

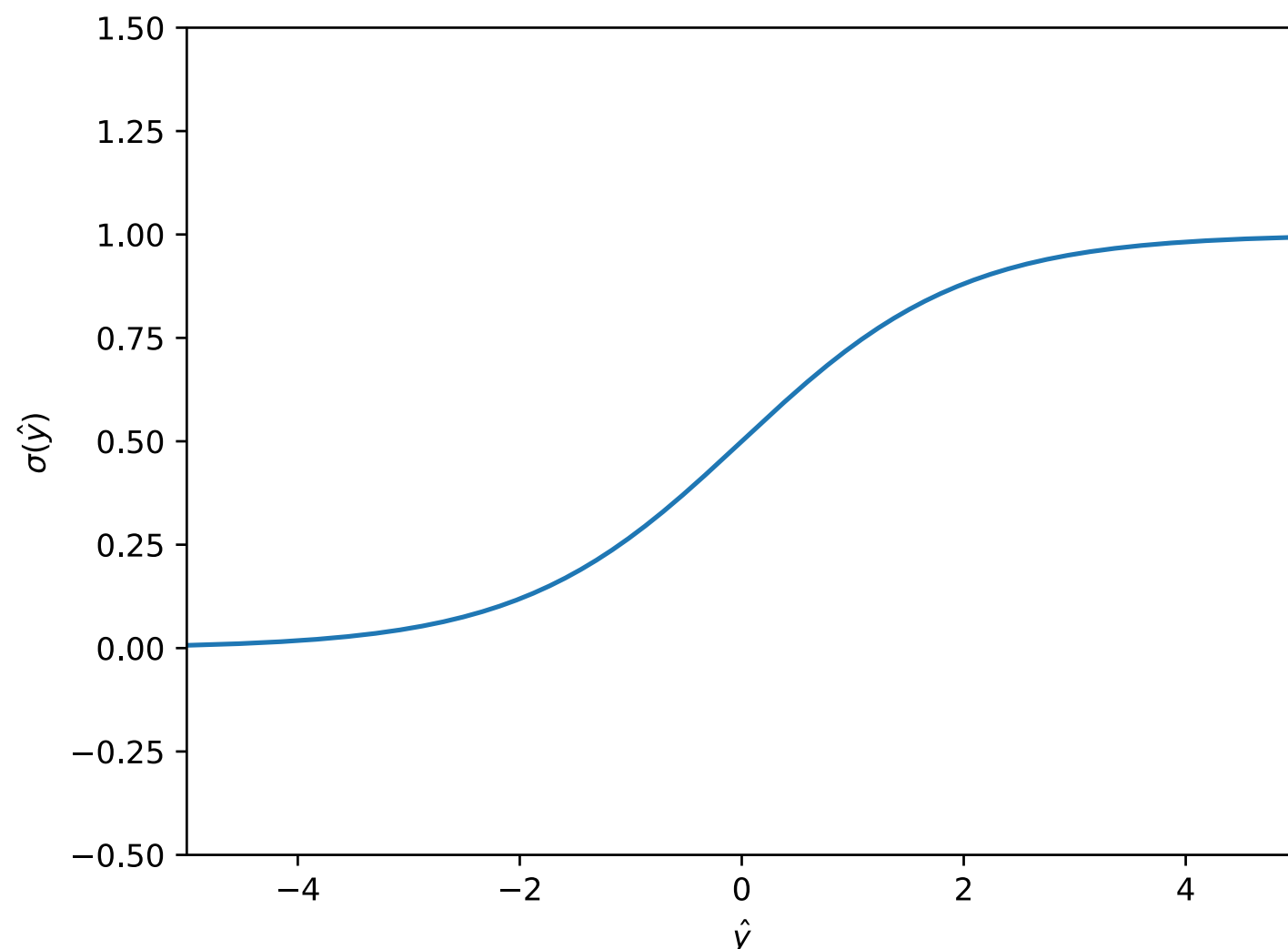
# CS 4342: Class 7

Jacob Whitehill

# Logistic regression

# Sigmoid: a “squashing” function

- A sigmoid function is an “s”-shaped, monotonically increasing and bounded function.
- Here is the **logistic sigmoid** function  $\sigma$ :



$$\frac{1}{1 + e^{-x}}$$

# Logistic sigmoid

- The logistic sigmoid function  $\sigma$  has some nice properties:
  - $\sigma(-z) = 1 - \sigma(z)$

$$\begin{aligned}\sigma(z) &= \frac{1}{1 + e^{-z}} \\ 1 - \sigma(z) &= 1 - \frac{1}{1 + e^{-z}} \\ &= \frac{1 + e^{-z}}{1 + e^{-z}} - \frac{1}{1 + e^{-z}} \\ &= \frac{e^{-z}}{1 + e^{-z}} \\ &= \frac{1}{1/e^{-z} + 1} \\ &= \frac{1}{1 + e^z} \\ &= \sigma(-z)\end{aligned}$$

# Logistic sigmoid

- The logistic sigmoid function  $\sigma$  has some nice properties:
  - $\sigma'(z) = \sigma(z)(1 - \sigma(z))$

$$\begin{aligned}\sigma(z) &= \frac{1}{1 + e^{-z}} \\ \frac{\partial \sigma}{\partial z} = \sigma'(z) &= -\frac{1}{(1 + e^{-z})^2} (e^{-z} \times (-1)) \\ &= \frac{e^{-z}}{(1 + e^{-z})^2} \\ &= \frac{e^{-z}}{1 + e^{-z}} \times \frac{1}{1 + e^{-z}} \\ &= \frac{1}{1/e^{-z} + 1} \times \frac{1}{1 + e^{-z}} \\ &= \frac{1}{1 + e^z} \times \frac{1}{1 + e^{-z}} \\ &= \sigma(z)(1 - \sigma(z))\end{aligned}$$

# Logistic regression

- With logistic regression, our predictions are defined as:

$$\hat{y} = \sigma(\mathbf{x}^\top \mathbf{w})$$

- Hence, they are forced to be in (0,1).
- For classification, we can interpret the real-valued outputs as probabilities that express how confident we are in a prediction, e.g.:
  - $\hat{y}=0.95$ : very confident that the class is a smile.
  - $\hat{y}=0.45$ : not very confident that the class is a non-smile.

# Exercise

- Suppose we want to predict lung cancer from a person's exposure to radon  $r$  and asbestos  $a$ :
  - $y = 1$  if person develops lung cancer;  $y = 0$  otherwise.
  - $\mathbf{x} = [a, r]^T$ , where:
    - $a$  = kilograms of asbestos inhaled
    - $r$  = average microCuries of radiation at home
  - Machine (with parameters  $\mathbf{w}$ ):  $\hat{y} = \sigma(\mathbf{x}^T \mathbf{w})$

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  - Machine (with parameters  $\mathbf{w}$ ):  $\hat{y} = \sigma(\mathbf{x}^T \mathbf{w})$
- Suppose we train the machine so that  $\mathbf{w} = [1.5 \ .22]^T$ .
- What is the machine's prediction for a person who inhales 2 grams of asbestos and whose home has an average of 4 microCuries?



# Solution

- Just plug in values for  $\mathbf{w}$  and  $\mathbf{x}$  (making sure to convert from grams to kilograms) and then pass through  $\sigma$ :
- $\hat{y} = \sigma(\mathbf{x}^T \mathbf{w}) = \sigma(.002 * 1.5 + 4 * .22) = \sigma(0.883) = 0.707.$
- In other words, the person is predicted to have a 70.7% probability of getting lung cancer.

# Logistic regression

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- Could we use grid search (like in homework 1)?

# Logistic regression

- How to train? Unlike linear regression, logistic regression has no analytical (“one-shot”) solution.
- Could we use grid search (like in homework 1)? No — intractable and unclear how to determine the grid.

# Logistic regression

- How to train? Unlike linear regression, logistic regression has no analytical (“one-shot”) solution.
- We can use gradient descent instead.
- We have to apply the **chain-rule of differentiation** to handle the sigmoid function.

# Gradient descent for logistic regression

- Let's compute the gradient of  $f_{\text{MSE}}$  for logistic regression.
- For simplicity, we'll consider just a single example:

$$\begin{aligned} f_{\text{MSE}}(\mathbf{w}) &= \frac{1}{2} (\hat{y} - y)^2 \\ &= \frac{1}{2} (\sigma(\mathbf{x}^\top \mathbf{w}) - y)^2 \\ \nabla_{\mathbf{w}} f_{\text{MSE}}(\mathbf{w}) &= \nabla_{\mathbf{w}} \left[ \frac{1}{2} (\sigma(\mathbf{x}^\top \mathbf{w}) - y)^2 \right] \\ &= \mathbf{x} (\sigma(\mathbf{x}^\top \mathbf{w}) - y) \sigma(\mathbf{x}^\top \mathbf{w}) (1 - \sigma(\mathbf{x}^\top \mathbf{w})) \\ &= \mathbf{x} (\hat{y} - y) \hat{y} (1 - \hat{y}) \end{aligned}$$

Notice the extra multiplicative terms compared to the gradient for *linear* regression:  $\mathbf{x}(\hat{y} - y)$

# Attenuated gradient

- What if the weights  $\mathbf{w}$  are initially chosen badly, so that  $\hat{y}$  is very close to 1, even though  $y = 0$  (or vice-versa)?
  - Then  $\hat{y}(1 - \hat{y})$  is close to 0.
- In this case, the gradient:

$$\nabla_{\mathbf{w}} f_{\text{MSE}}(\mathbf{w}) = \mathbf{x} (\hat{y} - y) \hat{y} (1 - \hat{y})$$

will be very close to 0.

- If the gradient is 0, then no learning will occur!

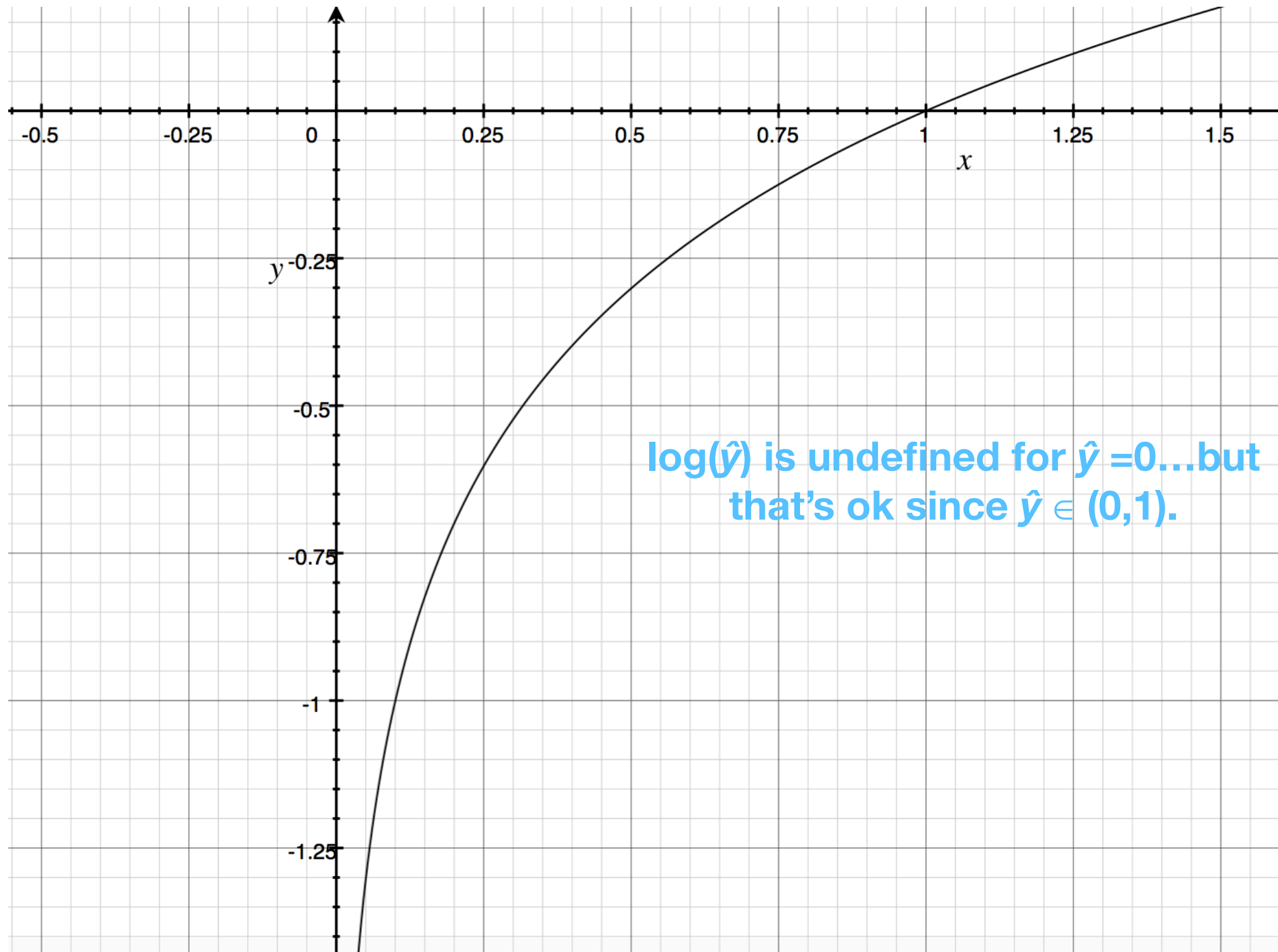
# Different cost function

- For this reason, logistic regression is typically trained using a different cost function from  $f_{\text{MSE}}$ .
- One particularly well-suited cost function uses logarithms.
- Logarithms and the logistic sigmoid interact well:

$$\begin{aligned}\frac{\partial}{\partial z} [\log \sigma(z)] &= \frac{1}{\sigma(z)} \sigma'(z) \\ &= \frac{1}{\sigma(z)} \sigma(z)(1 - \sigma(z)) \\ &= 1 - \sigma(z)\end{aligned}$$

The gradient of  $\log(\sigma)$  is surprisingly simple.

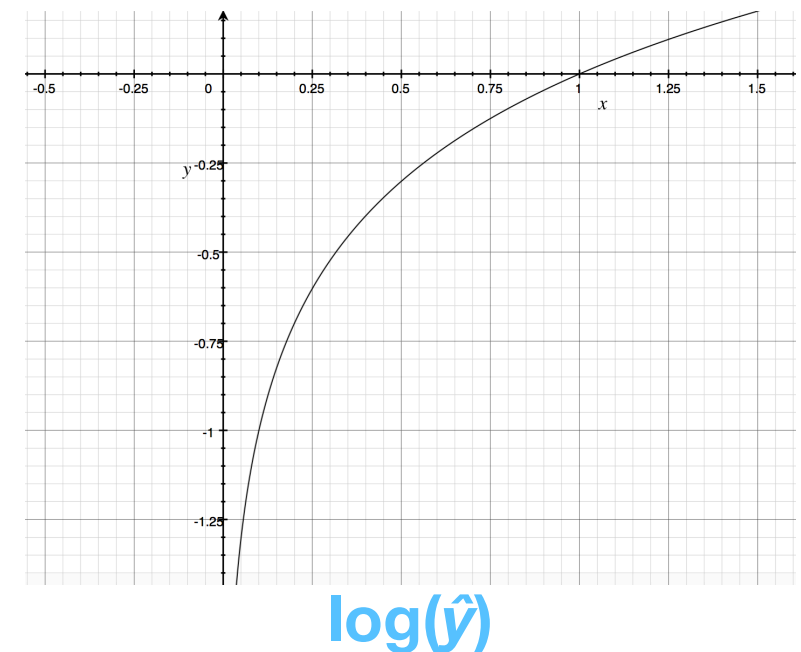
# Logarithm function





# Log loss

- How could we define a “log-loss” function  $f_{\log}$  so that:
    - $f_{\log}(y, \hat{y})$  is small when  $\hat{y} \approx y$  and large when they are far apart.
1.  $-y \log \hat{y} - \hat{y} \log y$
  2.  $-y \log \hat{y} - (1 - y) \log \hat{y}$
  3.  $-y \log \hat{y} - (1 - y) \log(1 - \hat{y})$
  4.  $-(1 - y) \log \hat{y} - y \log(1 - \hat{y})$



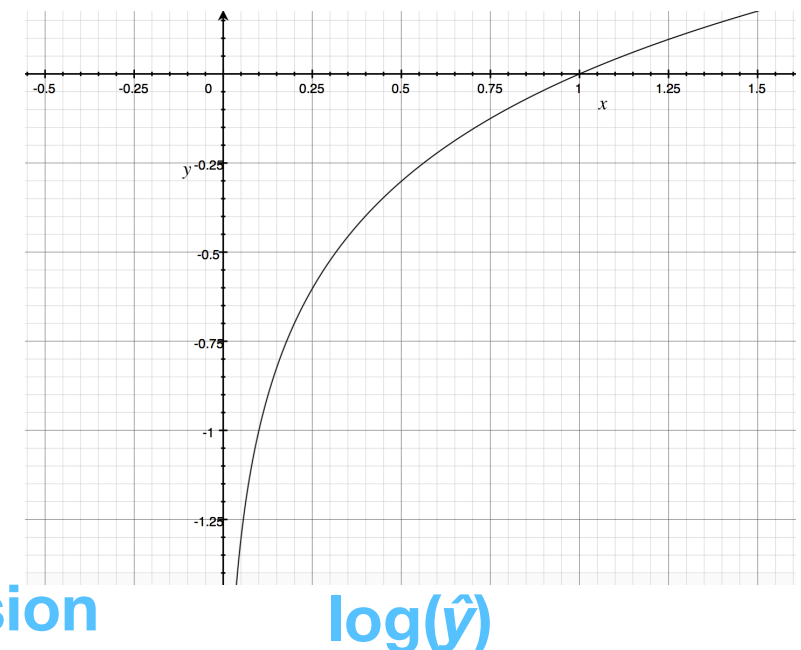
# Log loss

- How could we define a “log-loss” function  $f_{\log}$  so that:
- $f_{\log}(y, \hat{y})$  is small when  $\hat{y} \approx y$  and large when they are far apart.

This expression is known as the *log-loss*.

$$3. \quad -y \log \hat{y} - (1 - y) \log(1 - \hat{y})$$

The  $y$  or  $(1-y)$  “selects” which term in the expression is active, based on the ground-truth label.



# Gradient descent for logistic regression with log-loss

$$\nabla_{\mathbf{w}} f_{\log}(\mathbf{w}) = \nabla_{\mathbf{w}} [- (y \log \hat{y} - (1 - y) \log(1 - \hat{y}))]$$

# Gradient descent for logistic regression with log-loss

$$\begin{aligned}\nabla_{\mathbf{w}} f_{\log}(\mathbf{w}) &= \nabla_{\mathbf{w}} [- (y \log \hat{y} - (1 - y) \log(1 - \hat{y}))] \\ &= -\nabla_{\mathbf{w}} (y \log \sigma(\mathbf{x}^{\top} \mathbf{w}) + (1 - y) \log(1 - \sigma(\mathbf{x}^{\top} \mathbf{w})))\end{aligned}$$

# Gradient descent for logistic regression with log-loss

$$\begin{aligned}\nabla_{\mathbf{w}} f_{\log}(\mathbf{w}) &= \nabla_{\mathbf{w}} [- (y \log \hat{y} - (1 - y) \log(1 - \hat{y}))] \\ &= -\nabla_{\mathbf{w}} (y \log \sigma(\mathbf{x}^{\top} \mathbf{w}) + (1 - y) \log(1 - \sigma(\mathbf{x}^{\top} \mathbf{w}))) \\ &= - \left( y \frac{\mathbf{x} \sigma(\mathbf{x}^{\top} \mathbf{w})(1 - \sigma(\mathbf{x}^{\top} \mathbf{w}))}{\sigma(\mathbf{x}^{\top} \mathbf{w})} \right)\end{aligned}$$

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# Gradient descent for logistic regression with log-loss

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# Gradient descent for logistic regression with log-loss

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# Linear regression versus logistic regression

	Linear regression	Logistic regression
Primary use	Regression	Classification
Prediction ( $\hat{y}$ )	$\hat{y} = \mathbf{x}^T \mathbf{w}$	$\hat{y} = \sigma(\mathbf{x}^T \mathbf{w})$
Loss	$f_{\text{MSE}}$	$f_{\text{log}}$
Gradient	$\mathbf{x}(\hat{y} - y)$	$\mathbf{x}(\hat{y} - y)$

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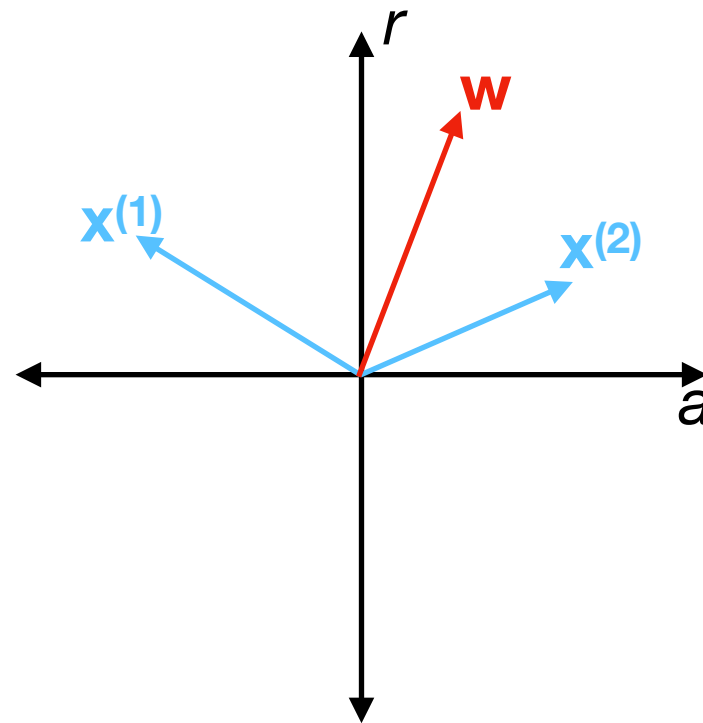
- Logistic regression is used primarily for *classification* even though it's called "regression".
- Logistic regression is an instance of a **generalized linear model** — a linear model combined with a **link function** (e.g., logistic sigmoid).
- In neural networks, link functions are typically called **activation functions**.

# Exercise

- Suppose we train a logistic regressor using  $f_{\log}$ , and our training set contains only **positive** examples.
- As before, we let  $\hat{y} = \sigma(\mathbf{x}^T \mathbf{w})$  and  $\mathbf{x} = [a, r]^T$ .
- What will/could happen during training? Explain your reasoning based on a specific dataset that you create (2 training examples should suffice).
- $f_{\log}$ :  $-y \log \hat{y} - (1 - y) \log(1 - \hat{y})$

# Solution

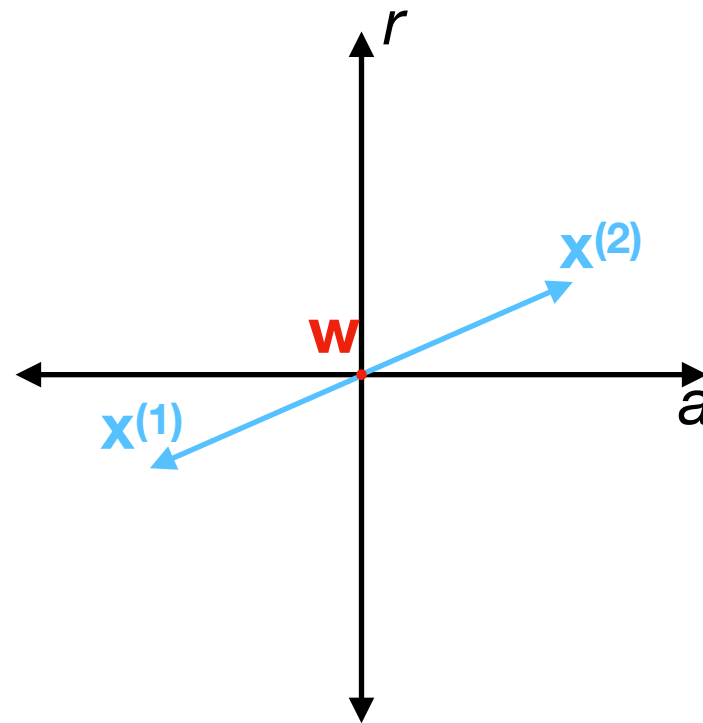
- Possibility 1: there exists a vector  $\mathbf{w}$  with positive inner-product with *every*  $\mathbf{x}^{(i)}$  in the training set, e.g.:



- In this case,  $f_{\log}$  can be made arbitrarily small by making  $\mathbf{w}$  be any vector with positive inner-product with the training examples.

# Solution

- Possibility 2: there exists *no* vector  $\mathbf{w}$  with positive inner-product with every  $\mathbf{x}^{(i)}$  in the training set, e.g.:



- In this case, a best  $\mathbf{w}$  may exist. For a dataset with 2 examples where  $\mathbf{x}^{(1)} = \mathbf{x}^{(2)}$ , then the best  $\mathbf{w}$  is  $\mathbf{0}$ .

# Exercise

- Now let's change our prediction model to be  $\hat{y} = \sigma(\mathbf{x}^T \mathbf{w} + b)$  and  $\mathbf{x} = [a, r]^T$ .
- What will/could happen now during training if all the training examples are positive?

# Solution

- We can make  $f_{\log}$  arbitrarily small by setting  $\mathbf{w}=\mathbf{0}$  and making  $b$  a large positive number.
- $f_{\log}$ :  $-y \log \hat{y} - (1 - y) \log(1 - \hat{y})$

# **Softmax regression (aka multinomial logistic regression)**



# Multi-class classification

- So far we have talked about classifying only 2 classes (e.g., smile versus non-smile).
  - This is sometimes called **binary classification**.
- But there are many settings in which multiple ( $>2$ ) classes exist, e.g., emotion recognition, hand-written digit recognition:



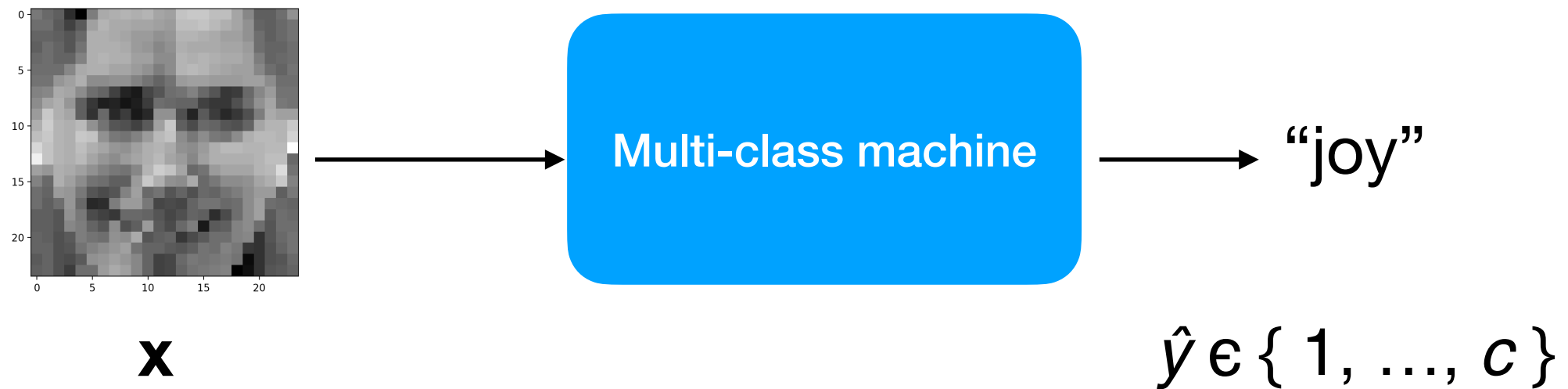
6 classes (fear, anger, sadness, happiness, disgust, surprise)



10 classes (0-9)

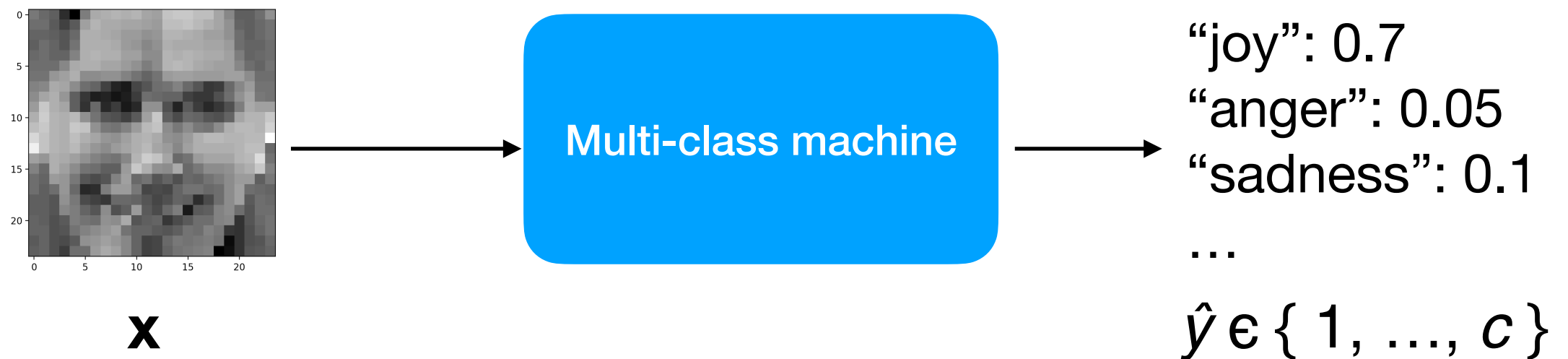
# Multi-class classification

- In one form of multi-classification (over  $c$  classes), we map every input  $\mathbf{x}$  into exactly 1 class:



# Multi-class classification

- In another, we map  $\mathbf{x}$  into a **probability distribution** over the  $c$  classes:



This is the approach we will use.

# Classification versus regression

- Note that, in contrast to regression problems (e.g., age estimation), there is no sense of “distance” between classes:
- Misclassifying a “joyful” face as “sad” is just as bad as misclassifying a “joyful” face as “angry”.

# Multi-class classification

- It turns out that logistic regression can easily be extended to support an arbitrary number ( $\geq 2$ ) of classes.
  - The multi-class case is called **softmax regression** or sometimes **multinomial logistic regression**.
- How to represent the ground-truth  $y$  and prediction  $\hat{y}$ ?
  - Instead of just a scalar  $y$ , we will use a vector  $\mathbf{y}$ .

# Example: 2 classes

- Suppose we have a dataset of 3 examples and 2 classes, where the ground-truth class labels are 0, 1, 0.
- Then we would define our ground-truth vectors as:

$$\mathbf{y}^{(1)} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\mathbf{y}^{(2)} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\mathbf{y}^{(3)} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- Exactly 1 coordinate of each  $\mathbf{y}$  is 1; the others are 0.

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$$\begin{aligned} \mathbf{y}^{(1)} &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \leftarrow \text{This "slot" is for class 0.} \\ \mathbf{y}^{(2)} &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ \mathbf{y}^{(3)} &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{aligned}$$

- This is called a **one-hot encoding** of the class label.

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- This is called a **one-hot encoding** of the class label.



# Example: 2 classes

- The machine's predictions  $\hat{\mathbf{y}}$  about each example's label are also **probabilistic**.

- They could consist of:

$$\hat{\mathbf{y}}^{(1)} = \begin{bmatrix} 0.93 \\ 0.07 \end{bmatrix}$$

$$\hat{\mathbf{y}}^{(2)} = \begin{bmatrix} 0.4 \\ 0.6 \end{bmatrix}$$

$$\hat{\mathbf{y}}^{(3)} = \begin{bmatrix} 0.99 \\ 0.01 \end{bmatrix}$$

← Machine's "belief" that the label is 0.

- Each coordinate of  $\hat{\mathbf{y}}$  is a probability.

# Example: 2 classes

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- They could consist of:

$$\hat{\mathbf{y}}^{(1)} = \begin{bmatrix} 0.93 \\ 0.07 \end{bmatrix} \leftarrow \text{Machine's "belief" that the label is 1.}$$

$$\hat{\mathbf{y}}^{(2)} = \begin{bmatrix} 0.4 \\ 0.6 \end{bmatrix}$$

$$\hat{\mathbf{y}}^{(3)} = \begin{bmatrix} 0.99 \\ 0.01 \end{bmatrix}$$

- The sum of the coordinates in each  $\hat{\mathbf{y}}$  is 1.

# Cross-entropy loss

- We need a loss function that can support  $c \geq 2$  classes.
- We will use the **cross-entropy** loss (aka **negative log-likelihood**):

$$f_{\text{CE}} = - \sum_{i=1}^n \sum_{k=1}^c y_k^{(i)} \log \hat{y}_k^{(i)}$$

# Cross-entropy loss

- Note that the  $f_{\log}$  (for logistic regression) is a special case of  $f_{\text{CE}}$  (for softmax regression) for  $c=2$ .
- To see how, consider just a simple example:

$$f_{\text{CE}} = - \sum_{k=0}^1 y_k \log \hat{y}_k$$

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$$f_{\text{CE}} = - \sum_{k=0}^1 y_k \log \hat{y}_k$$

Note: the sum from  $k=1$  to  $c$  is  
renumbered from 0 to  $c-1$ .

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$$\begin{aligned} f_{\text{CE}} &= - \sum_{k=0}^1 y_k \log \hat{y}_k \\ &= -y_1 \log \hat{y}_1 - y_0 \log \hat{y}_0 \end{aligned}$$

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$$\hat{\mathbf{y}}^{(1)} = \begin{bmatrix} 0.93 \\ 0.07 \end{bmatrix}$$

Recall that the sum over all coordinates of each  $\hat{\mathbf{y}}$  (and each  $\mathbf{y}$ ) must equal 1. Since there are only 2 classes, then  $\hat{y}_0 = 1 - \hat{y}_1$  (and  $y_0 = 1 - y_1$ ).

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For  $c=2$  classes, we can define  $\hat{\mathbf{y}}$  (and  $\mathbf{y}$ ) simply as probability that the example is class 1.



# Cross-entropy loss

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- To see how, consider just a simple example:

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# Softmax activation function

- Softmax regression outputs a *vector* of probabilistic class labels  $\hat{\mathbf{y}}$  containing  $c$  components.
  - We need  $c$  different vectors of weights  $\mathbf{w}^{(1)}, \dots, \mathbf{w}^{(c)}$ .
  - Each weight vector  $\mathbf{w}^{(i)}$  measures how “compatible”  $\mathbf{x}$  is with class  $i$ .

# Softmax activation function

- With softmax regression, we first compute:

$$\mathbf{z}_1 = \mathbf{x}^\top \mathbf{w}^{(1)}$$

$$\mathbf{z}_2 = \mathbf{x}^\top \mathbf{w}^{(2)}$$

...

$$\mathbf{z}_c = \mathbf{x}^\top \mathbf{w}^{(c)}$$

I will refer to the  $\mathbf{z}$ 's as “pre-activation scores”.

# Softmax activation function

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...

$$\mathbf{z}_c = \mathbf{x}^\top \mathbf{w}^{(c)}$$

- Since we want to output probabilities, we then **normalize** across all  $c$  classes so that:
  1. Each output  $\hat{\mathbf{y}}_k$  is non-negative.
  2. The sum of  $\hat{\mathbf{y}}_k$  over all  $c$  classes is 1.

# Normalization of the $\hat{y}_k$

1. To enforce non-negativity, we can exponentiate each  $\mathbf{z}_k$ :

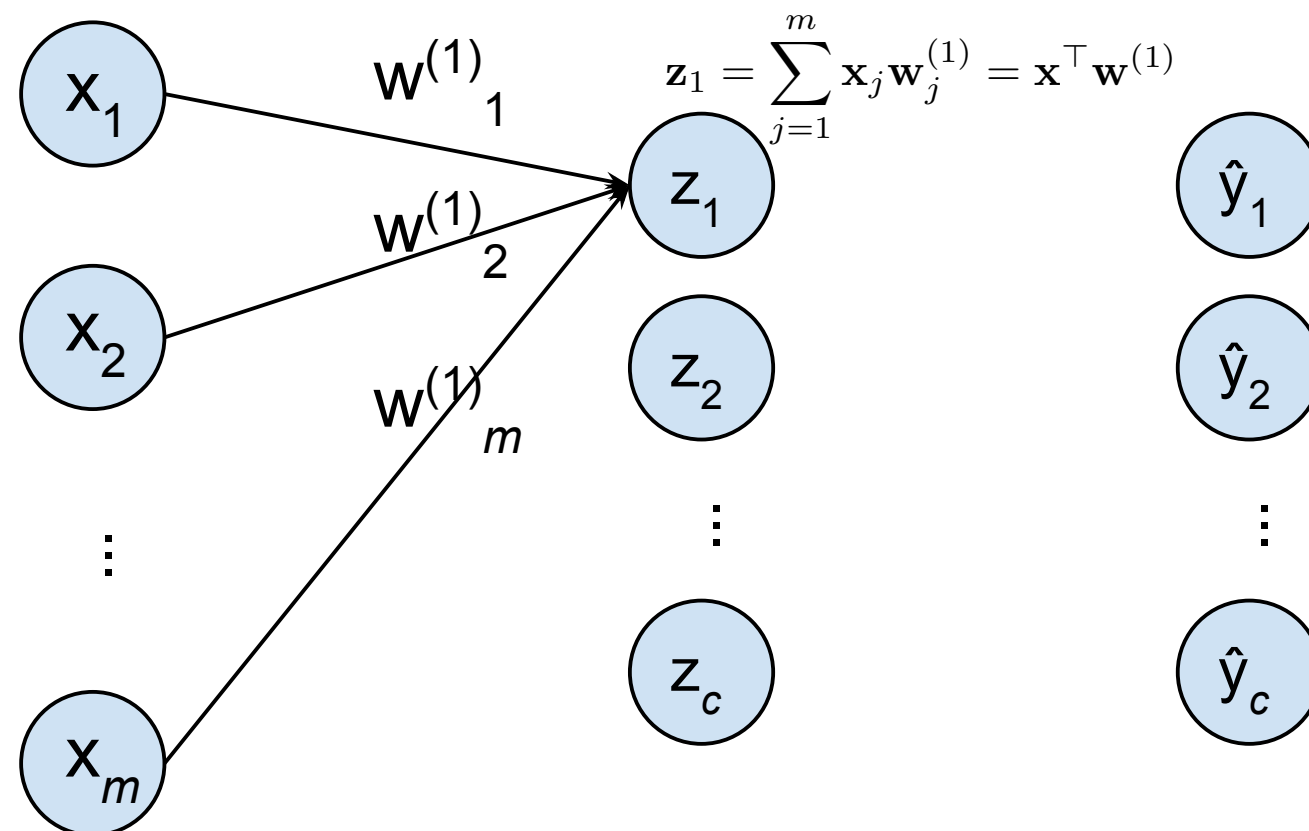
$$\hat{y}_k = \exp(\mathbf{z}_k)$$

# Normalization of the $\hat{y}_k$

2. To enforce that the  $\hat{y}_k$  sum to 1, we can divide each entry by the sum:

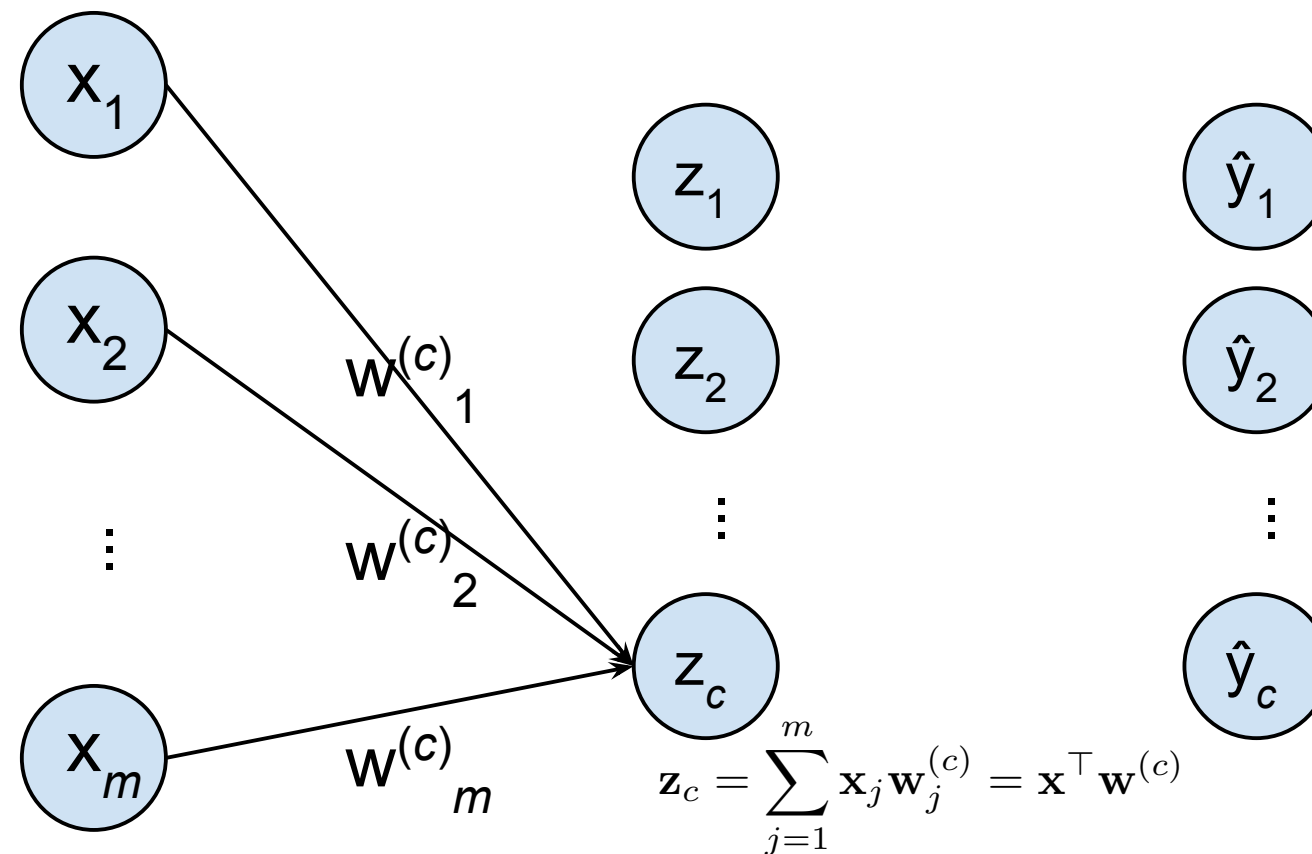
$$\hat{y}_k = \frac{\exp(\mathbf{z}_k)}{\sum_{k'=1}^c \exp(\mathbf{z}_{k'})}$$

# Softmax regression diagram



- With softmax regression, we first compute:  
$$\mathbf{z}_1 = \mathbf{x}^\top \mathbf{w}^{(1)}$$

# Softmax regression diagram



- With softmax regression, we first compute:

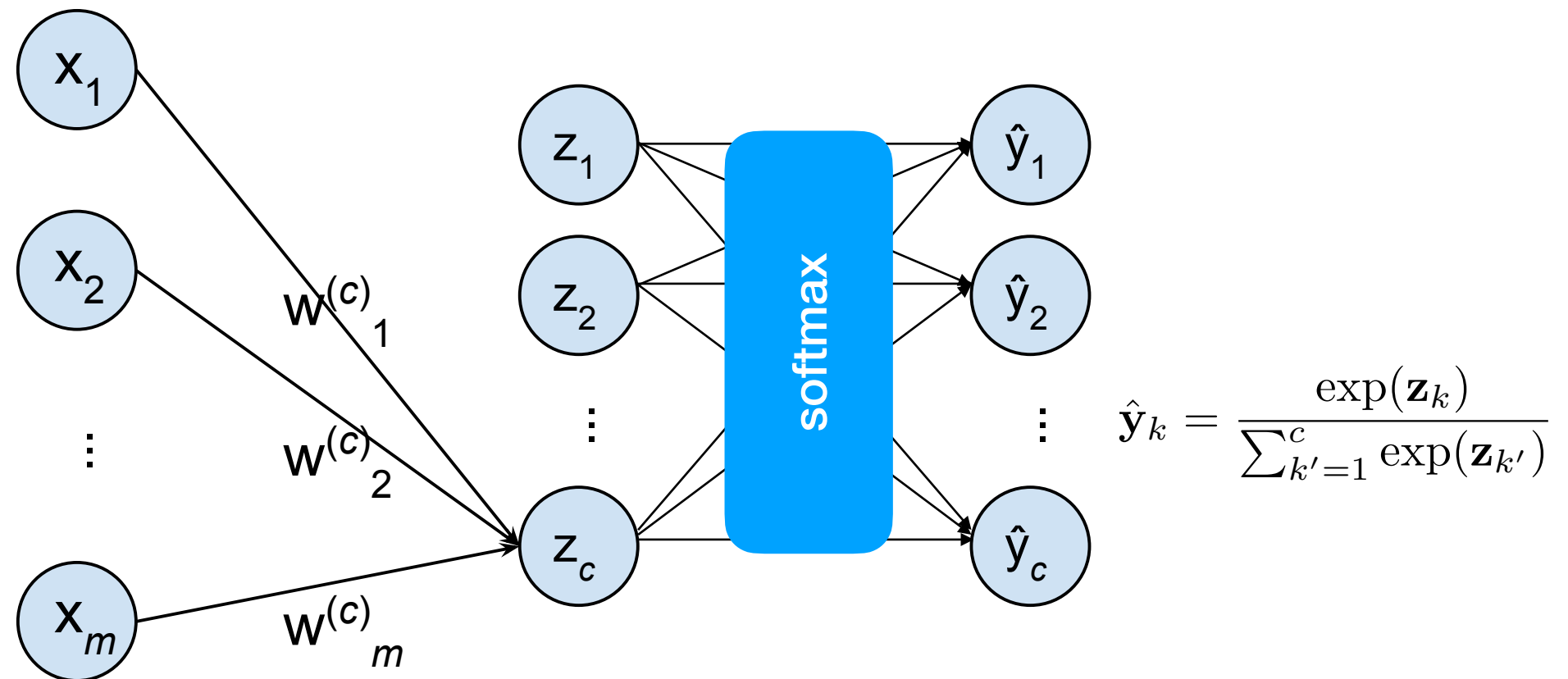
$$\mathbf{z}_1 = \mathbf{x}^\top \mathbf{w}^{(1)}$$

...

$$\mathbf{z}_c = \mathbf{x}^\top \mathbf{w}^{(c)}$$



# Softmax regression diagram



- We then **normalize** across all  $c$  classes.

# Illustration

- Let  $m=2, c=3$ .

- Let:  $\mathbf{x} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$

$$\mathbf{w}^{(1)} = \begin{bmatrix} -2.5 \\ -1 \end{bmatrix} \quad \mathbf{w}^{(2)} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \quad \mathbf{w}^{(3)} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- Which class will have highest estimated probability?

$$\mathbf{z} = \begin{bmatrix} \phantom{0} \\ \phantom{0} \end{bmatrix}$$

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- Which class will have highest estimated probability?

$$\mathbf{z} = \begin{bmatrix} 1.5 \\ 1 \\ -1 \end{bmatrix}$$

# Illustration

- Let  $m=2$ ,  $c=3$ .

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- Which class will have highest estimated probability?

$$\mathbf{z} = \begin{bmatrix} 1.5 \\ 1 \\ -1 \end{bmatrix} \quad \hat{\mathbf{y}} = \begin{bmatrix} .592 \\ .359 \\ .049 \end{bmatrix}$$