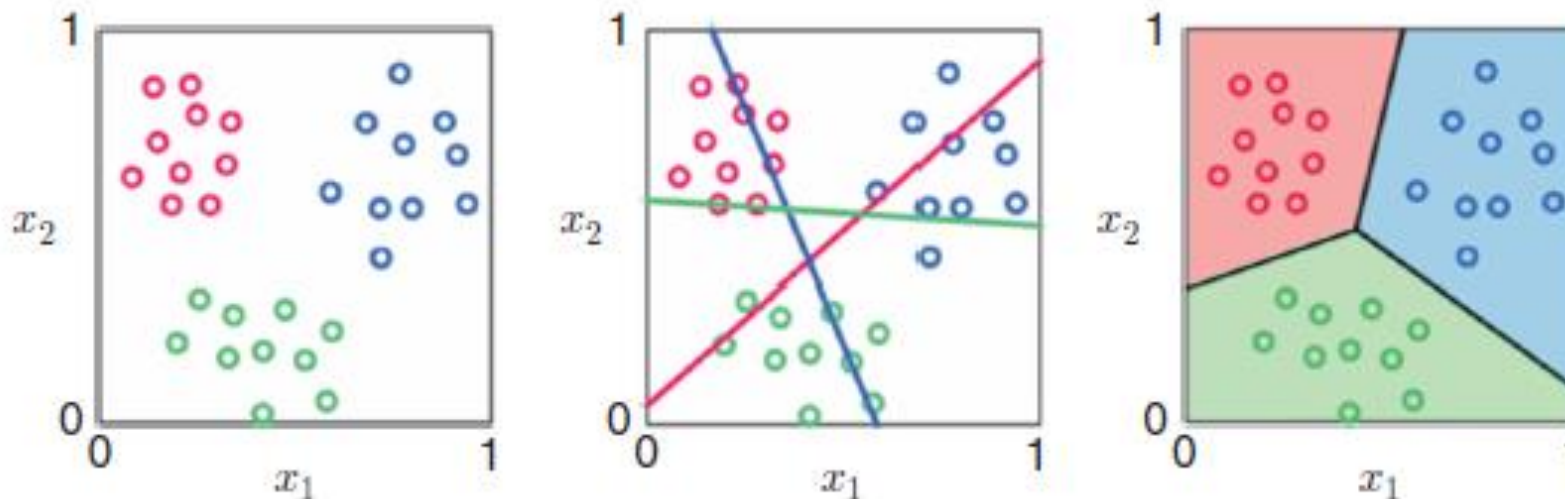
- A new loss function

$$\begin{aligned} E(\mathbf{w}_0, \dots, \mathbf{w}_{C-1}) &= \sum_{i=1}^N \left\{ \left( \operatorname{softmax}_{j=0, \dots, C-1} \mathbf{w}_j^T \mathbf{x}^{(i)} \right) - \mathbf{w}_{y^{(i)}}^T \mathbf{x}^{(i)} \right\} \\ &= \sum_{i=1}^N \left\{ \log \left( \sum_{j=0}^{C-1} e^{\mathbf{w}_j^T \mathbf{x}^{(i)}} \right) - \mathbf{w}_{y^{(i)}}^T \mathbf{x}^{(i)} \right\} \\ &= - \sum_{i=1}^N \left\{ \log \left( \frac{e^{\mathbf{w}_{y^{(i)}}^T \mathbf{x}^{(i)}}}{\sum_{j=0}^{C-1} e^{\mathbf{w}_j^T \mathbf{x}^{(i)}}} \right) \right\} \end{aligned}$$

- This is convex and smooth!

# Classification Boundaries

- Multi-class perceptron learns all  $C$  binary classifiers **simultaneously**
  - Each single binary classifier may not be the best OvA classifier, but the fused classifier is usually better than the naïve fusion of  $C$  independently trained OvA classifiers



(Fig. 4.20 in WBK 1<sup>st</sup> ed.)

# Summary

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- Classification boundaries of linear classifiers are linear functions of the input features. They are hyperplanes.
- Perceptron uses a **step function** across the classification boundary. Its optimization has two main variants
  - Perceptron criterion function (**max**, hinge loss, ReLU) → perceptron update rule
  - Perceptron with squared error → delta rule
- Logistic regression uses **hyperbolic tangent function** to replace the step function. Its optimization has two main variants
  - Logistic regression with squared error (not convex)
  - Logistic regression with log error (**softmax**)
- Loss comparisons  $E(\mathbf{w})$  vs.  $-y\mathbf{w}^T \mathbf{x}$

# Summary

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- Multi-class classification
  - One-versus-All (OvA): train binary classifiers **independently**, then fuse based on **signed distance** from classification boundaries
  - Multi-class perceptron: train binary classifiers **simultaneously**; **fusion is inside** the model.  
Two variants of loss functions:
    - Max: extension of the binary-class perceptron criterion function (i.e., perceptron update rule)
    - Softmax: extension of the binary-class logistic regression with log error
    - The learned binary classifiers may not be the optimal OvA classifiers, but the learned multi-class classifier is usually better than the post fusion of independently trained OvA classifiers