Machine Learning Classification 3 and 4

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### Classification with a linear classifier

•  $S = \{(x_1, y_1), \dots, (x_N, y_N)\}$ : data set

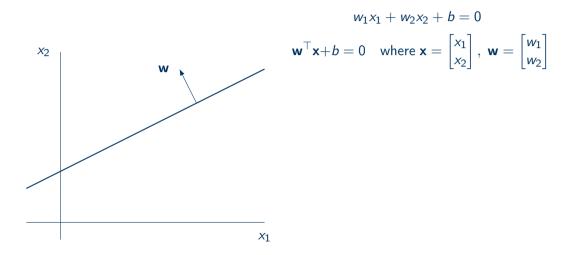
•  $\mathbf{x}_i = \begin{bmatrix} x_{i1} & \cdots & x_{id} \end{bmatrix}^\top$ ,  $i = 1, \dots, n$ : input, feature vector, *features* 

• y<sub>i</sub>: ground truth, *label*, gold reference, for x<sub>i</sub>.

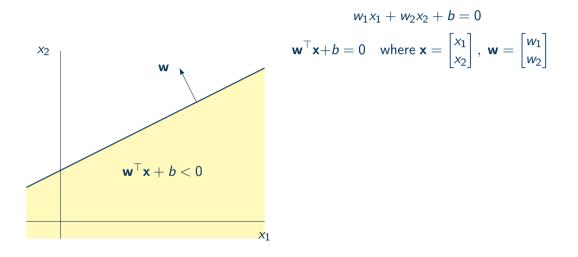
- $f(\mathbf{x}) = \mathbf{w}^{\top}\mathbf{x} + b$ : linear separator, linear predictor
  - $\boldsymbol{w} = \begin{bmatrix} w_1 & \cdots & w_d \end{bmatrix}^\top$ : weights, weight vector
  - $b \in \mathbb{R}$ : bias
  - $\{\boldsymbol{w}, b\}$ : parameters  $\cdots$   $(\boldsymbol{\theta} = [b \ \boldsymbol{w}^{\top}]^{\top})$

• 
$$h(\mathbf{x}) = \operatorname{sgn}(f(\mathbf{x}))$$
, where  $\operatorname{sgn}(z) = \begin{cases} -1 & \text{if } z < 0 \\ +1 & \text{if } z \ge 0 \end{cases}$   
NB: This is a non-standard definition of a sign function

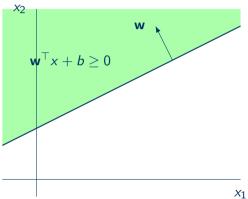
#### Geometry of linear classification



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$$w_1 x_1 + w_2 x_2 + b = 0$$
  
 $\mathbf{w}^\top \mathbf{x} + b = 0$  where  $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ ,  $\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$ 

hyperplane, decision boundary, . . . splitting the space into decision regions

NB:  $\boldsymbol{w}$  is a normal vector of the hyper**plane**. b is not the  $x_2$  intercept.

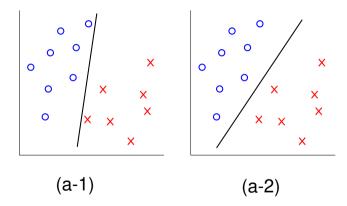
#### Geometry of linear classification (cont.)

 $f(\mathbf{x}) = w_1 x_1 + w_2 x_2 + b$ 15 10 5 f(**x**) 0 -5 -10-15 15 10 5 0 <u>+</u>5 -5 -10

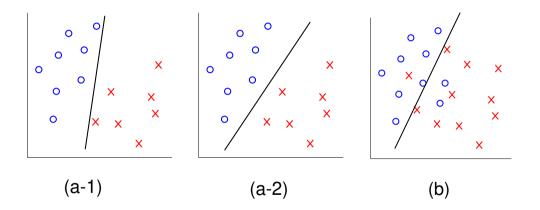
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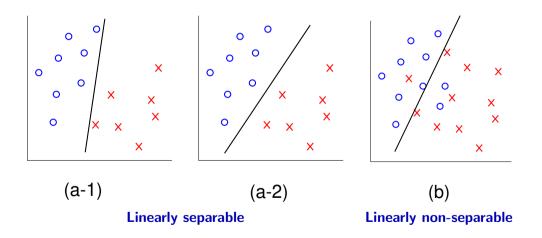
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- The task is called *binary classification*, because there are two classes.
- Why not finding the model parameters {**w**, b} directly based on a misclassification *loss*?

$$\min_{\boldsymbol{w},b}\sum_{i=1}^{N}\ell(\hat{y}_{i},y_{i}), \quad \text{where } \hat{y}_{i}=h(\boldsymbol{x}_{i})$$

#### Zero-one loss

$$\ell_{01}(\hat{y},y) = egin{cases} 1 & ext{if } \hat{y} 
eq y \ 0 & ext{otherwise} \end{bmatrix} = \mathbb{1}_{\hat{y} 
eq y}$$

(2)

- Think  $\hat{y}$  as the prediction and y as the label.
- We suffer a loss of 1 if we predict the label wrong.
- In the binary case,  $\ell_{01}(\hat{y}, y) = \mathbb{1}_{\hat{y}y < 0}$ .

### Discriminative training of a classifier

• Given  $S = \{(x_1, y_1), \dots, (x_N, y_N)\}$ , find  $\theta$  such that the **zero-one loss** 

$$L = \frac{1}{N} \sum_{i=1}^{N} \ell_{01}(h(\mathbf{x}_i), y_i)$$
(3)

is minimised. NB: L is called a **cost function**.

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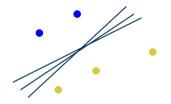
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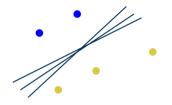
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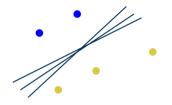
$$L = \frac{1}{N} \sum_{i=1}^{N} \ell_{01}(\text{sgn}(\mathbf{w}^{\top} \mathbf{x}_{i} + b), y_{i}) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{y_{i}(\text{sgn}(\mathbf{w}^{\top} \mathbf{x}_{i} + b)) < 0}$$
(4)



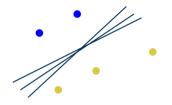
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- The loss function (with respect to **w** and b) is like step functions, flat everywhere with discontinuity when the value changes.
- Finding the optimal **w** and b is inherently combinatorial and hard.

# What about using linear regression?

$$\min_{\boldsymbol{w},b} \sum_{i=1}^{N} \left( (\boldsymbol{w}^{\top} \boldsymbol{x}_i + b) - y_i \right)^2, \quad y_i \in \{-1,+1\}$$

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- We know we can find a solution in closed form.
- Any problems?

# **Types of linear classifiers**

- Linear Discriminant Analysis (LDA)
- Template-based matching with Euclidean distance
- Fisher's linear discriminant
- Logistic regression
- Support Vector Machine (linear version)
- Perceptron (original version)
- Single-layer neural networks with no hidden nodes

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#### Q: Which of the above are from a generative approach?

- The range of  $f(\mathbf{x}) = \mathbf{w}^{\top}\mathbf{x} + b : (-\infty, +\infty)$
- We want to squeeze the range into [0,1] with a function g(s) so that it can be treated as a probability.

$$g(f(\mathbf{x})) = g(\mathbf{w}^{\top}\mathbf{x} + b) \rightarrow p(y = +1|\mathbf{x})$$

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• Logistic regression model:

$$p(y=+1|\mathbf{x}, \boldsymbol{\theta}) = \frac{1}{1 + \exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}$$
(6)  
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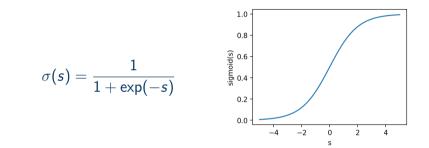
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$$= \frac{\exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}{1 + \exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}$$
(8)

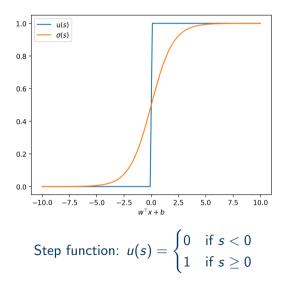
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# **Sigmoid function**

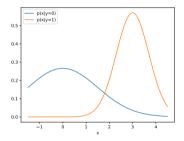


- When  $s \to \infty$ ,  $\sigma(s) \to 1$ .
- When  $s \to -\infty$ ,  $\sigma(s) \to 0$ .

#### Sigmoid function vs step function

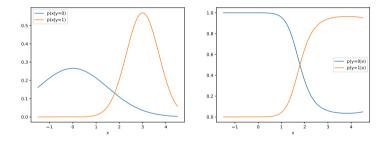


#### Data distributions p(x|y)



Data distributions p(x|y) Poste

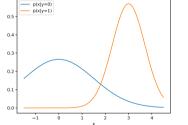
Posterior prob. p(y|x)

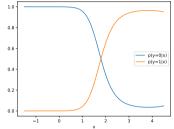


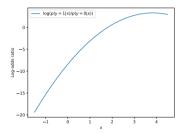
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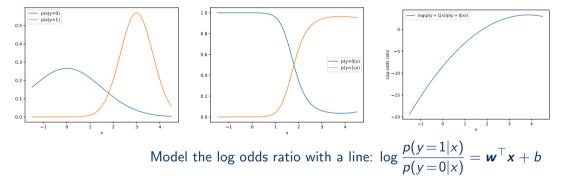




Data distributions p(x|y)

#### Posterior prob. p(y|x)





### Classification with the logistic regression model

For a test input x,

 $1. \ \mbox{calculate the posterior probability with the model.}$ 

$$p(y=1|\boldsymbol{x}, \boldsymbol{ heta}) = rac{1}{1+\exp(-(\boldsymbol{w}^{ op}\boldsymbol{x}+b))}$$

2. make a prediction:

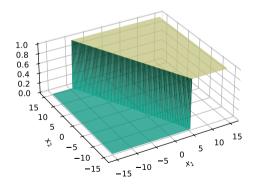
.

$$\hat{y} = \begin{cases}
+1 & p(y = +1 | \mathbf{x}, \theta) > \text{threshold}, \\
-1 & p(y = +1 | \mathbf{x}, \theta) \le \text{threshold}
\end{cases}$$
(9)

NB: threshold = 0.5 normally – it gives a minimum misclassification rate.

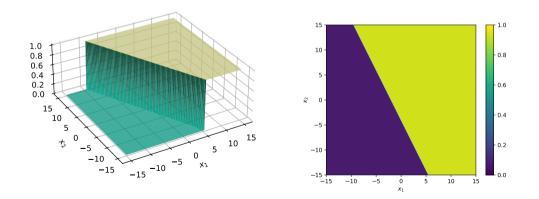
#### **Decision surface - step function version**

 $u(w^{\top}x+b)$ 



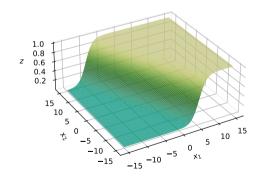
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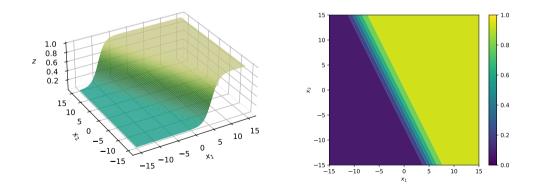
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# A logistic regression model

$$p(y=+1|\mathbf{x}, \theta) = \frac{1}{1 + \exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}$$
(10)  
$$p(y=-1|\mathbf{x}, \theta) = 1 - \frac{1}{1 + \exp(-(\mathbf{w}^{\top}\mathbf{x} + b))} = \frac{\exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}{1 + \exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}$$
(11)  
$$= \frac{1}{\exp(\mathbf{w}^{\top}\mathbf{x} + b) + 1}$$
(12)

Thus,

$$p(y|\boldsymbol{x},\boldsymbol{\theta}) = \frac{1}{1 + \exp(-\boldsymbol{y}(\boldsymbol{w}^{\top}\boldsymbol{x} + b))}$$
(13)

#### How to train the logistic regression model?

• Use MSE? 
$$\min_{\boldsymbol{w},\boldsymbol{b}} \sum_{i=1}^{n} (p(y=+1|\boldsymbol{x}_i,\boldsymbol{\theta}) - y_i)^2$$
 NB: the label  $y_i$  needs to be changed to  $\{0,1\}$ .

• Apply the *maximum likelihood estimation (MLE*):

Given a data set  $\{(x_1, y_1), \dots, (x_N, y_N)\}$ , maximise the likelihood *L* of *w* and *b*.

n

$$\max_{\boldsymbol{w},b} L$$
(14)  
$$L = \log \prod_{i=1}^{N} p(y_i | \boldsymbol{x}_i, \boldsymbol{\theta}) = \sum_{i=1}^{N} \log \frac{1}{1 + \exp(-y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b))}$$
(15)  
$$= \sum_{i=1}^{N} -\log \left(1 + \exp(-y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + b))\right)$$
(16)

### How to find the optimal solutions w and b?

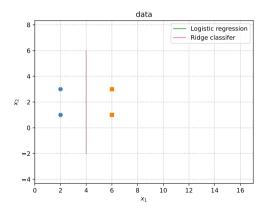
- The zero-one loss  $\sum_{i=1}^{N} \mathbb{1}_{y_i(\boldsymbol{w}^{\top}\boldsymbol{x}_i+b)<0}$  is flat, and is hard to optimise.
- The log likelihood of the logistic regression model  $L = \sum_{i=1}^{N} -\log(1 + \exp(-y_i(\boldsymbol{w}^{\top}\boldsymbol{x}_i + b)) \text{ is differentiable.}$
- However,

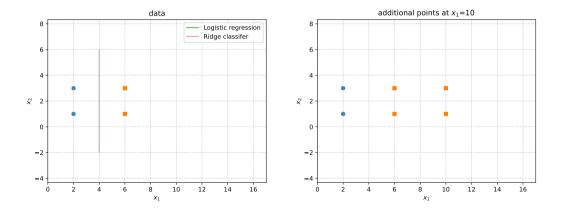
$$\frac{\partial L}{\partial w_i} = 0, \ i = 1, \dots, d$$
 and  $\frac{\partial L}{\partial b} = 0$ 

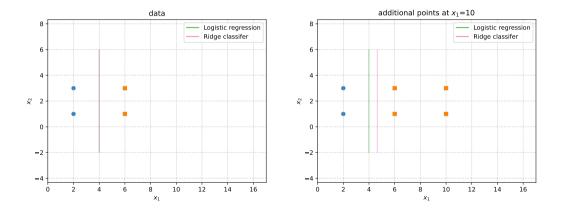
do not have *closed-form* solutions.  $\rightarrow$  employ *gradient ascent*.

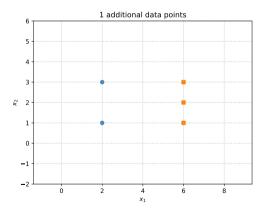
• We will come back to this in a lecture on optimisation.

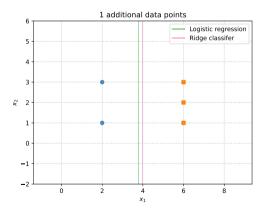
(17)

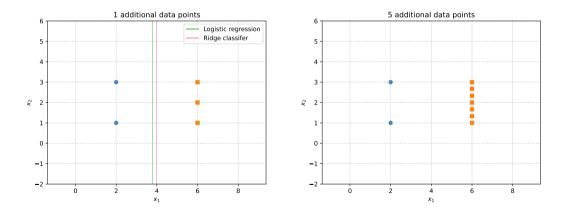


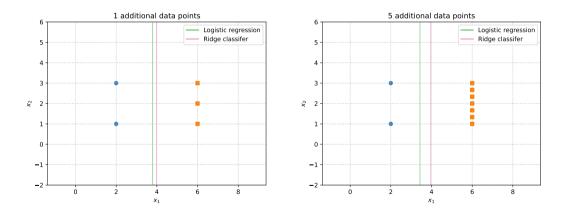












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(19)

$$p(y \mid \mathbf{x}) = \left(\frac{1}{1 + \exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}\right)^{y} \left(1 - \frac{1}{1 + \exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}\right)^{1-y}$$
(20)  
=  $s^{y}(1 - s)^{1-y}$ (21)  
where  $s = \frac{1}{1 + \exp(-(\mathbf{w}^{\top}\mathbf{x} + b))}$ .

# What if we use 0/1 labels instead of -1/+1? (cont.)

Training with MLE,

$$L = \log \prod_{i=1}^{N} p(y_i | \mathbf{x}_i, \theta)$$
(22)  
=  $\log \prod_{i=1}^{N} s_i^{y_i} (1 - s_i)^{1 - y_i}$ (23)  
=  $\sum_{i=1}^{N} y_i \log s_i + (1 - y_i) \log(1 - s_i)$ (24)  
=  $-\sum_{i=1}^{N} H(y_i, s_i)$ (25)

where  $H(p,q) = -\sum_{x} p(x) \log q(x)$  is a cross entropy between the two probability distributions p and q. For a binary case,  $H(p,q) = -(p \log q + (1-p) \log(1-q))$ .

# **Classification losses**

Suppose we have a labelled data point (x, y).

• Zero-one loss

$$\mathbb{1}_{y(\boldsymbol{w}^{\top}\boldsymbol{x}+b)<0} \tag{26}$$

• Log loss (logistic loss)

$$-\log p(y|\mathbf{x}) = \log(1 + \exp(-y(\mathbf{w}^{\top}\mathbf{x} + b))$$
(27)

#### **Notation caveat**

- The log loss notation  $-\log p(y|\mathbf{x})$  can be misleading.
- Is y the ground truth or is it a free variable?
- What it really means is  $-\log p(y=y^*|\mathbf{x})$  given a pair  $(x, \mathbf{y}^*)$ .
- Or  $-\log p(y=y_i|\mathbf{x}_i)$  given a pair  $(\mathbf{x}_i, y_i)$  in a data set.

### How to resolve a linearly non-separable case?

#### Feature transformation

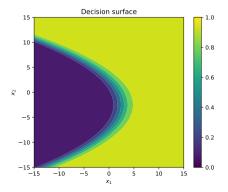
$$h(\mathbf{x}) = \begin{cases} -1 & \text{if } \mathbf{w}^{\top} \mathbf{x} + b < 0 \\ +1 & \text{if } \mathbf{w}^{\top} \mathbf{x} + b \ge 0 \end{cases} = \operatorname{sgn}(\mathbf{w}^{\top} \mathbf{x} + b)$$
(28)  
$$\downarrow$$
$$h(\mathbf{x}) = \begin{cases} -1 & \text{if } \mathbf{w}^{\top} \phi(\mathbf{x}) < 0 \\ +1 & \text{if } \mathbf{w}^{\top} \phi(\mathbf{x}) \ge 0 \end{cases} = \operatorname{sgn}(\mathbf{w}^{\top} \phi(\mathbf{x}))$$
(29)

#### Feature transformation (cont.)

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \frac{1}{1 + \exp(-y(\mathbf{w}^{\top}\mathbf{x} + b))}$$
(30)  
$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \frac{1}{1 + \exp(-y(\mathbf{w}^{\top}\phi(\mathbf{x})))}$$
(31)

#### **Feature transformation - examples**

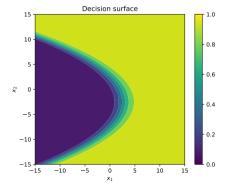
 $(x_1, x_2) \rightarrow (x_1, x_2, x_2^2)$ 

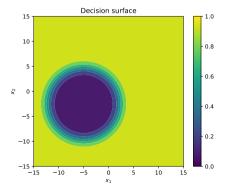


#### **Feature transformation - examples**

 $(x_1, x_2) \rightarrow (x_1, x_2, x_2^2)$ 

 $(x_1, x_2) \rightarrow (x_1, x_2, x_1^2, x_2^2)$ 

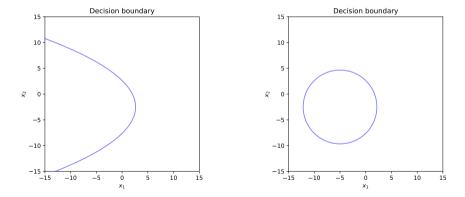




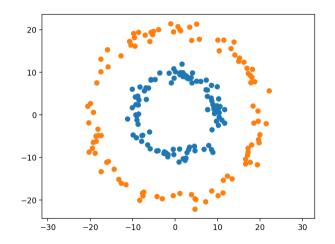
#### **Feature transformation - examples**

 $(x_1, x_2) \rightarrow (x_1, x_2, x_2^2)$ 

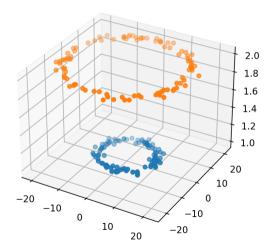
 $(x_1, x_2) \rightarrow (x_1, x_2, x_1^2, x_2^2)$ 



# **Two-circle example**



#### **Two-circle example**



## What is it meant by linear classifiers?

- A linear classifier is linear in the parameters w, **not** in the features.
- A linear classifier can have arbitrary nonlinear features.

# Should we consider very complex transformation?

- Not necessarily so.
- Complex models may overfit the training data and may not generalise very well.
- We will come back to this in some lectures later.

### How to extend the model to multiclass classification?

- one-vs.-all (one-against-all)
- one-vs.-one

### Multiclass classification with logistic regression

Replace the sigmoid with the softmax function letting  $\mathbf{x} = [1 x_1 x_2 \cdots, x_d]$  and  $\mathbf{w} = [w_0 w_1 \cdots w_d]$ 

• w/o transformation

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \frac{\exp(\mathbf{w}_{y}^{\top} \mathbf{x})}{\sum_{y' \in \mathbf{y}} \exp(\mathbf{w}_{y'}^{\top} \mathbf{x})}$$
(32)

• w transformation

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \frac{\exp(\mathbf{w}_{y}^{\top} \phi(\mathbf{x}))}{\sum_{y' \in \boldsymbol{\mathcal{Y}}} \exp(\mathbf{w}_{y'}^{\top} \phi(\mathbf{x}))}$$
(33)

NB: we can just use and compare " $\boldsymbol{w}_{y}^{\top}\phi(\boldsymbol{x})$ " for classification – the denominator is a constant for  $y \in \mathcal{Y}$  and exp() is a monotonically increasing function.

#### Softmax for binary classification

$$p(y=+1|\mathbf{x},\theta) = \frac{\exp(\mathbf{w}_{+1}^{\top}\mathbf{x})}{\exp(\mathbf{w}_{+1}^{\top}\mathbf{x}) + \exp(\mathbf{w}_{-1}^{\top}\mathbf{x})}$$
(34)  
$$= \frac{1}{1 + \exp(-(\mathbf{w}_{+1} - \mathbf{w}_{+1})^{\top}\mathbf{x})} = \frac{1}{1 + \exp(-\mathbf{w}^{\top}\mathbf{x})}$$
(35)  
$$p(y=-1|\mathbf{x},\theta) = \frac{\exp(\mathbf{w}_{-1}^{\top}\mathbf{x})}{\exp(\mathbf{w}_{+1}^{\top}\mathbf{x}) + \exp(\mathbf{w}_{-1}^{\top}\mathbf{x})}$$
(36)  
$$= \frac{\exp(-(\mathbf{w}_{+1} - \mathbf{w}_{-1})^{\top}\mathbf{x})}{1 + \exp(-(\mathbf{w}_{+1} - \mathbf{w}_{-1})^{\top}\mathbf{x})} = \frac{\exp(-\mathbf{w}^{\top}\mathbf{x})}{1 + \exp(-\mathbf{w})^{\top}\mathbf{x}}$$
(37)

where  $w = w_{+1} - w_{-1}$ .

 $\rightarrow$  the same as the sigmoid.

# Logistic regression model vs LDA

- Logistic regression:
- LDA

$$\log p(C_k | \mathbf{x}, \theta) = \mathbf{w}_k^\top \mathbf{x} + w_{k0} + \text{const}$$
(38)  
$$p(C_k | \mathbf{x}, \theta) = \frac{\exp(\mathbf{w}_k^\top \mathbf{x} + w_{k0})}{\sum_{k'} \exp(\mathbf{w}_{k'}^\top \mathbf{x} + w_{k'0})}$$
(39)

# Summary

• Log loss in the binary case

$$\sum_{i=1}^{N} \log \left( 1 + \exp(-y_i \boldsymbol{w}^{\top} \boldsymbol{\phi}(\boldsymbol{x}_i)) \right)$$
(40)

• Log loss in the multiclass case

$$\sum_{i=1}^{N} - \boldsymbol{w}_{y_i}^{\top} \phi(\boldsymbol{x}_i) + \log \left( \sum_{y' \in \mathcal{Y}} \exp(\boldsymbol{w}_{y'}^{\top} \phi(\boldsymbol{x}_i)) \right)$$

(41)

# Summary (cont.)

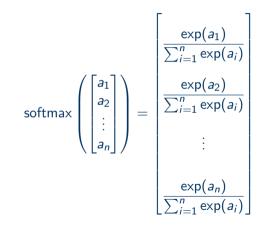
#### binary classification

#### multiclass classification

$$h(\boldsymbol{x}) = \begin{cases} -1 & \text{if } \boldsymbol{w}^\top \phi(\boldsymbol{x}) < 0 \\ +1 & \text{if } \boldsymbol{w}^\top \phi(\boldsymbol{x}) \ge 0 \end{cases} \qquad \qquad h(\boldsymbol{x}) = \underset{\boldsymbol{y} \in \mathcal{Y}}{\arg \max} \ \boldsymbol{w}_{\boldsymbol{y}}^\top \phi(\boldsymbol{x})$$

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \frac{1}{1 + \exp(-y \mathbf{w}^\top \phi(\mathbf{x}))} \qquad p(y|\mathbf{x}, \boldsymbol{\theta}) = \frac{\exp(\mathbf{w}_y^\top \phi(\mathbf{x}))}{\sum_{y' \in \mathcal{Y}} \exp(\mathbf{w}_{y'}^\top \phi(\mathbf{x}))}$$

#### Appendix – softmax





#### Appendix – softmax (cont.)

- softmax( $\begin{bmatrix} 1 & 2 & 3 \end{bmatrix}^{\top}$ ) =  $\begin{bmatrix} 0.09 & 0.24 & 0.67 \end{bmatrix}^{\top}$
- softmax( $\begin{bmatrix} 100 & 200 & 300 \end{bmatrix}^{\top}$ ) =  $\begin{bmatrix} 10^{-87} & 10^{-44} & 1.0 \end{bmatrix}^{\top}$
- Softmax always returns a probability distribution.
- When the dynamic range of the input is large, the result of softmax becomes "sharp."

#### Appendix – softmax (cont.)

• Claim: 
$$\frac{\exp(a_{\max}/\tau)}{\sum_{i=1}^{n} \exp(a_i/\tau)} \to 1$$
 when  $\tau \to 0$ .

• That means  $\frac{\exp(a_j/\tau)}{\sum_{i=1}^{n} \exp(a_i/\tau)} \to 0$  when  $\tau \to 0$  for any  $a_j$  that is not the max.

• We have

$$\frac{\exp(a_m/\tau)}{\sum_{i=1}^{n} \exp(a_i/\tau)} = \frac{\exp(a_m/\tau)}{\exp(a_m/\tau) + \sum_{i \neq m} \exp(a_i/\tau)}$$
(43)
$$= \frac{1}{1 + \sum_{i \neq m} \exp((a_i - a_m)/\tau)} \to 1$$
(44)

when  $\tau \rightarrow 0$  because  $a_m$  is the largest and  $a_i - a_m < 0$ .

# Quizzes

- 1. Consider two column vectors such that  $\mathbf{a} = (1,2,3)^{\top}$  and  $\mathbf{b} = (-3,3,-1)^{\top}$ .
  - Find  $\mathbf{a} + \mathbf{b}$ .
  - Find **a b**.
  - Find  $\|\mathbf{a}\|, \|\mathbf{b}\|, \text{and } \|\mathbf{a} \mathbf{b}\|.$
  - Find  $\mathbf{a}^{\top}\mathbf{b}$ .
  - Find  $\mathbf{a}\mathbf{b}^{\top}$ .
  - What is the geometric relationship between  $\mathbf{a}$  and  $\mathbf{b}$ ?
- 2. Considering a classification problem of two classes, whose discriminant function takes the form,  $y(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} + w_0$ .
  - Show that the decision boundary is a straight line when D = 2.
  - $\bullet\,$  Show that the weight vector w is a normal vector to the decision boundary.
- 3. Derive a formula for the Euclidean distance between the origin (0,0) and a line y = ax + b, where a and b are arbitrary constants.

# Quizzes (cont.)

- 4. Considering a linear classifier of binary classification in a two-dimensional vector space, such that the points (-2, -3) and (4, 1) are on the decision boundary, and the point (2, -3) lies in the -1 class region.
  - Find the parameters (w, b) of the classifier.
  - Find the unit normal vector of **w**.
- 5. Consider the following logistic regression model:

$$p(y=+1|x) = rac{1}{1+\exp(-(wx+b))}$$

Plot p(y=+1|x) for each of the following cases, where you use a fixed plotting range or show all the plots on a single graph for comparison, and report your findings.

- w = 1, b = 0
- w = 1, b = 1
- w = -1, b = 1
- w = 0.5, b = 1
- w = 2, b = 1

# Quizzes (cont.)

6. Consider the logistic sigmoid function.

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

- Based on the graph of σ(x), make an educated guess about the shape of the derivative σ'(x) without performing any calculations and illustrate it by hand.
- Find the derivative of  $\sigma(x)$ .
- Plot the derivative on a graph.