

# Binary classification problems

Logistic regression from a neural  
networks perspective

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# Binary classification problems

- the response variable  $y$  is **qualitative** and takes up one of two values
- binary traits (e.g. cases/controls, resistant/susceptible, true/false, etc.)
- $y = \text{label}$  (a.k.a. target/dependent variable)
- $X = \text{matrix of features}$  (continuous, categorical)

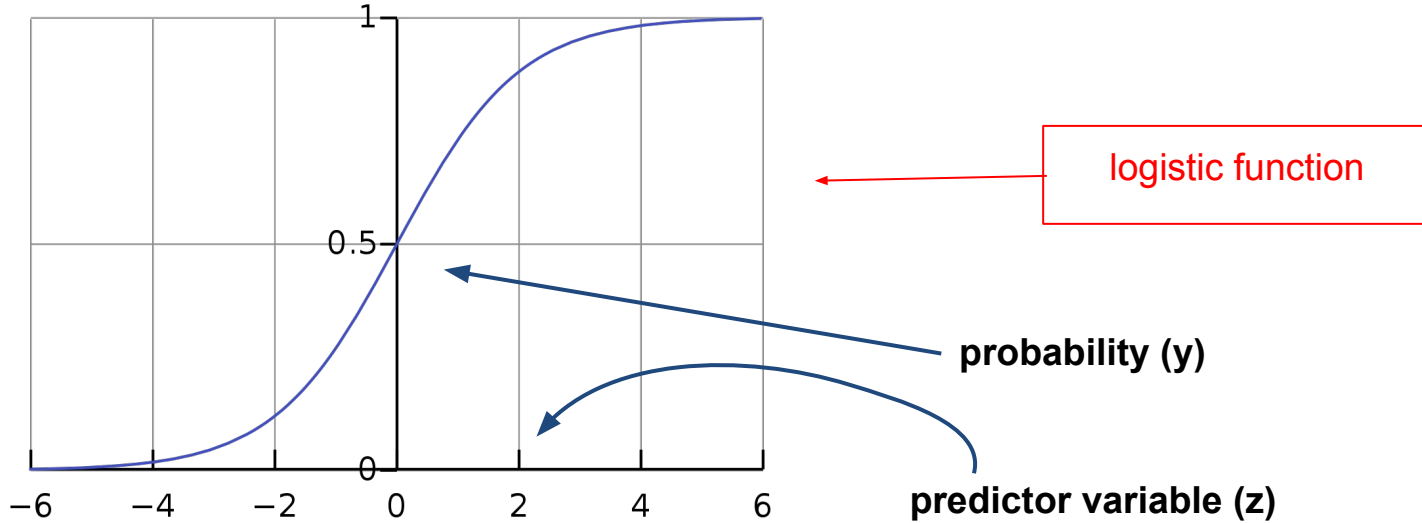


# Binary classification problems

- the response variable **y** is **qualitative** and takes up one of two values
- binary traits (e.g. cases/controls, resistant/susceptible, true/false, etc.)
- **y = label** (a.k.a. dependent variable)
- **X** = matrix of **features** (continuous, categorical)
- we don't model the response directly, rather its **probability**:  **$P(y=1|x)$**
- probabilities lie in  $[0,1]$  (not +/- infinity)



# Binary classification problems



$$\frac{1}{1+e^{-z}} = \frac{1}{1+\frac{1}{e^z}} = \frac{e^z}{1+e^z}$$



# Logistic regression

- the logistic function is the basis for **logistic regression**
- $P(y=1|x)$
- $Z = \beta_0 + \beta_1 x$

$$P(y = 1|x) = \sigma(z) = \frac{e^{\beta_0 + \beta_1 x}}{1 + e^{\beta_0 + \beta_1 x}}$$

we see here the familiar **model coefficients** (from linear regression) to be estimated and then used for predictions



# Logistic regression

- a little bit of algebra:

$$\sigma(z) = \frac{e^{\beta_0 + \beta_1 x}}{1 + e^{\beta_0 + \beta_1 x}} \longrightarrow \frac{\sigma(z)}{1 - \sigma(z)} = e^{\beta_0 + \beta_1 x}$$

odds



# Logistic regression

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$$\sigma(z) = \frac{e^{\beta_0 + \beta_1 x}}{1 + e^{\beta_0 + \beta_1 x}} \longrightarrow \frac{\sigma(z)}{1 - \sigma(z)} = e^{\beta_0 + \beta_1 x}$$

odds

log(odds): logit

$$\log \left( \frac{\sigma(z)}{1 - \sigma(z)} \right) = \text{logit}(\sigma(z)) = \beta_0 + \beta_1 x$$



# Logistic regression

- the **logit function** ( $\log(\text{odds})$ ) is the **link function** between a linear expression of  $X$  and the probabilities of  $Y$
- linear  $X$  expression ( $\beta_0 + \beta_1 x$ )  $\rightarrow$  logit scale (continuous)
- logistic function: converts values on the logit scale back to probabilities

$$\begin{cases} \text{logit}(\sigma(z)) = \beta_0 + \beta_1 x \\ \sigma(\beta_0 + \beta_1 x) = P(y = 1|x) \end{cases}$$

our objective!



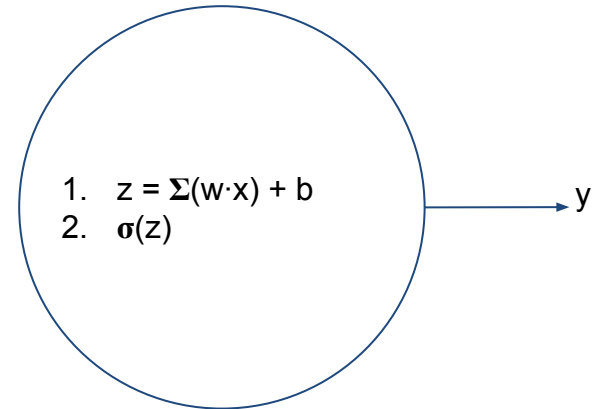


# Logistic regression

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$$\begin{cases} \text{logit}(\sigma(z)) = \beta_0 + \beta_1 x \\ \sigma(\beta_0 + \beta_1 x) = P(y = 1|x) \end{cases}$$

Looks familiar!



# Estimating the coefficients

## how do we obtain the model coefficients $\beta$ ?

- We introduced this question yesterday, when talking of **supervised** learning
- Did you think of possible answers?



# Estimating the coefficients

## how do we obtain the model coefficients $\beta$ ?

- we need to define a **loss function** and then minimise it

observations	predictions
$\mathbf{y}$	$\hat{y} = \sigma(\beta_0 + \beta_1 x)$

difference between observed and  
predicted values



# Estimating the coefficients

## how do we obtain the model coefficients $\beta$ ?

- we need to define a **loss function** and then minimise it
- $\hat{y} = \sigma(z)$

$$J(\beta) = \text{loss}(\hat{y}, y) = \\ - (y \cdot \log(\hat{y}) + (1 - y) \cdot \log(1 - \hat{y}))$$



# Loss function for logistic regression

$$J(\beta) = \text{loss}(\hat{y}, y) =$$

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

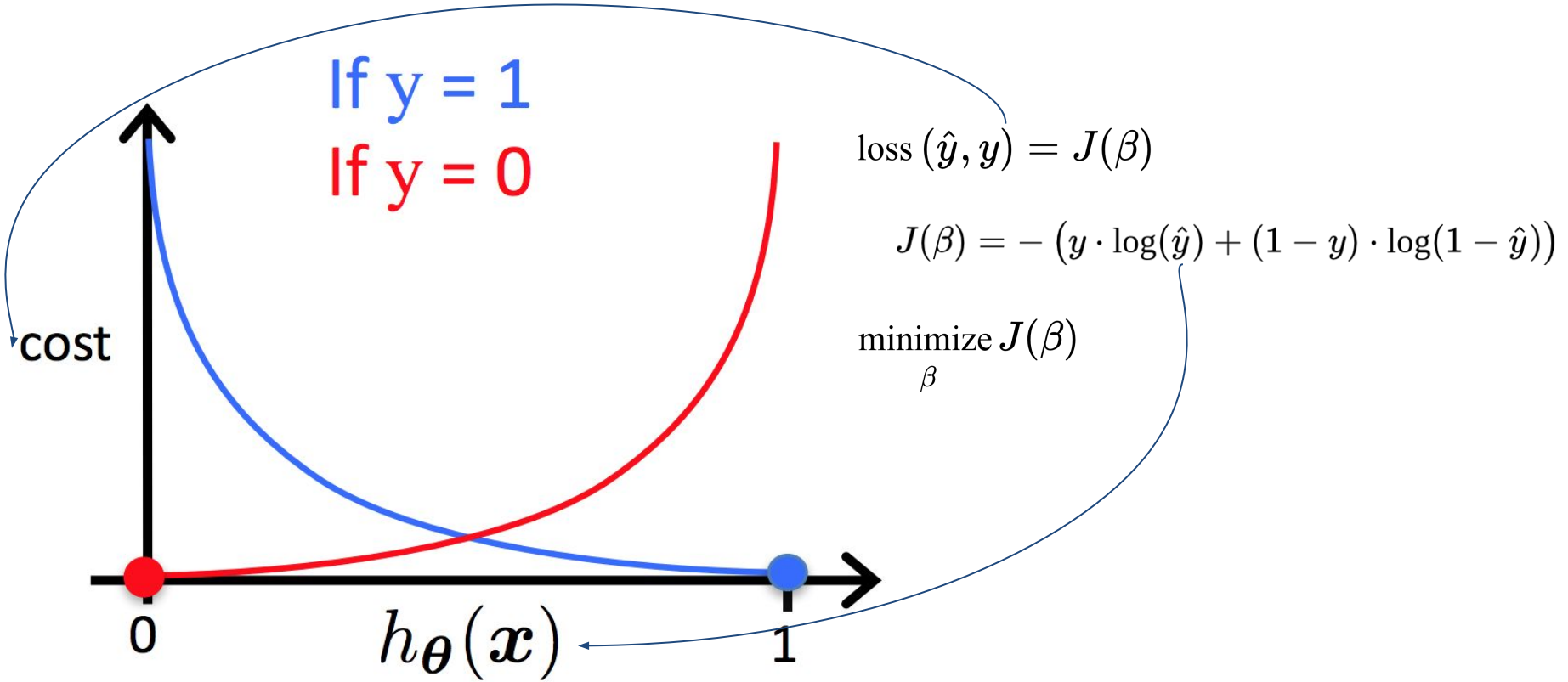
if  $y = 1$

- $y_{\text{hat}} \rightarrow 1$ , loss  $\rightarrow 0$
- $y_{\text{hat}} \rightarrow 0$  (but  $y = 1$ !), loss  $\rightarrow \text{infinity}$

the opposite holds if  $y = 0$



# Cost/loss function for logistic regression



From: <https://datascience.stackexchange.com/questions/40982/logistic-regression-cost-function>



# Minimising the cost function

$$J(\beta) = - (y \cdot \log(\hat{y}) + (1 - y) \cdot \log(1 - \hat{y}))$$

minimize  $J(\beta)$   
 $\beta$

How do we minimise the cost function?  
Any ideas?



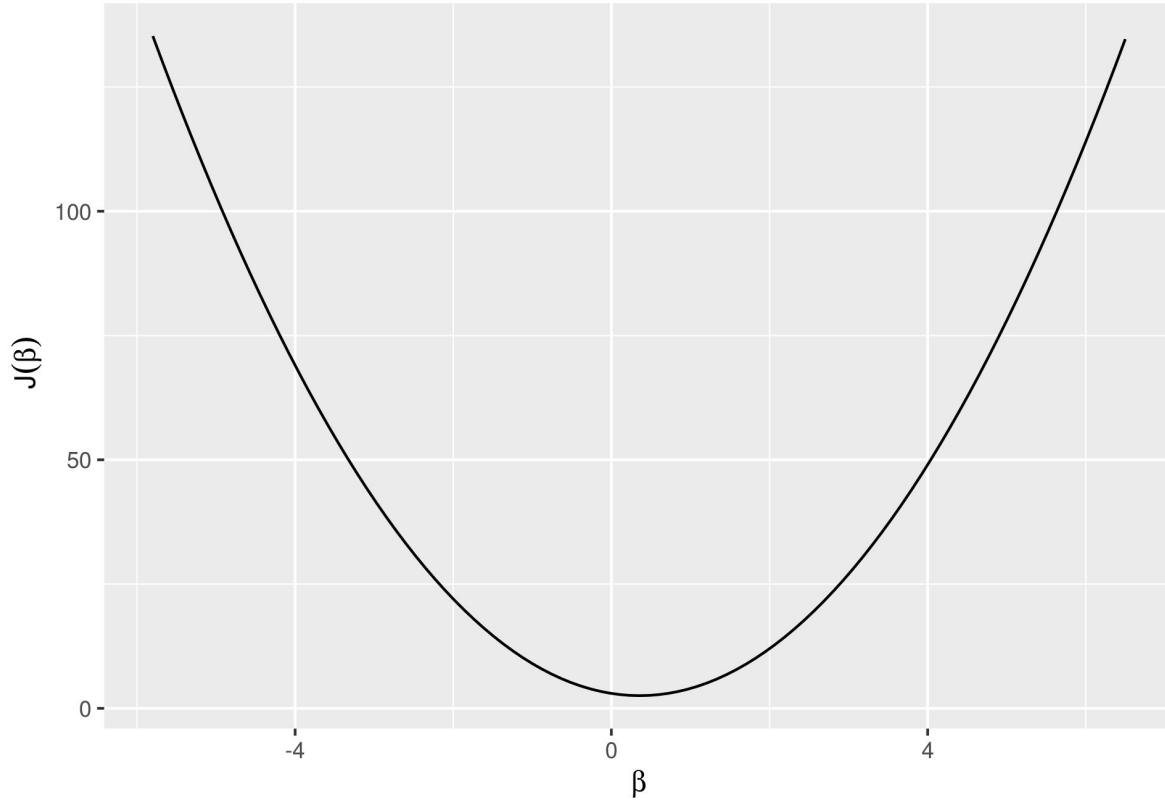
# Minimising the cost function

- the defined cost function is convex
- can be minimised by **gradient descent**
- machine learning perspective: gradient descent is a general algorithm to solve models
- alternatively:
  - maximum likelihood
  - non-linear least squares





# Minimise the cost function

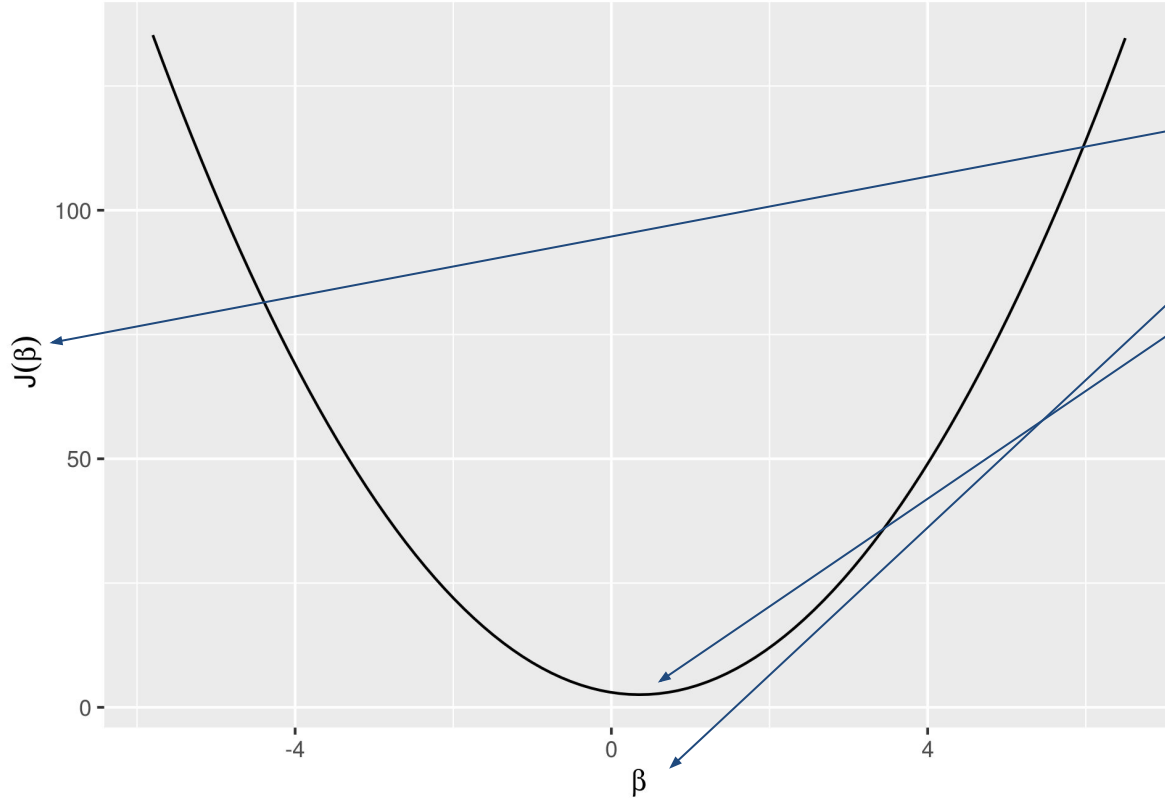


Simple logistic regression (1 parameter):

$$z = \beta \cdot x$$



# Minimise the cost function



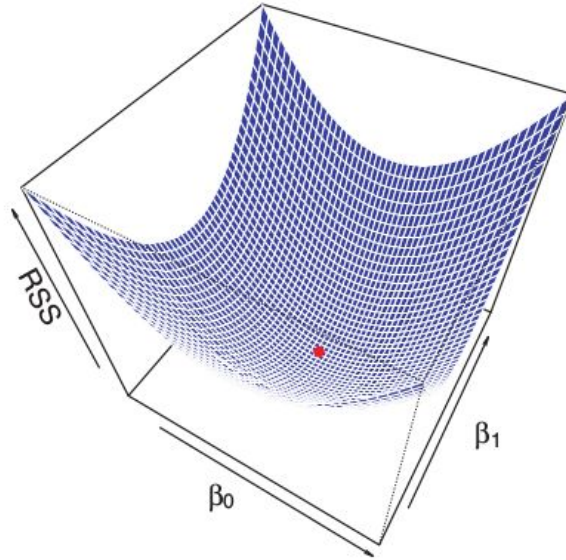
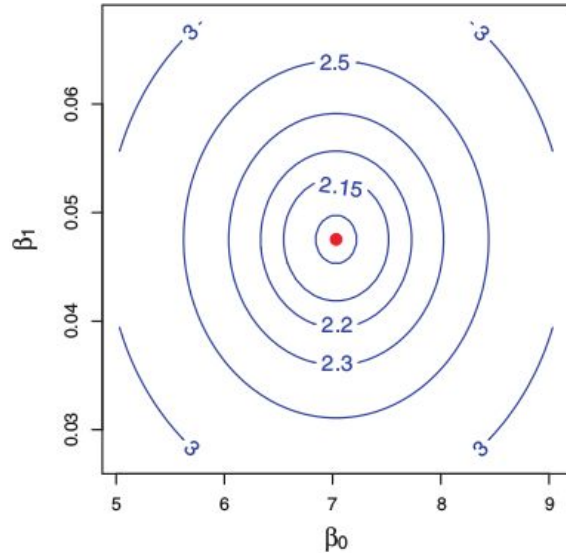
1. loss function
2. model parameters
3. minimum

Simple logistic regression (1 parameter):

$$z = \beta \cdot x$$



# Minimise the cost function



Multiple logistic regression

(e.g. 2 parameters):

$$y = \beta_0 + \beta_1 \cdot x$$

Multiple logistic regression (> 2 parameters):

→ m-dimensional hyperspace



# Cost function: finding the minimum?

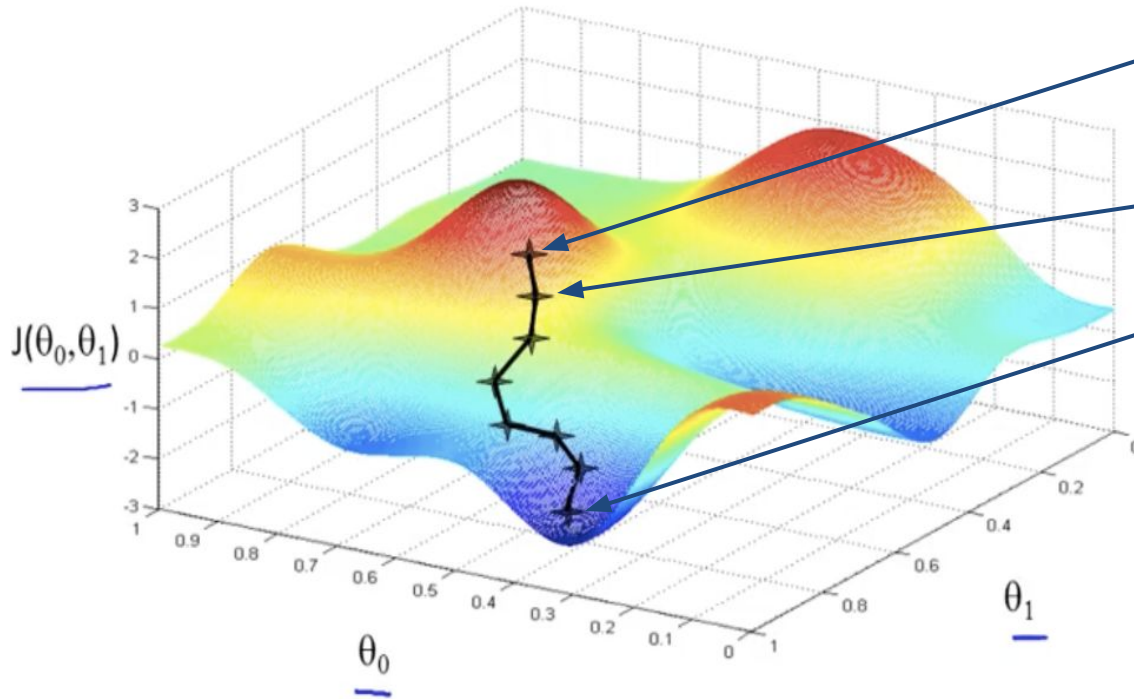
Gradient Descent:

minimize  $J(\beta)$   
 $\beta$

1. Start with initial values for  $\beta$  : (initialisation)
2. Change  $\beta$  in the direction of reducing  $J(\beta)$  : (descent)
3. Stop when the minimum is reached : (minimisation)



# Gradient descent



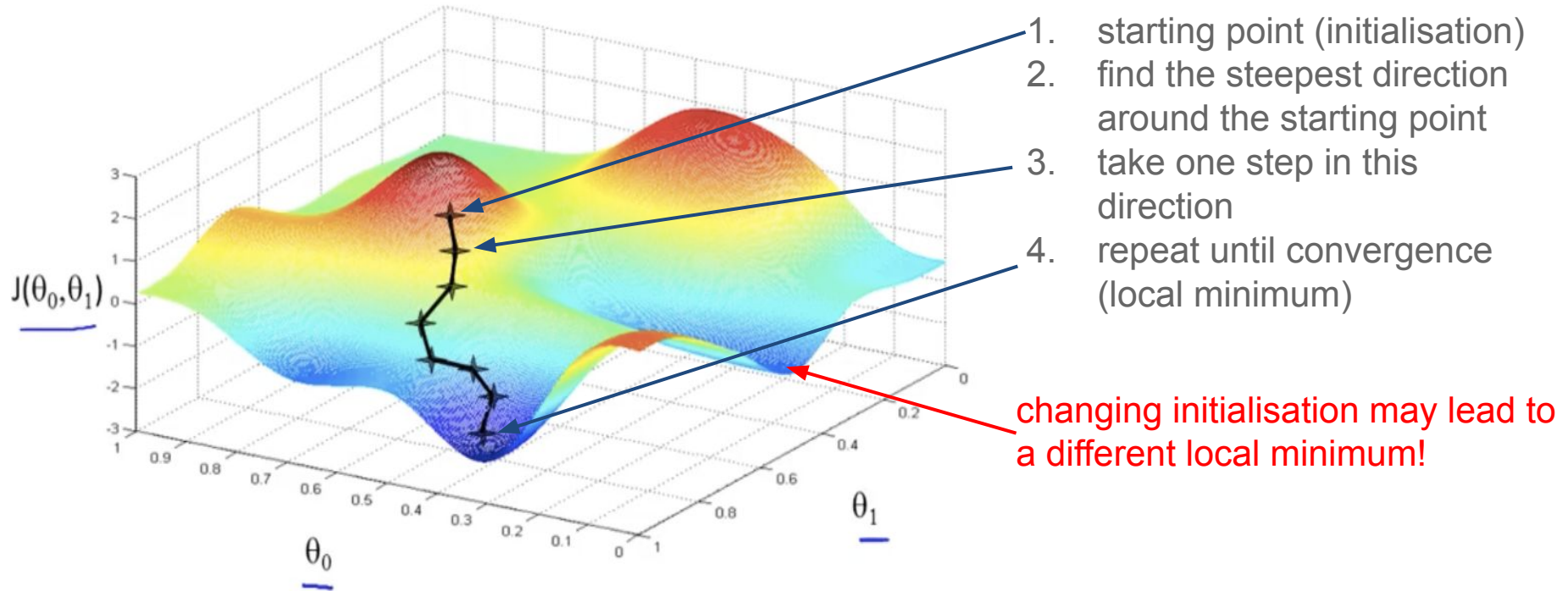
1. starting point (initialisation)
2. find the steepest direction around the starting point
3. take one step in this direction
4. repeat until convergence (local minimum)

Source: Andrew Ng

<https://medium.com/@DBCerigo/on-why-gradient-descent-is-even-needed-25160197a635>



# Gradient descent



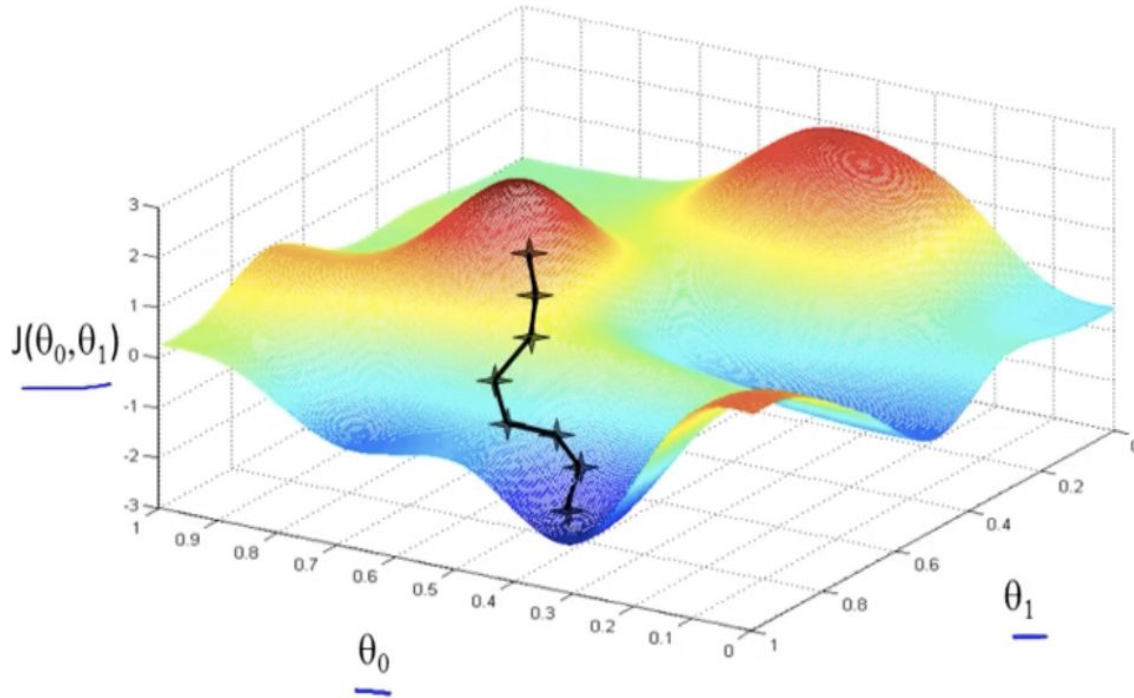
Source: Andrew Ng

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# Gradient descent

How do we find the steepest direction?

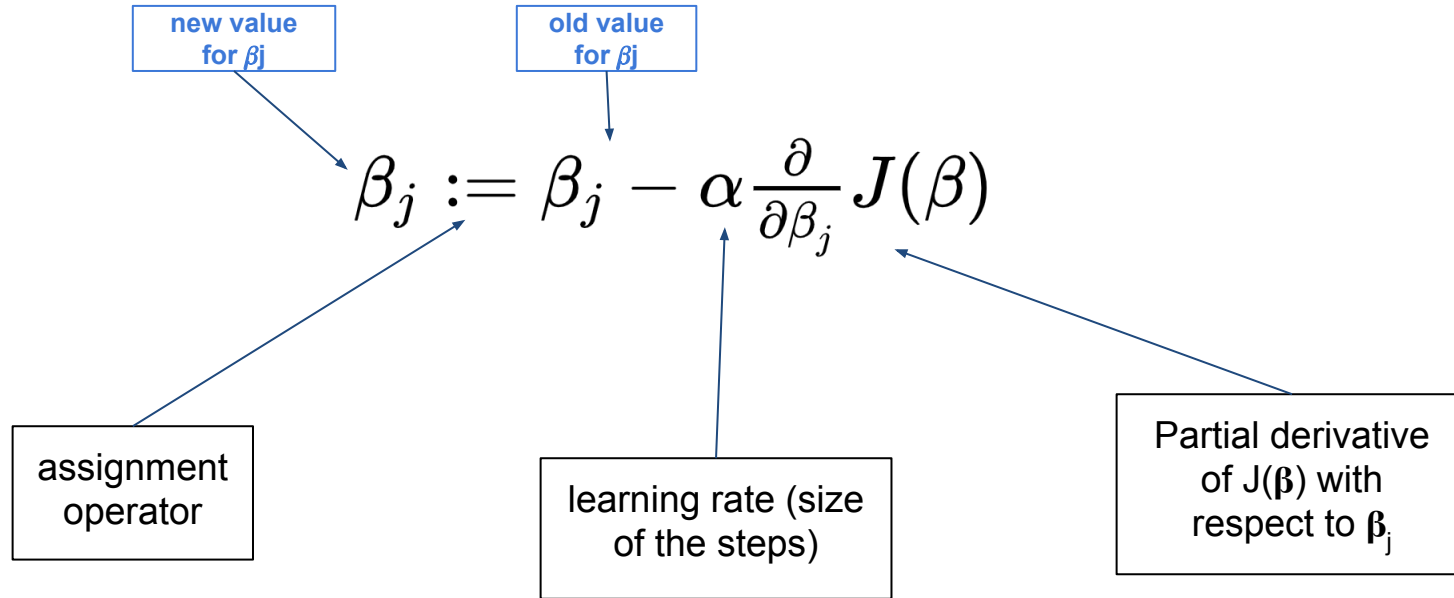


Source: Andrew Ng

<https://medium.com/@DBCerigo/on-why-gradient-descent-is-even-needed-25160197a635>

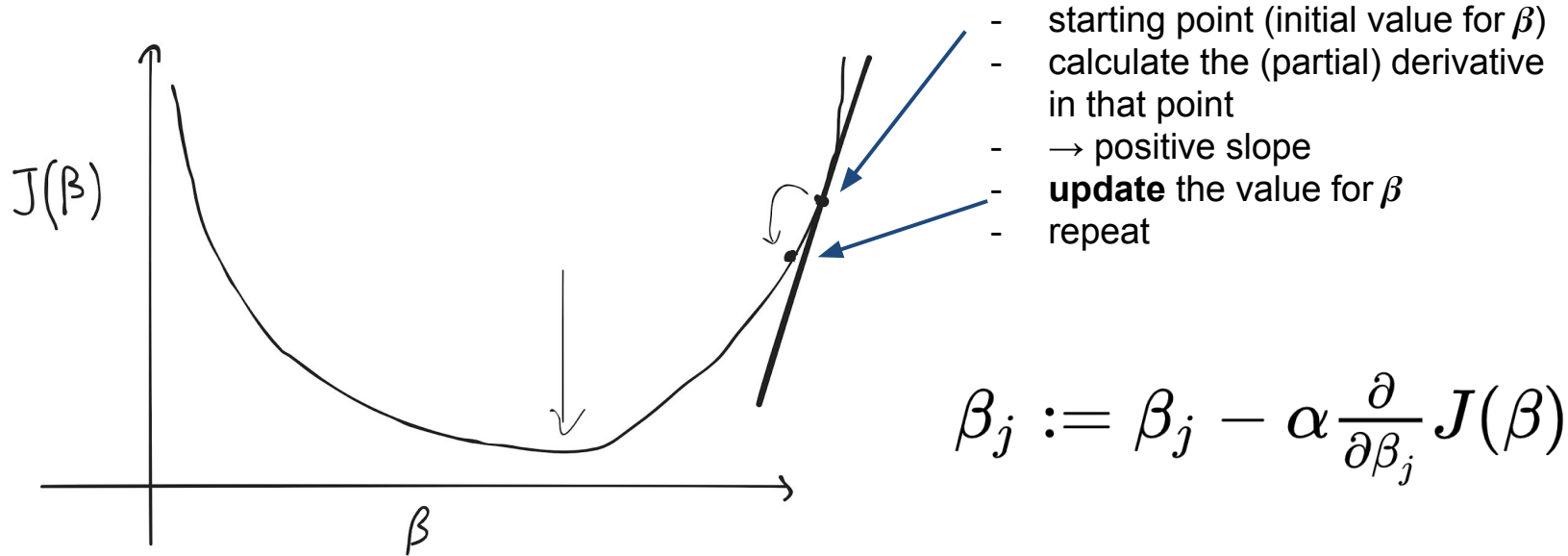


# Gradient descent





# Gradient descent

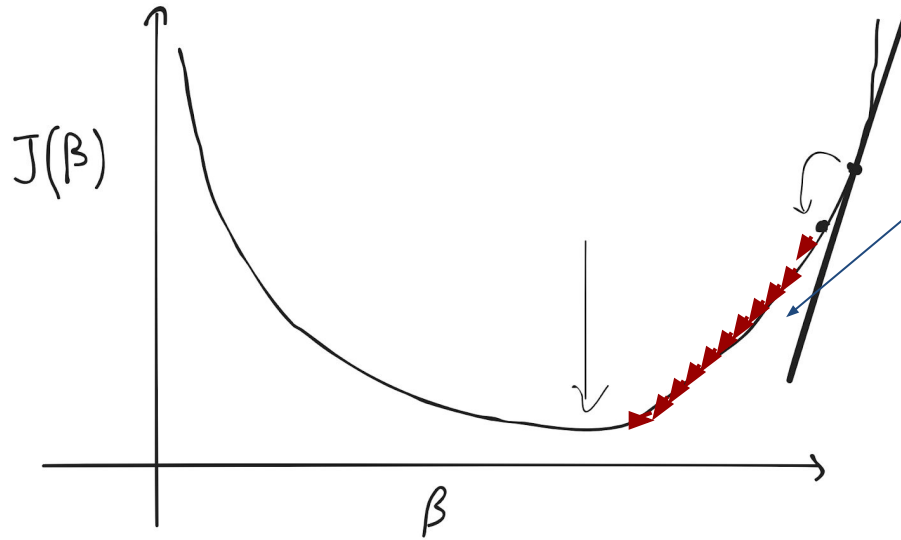


$$\beta_j := \beta_j - \alpha \frac{\partial}{\partial \beta_j} J(\beta)$$

- positive slope  $\rightarrow$  reducing the value of  $\beta$  (and the other way around)



# Gradient descent

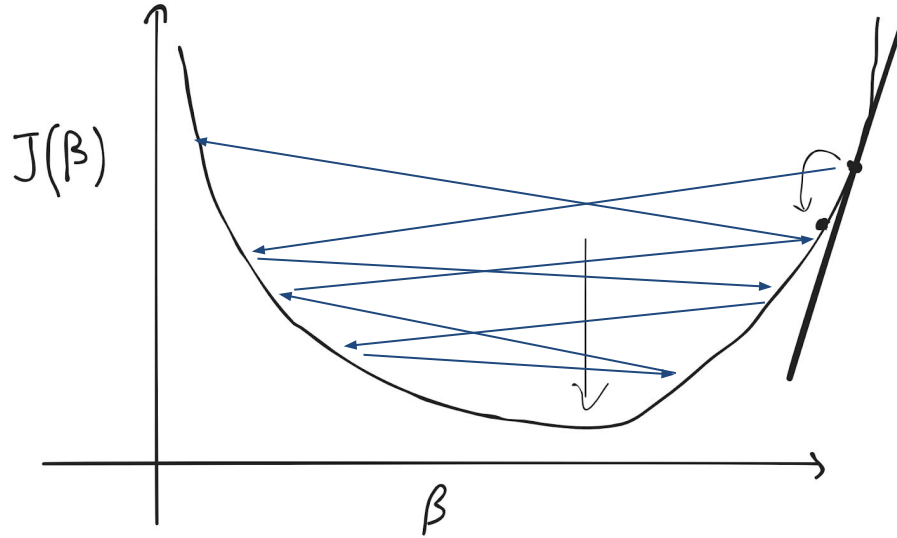


- $\alpha$  controls the size of the updating step
- small  $\alpha \rightarrow$  slow descent

$$\beta_j := \beta_j - \alpha \frac{\partial}{\partial \beta_j} J(\beta)$$



# Gradient descent



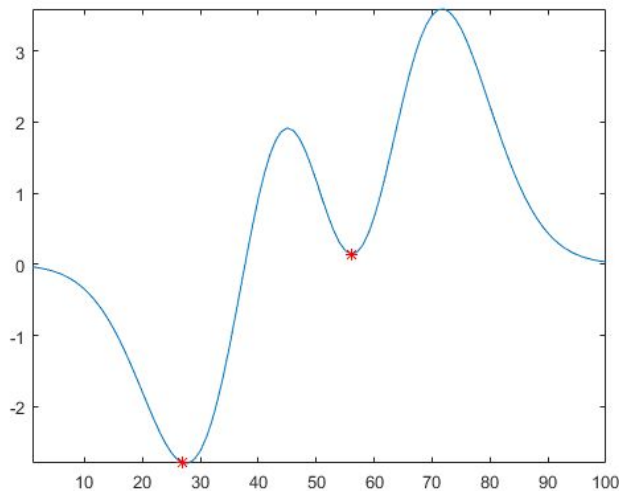
- $\alpha$  controls the size of the updating step
- large  $\alpha \rightarrow$  overshooting: failure to converge

$$\beta_j := \beta_j - \alpha \frac{\partial}{\partial \beta_j} J(\beta)$$



# Gradient descent - recap

- general method to **solve machine learning models** (e.g. multiple linear regression)
- optimise (minimise) the cost function → **optimiser**
- importance of the **learning rate**
- local minimum → **momentum**
- **initialization** values



# Logistic regression - recap

$$1) \quad z = w \cdot x + b$$

introduce **w** (weight) as  
parameter (+ b): NN notation

$$2) \quad \hat{y} = \sigma(z)$$

$$3) \quad J(w) = - (y \cdot \log(\hat{y}) + (1 - y) \cdot \log(1 - \hat{y}))$$

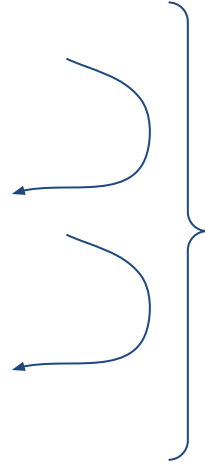


# Logistic regression - recap

1)  $z = w \cdot x + b$

2)  $\hat{y} = \sigma(z)$

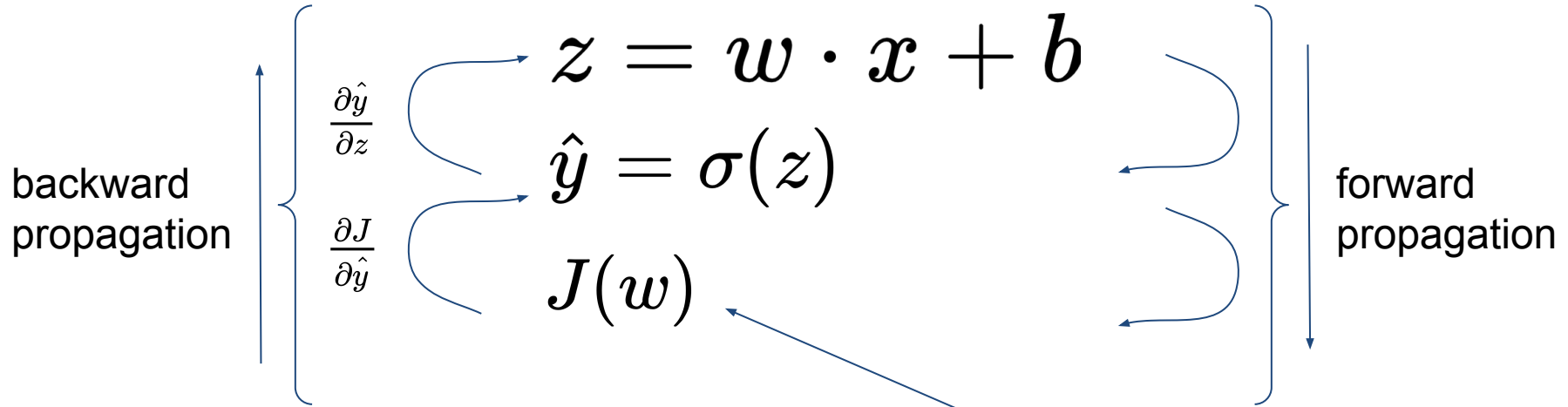
3)  $J(w)$



forward propagation



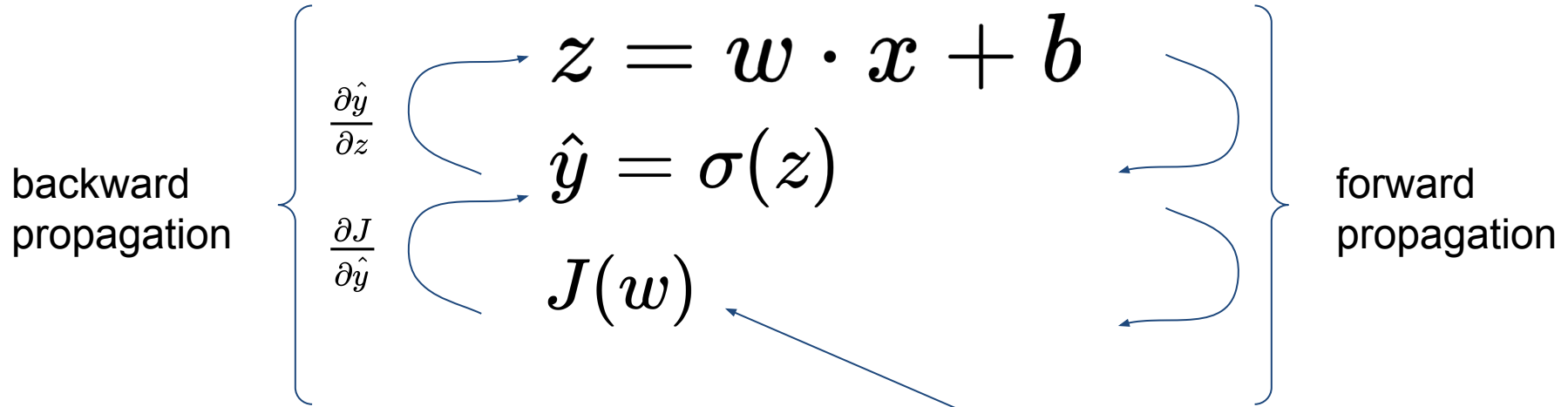
# Logistic regression - recap



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



# Logistic regression - recap



$$\frac{\partial J}{\partial z} = \frac{\partial J}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z} \quad \leftarrow \text{chain rule} \quad - (y \cdot \log(\hat{y}) + (1 - y) \cdot \log(1 - \hat{y}))$$





# Logistic regression - recap

$$\frac{\partial J}{\partial z} = \frac{\partial J}{\partial \hat{y}} \cdot \frac{\partial \hat{y}}{\partial z}$$

our objective!

$$\frac{\partial J}{\partial w_1} = \frac{\partial J}{\partial z} \cdot x_1$$

$$\frac{\partial J}{\partial w_2} = \frac{\partial J}{\partial z} \cdot x_2$$

$$\frac{\partial J}{\partial b} = \frac{\partial J}{\partial z}$$

$$w_1 := w_1 - \alpha \frac{\partial J}{\partial w_1}$$

$$w_2 := w_2 - \alpha \frac{\partial J}{\partial w_2}$$

$$b := b - \alpha \frac{\partial J}{\partial b}$$

updating step



# Take away message

- **back propagation** is a way (algorithm) to calculate partial derivatives (of the cost function with respect to the parameters) easily and efficiently
- partial derivatives are then used to **update** the values of the **parameters**
- in this way **gradient descent** can work to **minimise** the **cost function** and **estimate** the best values for the **parameters**
- this is very important to efficiently learn the weights (parameters) of deep neural networks



# Binary classification metrics



# Binary classification: measuring performance



- the most common metric to measure the performance of a binary classifier is the **error rate**:

$$\frac{1}{n} \sum_{i=1}^n I(y \neq \hat{y})$$



# Confusion matrix

		True observation	
		1	0
Prediction	1	TP	FP
	0	FN	TN

- **FPR** =  $FP / (FP + TN)$
- **FNR** =  $FN / (FN + TP)$
- **TER** =  $(FN + FP) / (FN + FP + TN + TP)$



# Confusion matrix

		True observation	
		1	0
Prediction	1	TP	FP
	0	FN	TN

Not only total error rate!

- $\text{FPR} = \text{FP}/(\text{FP}+\text{TN})$
- $\text{FNR} = \text{FN}/(\text{FN}+\text{TP})$
- $\text{TER} = (\text{FN}+\text{FP})/(\text{FN}+\text{FP}+\text{TN}+\text{TP})$



# Logistic regression

- lab 4

→ day2\_code01 logistic regression iris.ipynb

