

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)



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- probabilities lie in $[0,1]$ (not +/- infinity)

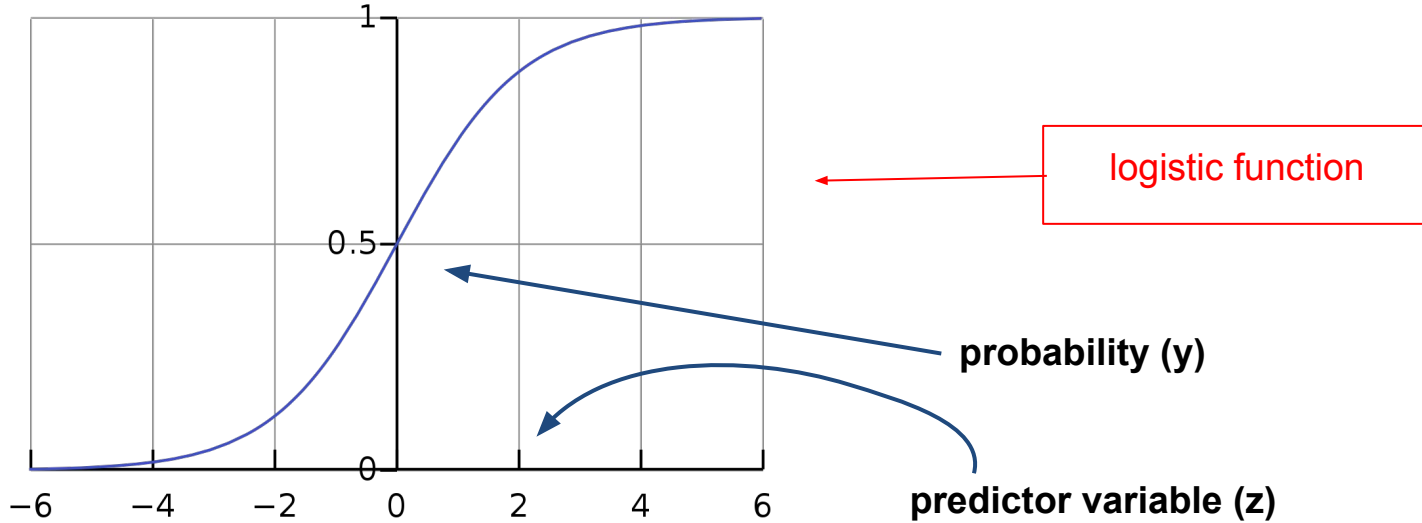


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- we don't model the response directly, rather its **probability**: $P(y=1|x)$
- probabilities lie in $[0,1]$ (not +/- infinity)
- **Q1: if you have n examples with m features X_{nm} , what would $f(X_{nm})$ look like? (shape of \hat{y})**



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 (but now they're exponents!)



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!

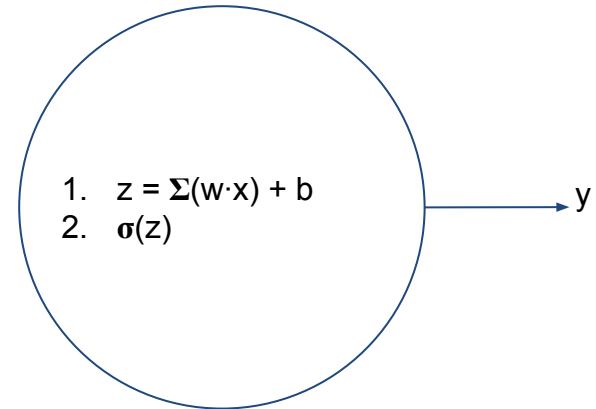


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Looks familiar!



Estimating the coefficients

how do we obtain the model coefficients β ?

- 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 β ?

- 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 β ?

- 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

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

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

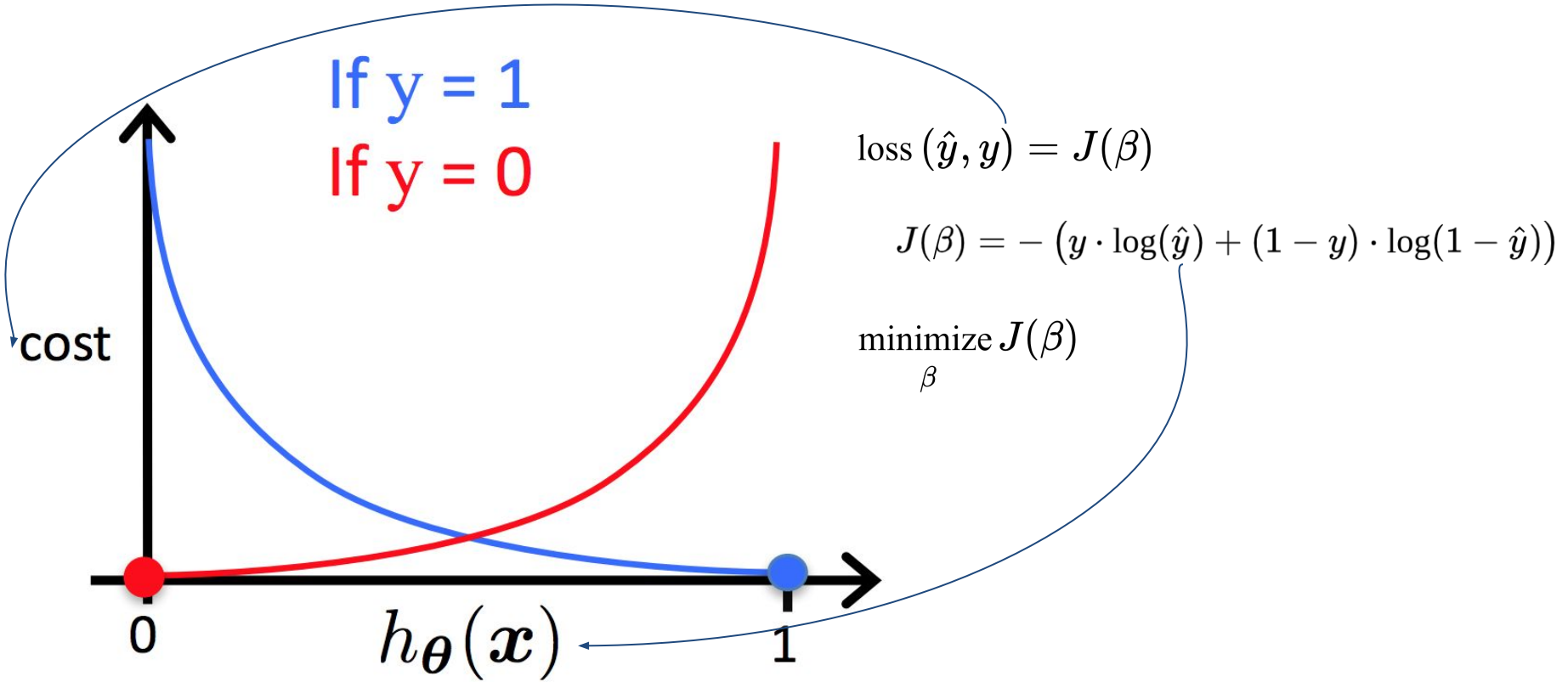
if $y = 1$

- $y_{\text{hat}} \rightarrow 1$, 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 $J(\beta)$
 β

OK: to obtain model coefficients we need to define and then minimise the cost function

How do we minimise the cost function?
Any ideas?

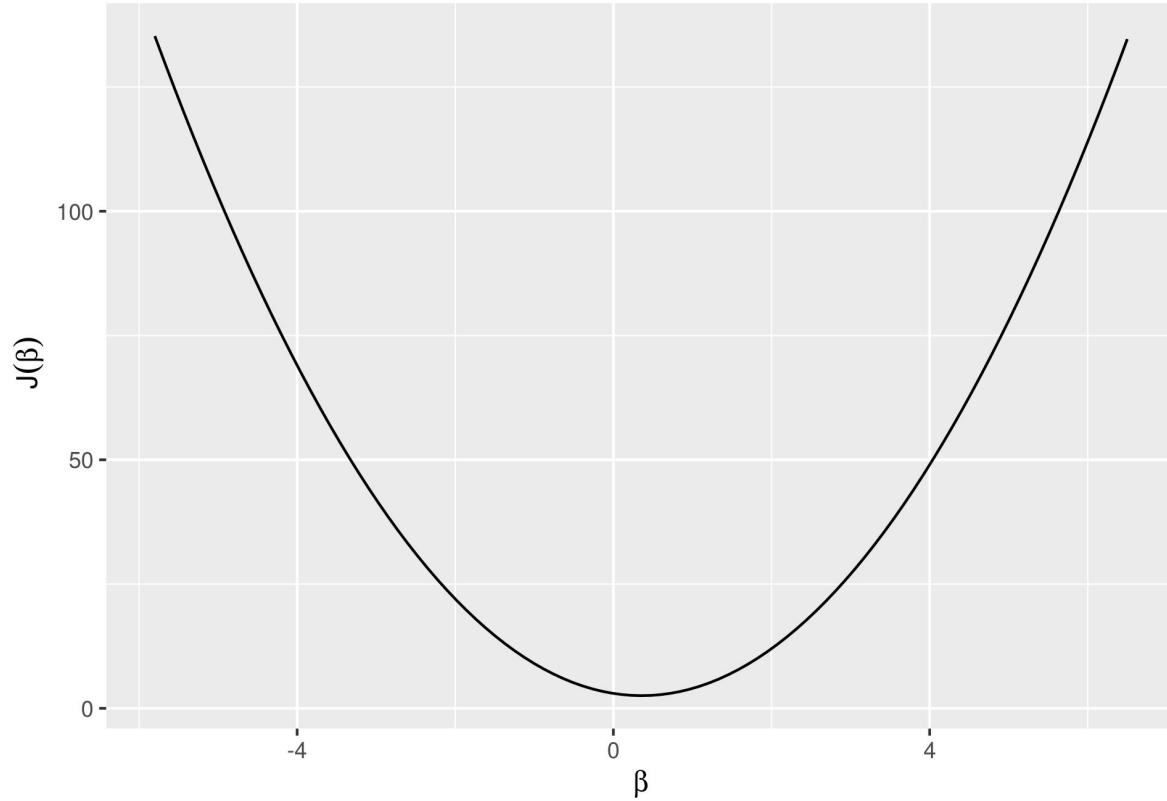


Minimising the cost function

- 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

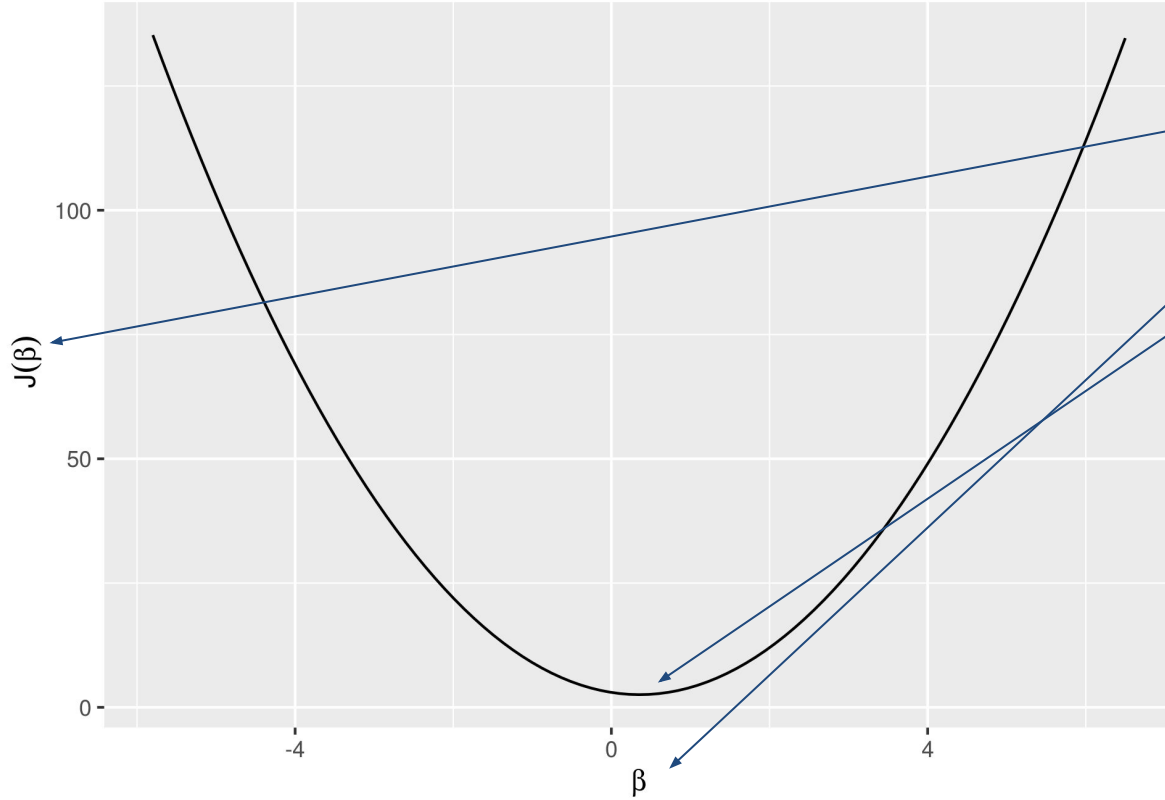


Simple logistic regression (1 parameter):

$$z = \beta \cdot x$$



Minimise the cost function



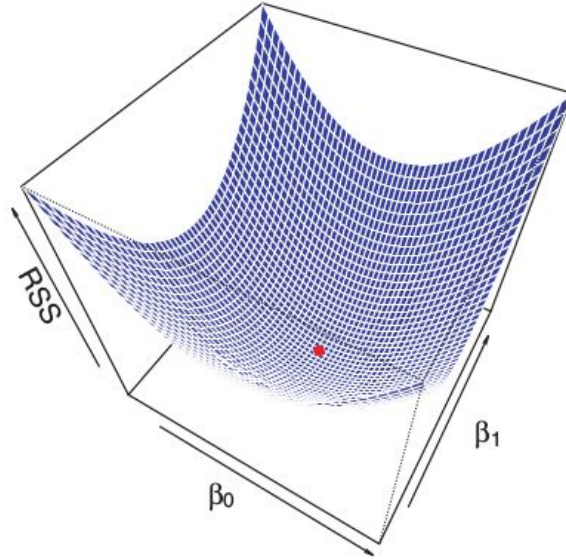
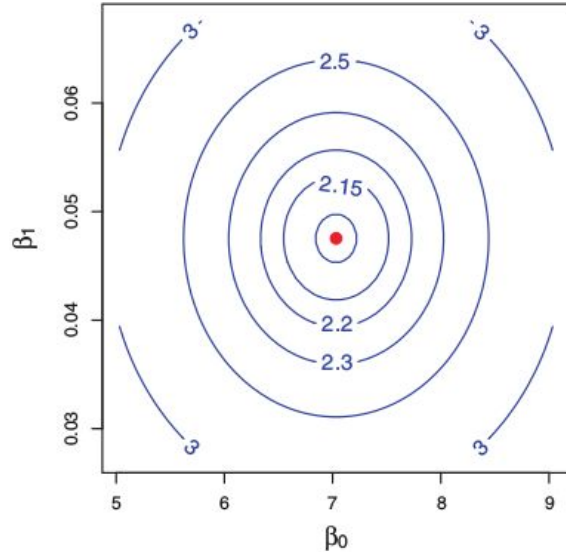
1. cost/loss function
2. model parameters
3. minimum

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 $J(\beta)$
 β

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



Cost function: finding the minimum?

Why algorithmic solution (series of steps) and not analytical solution?

- not always a closed form solution is available
- matrix derivatives are quite difficult and complex to calculate
- computational complexity (matrix inversion $\sim O(N^3)$); stepwise algorithm is more efficient
- algorithms are easier to program than analytical calculations
- etc.



Cost function: finding the minimum?

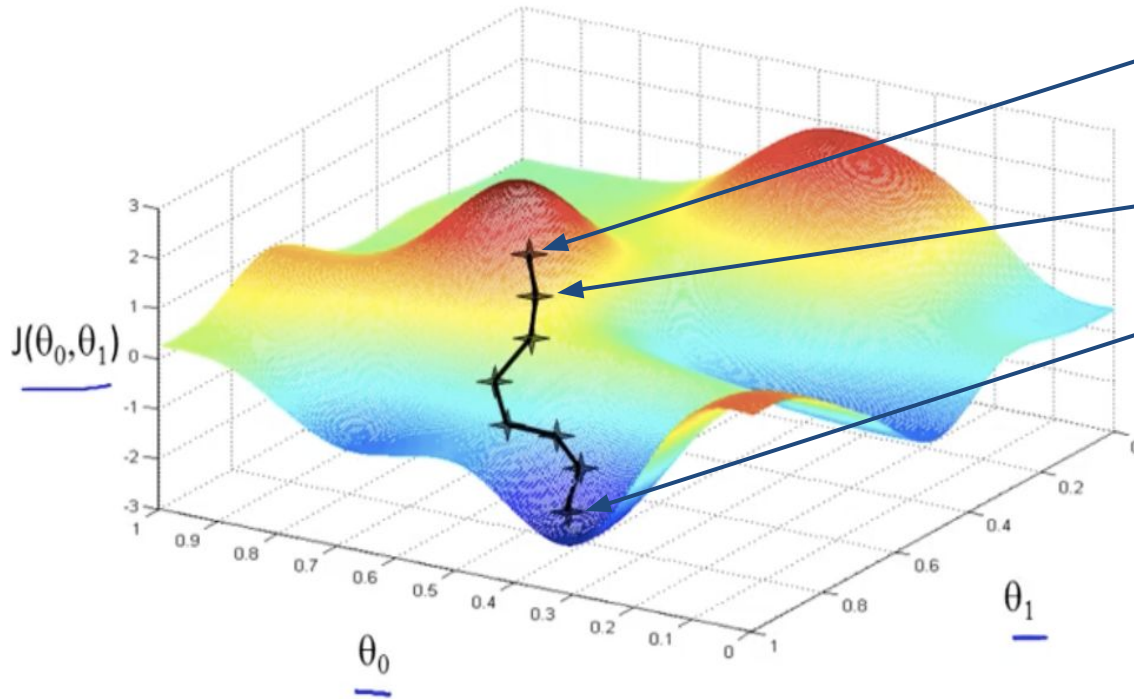
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- etc.

Mind you: in the algorithmic solution (gradient descent & co.) you will still need to take derivatives (but partial derivatives at specific data points)



Gradient descent



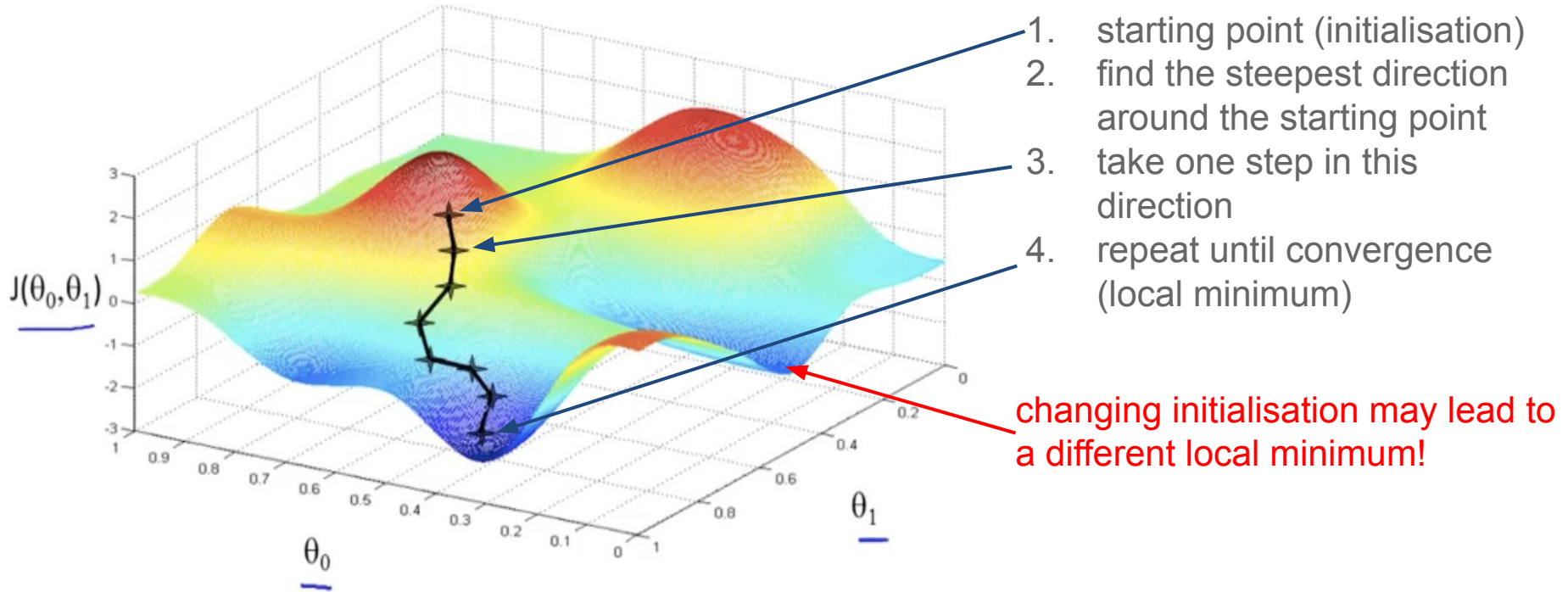
1. starting point (initialisation)
2. find the steepest direction around the starting point
3. take one step in this direction
4. repeat until convergence (local minimum)

Source: Andrew Ng

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



Gradient descent

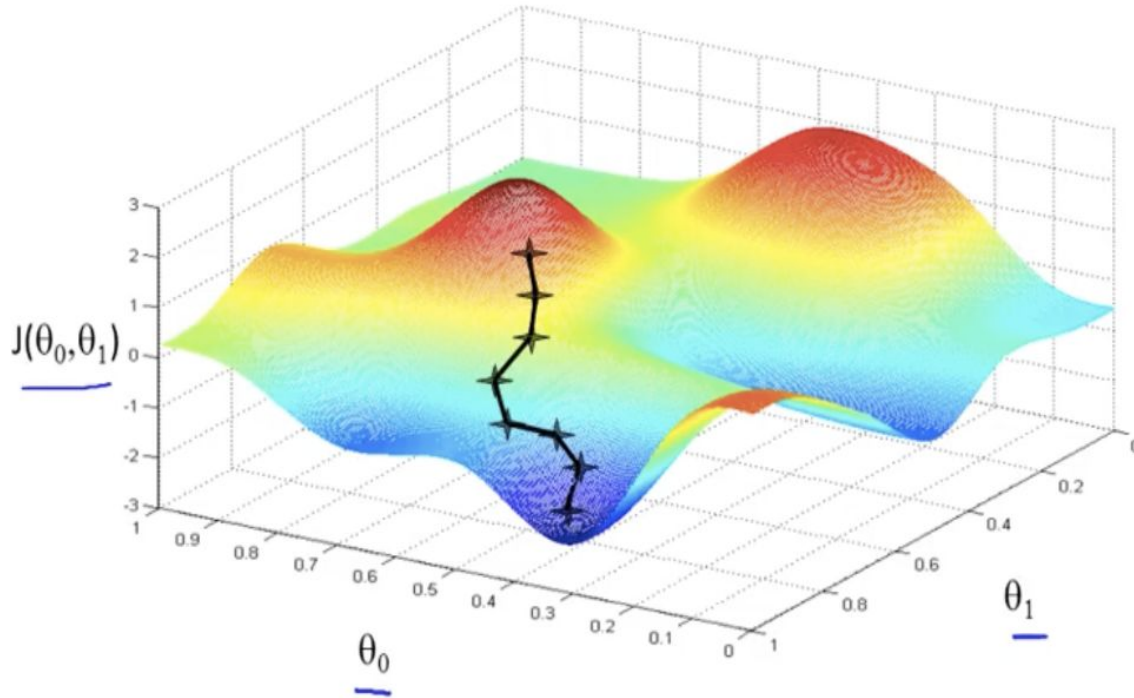


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Gradient descent



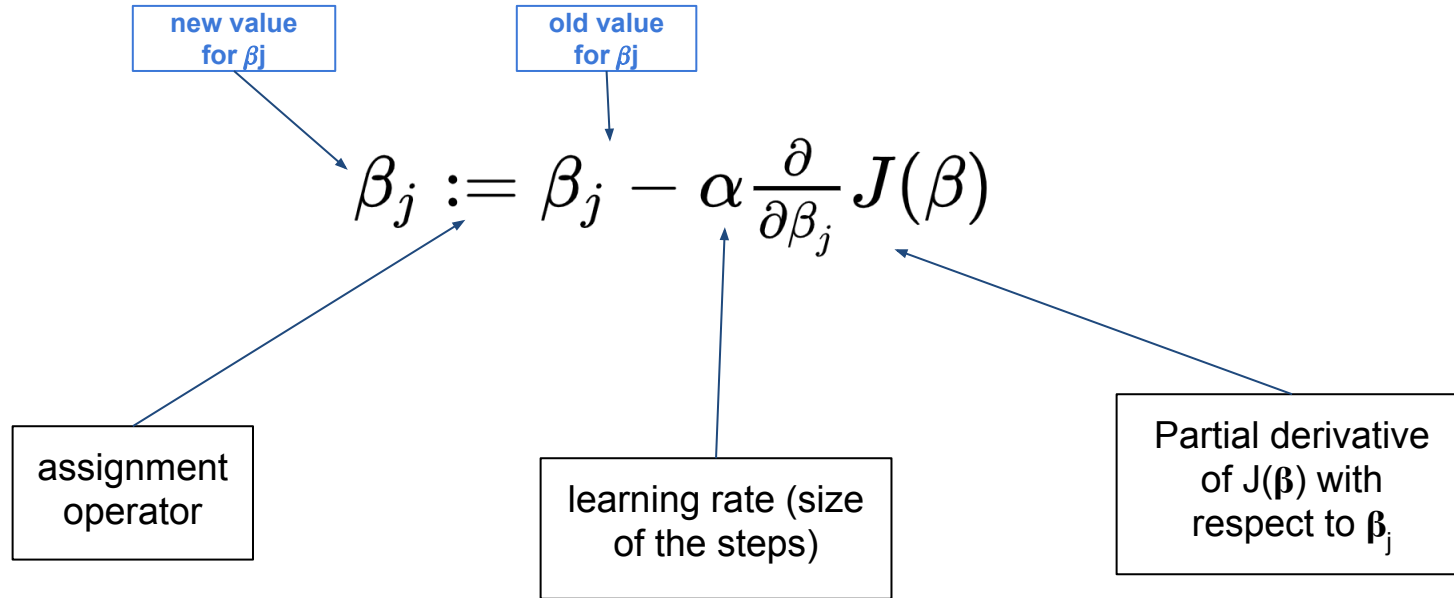
How do we find the steepest direction?

Source: Andrew Ng

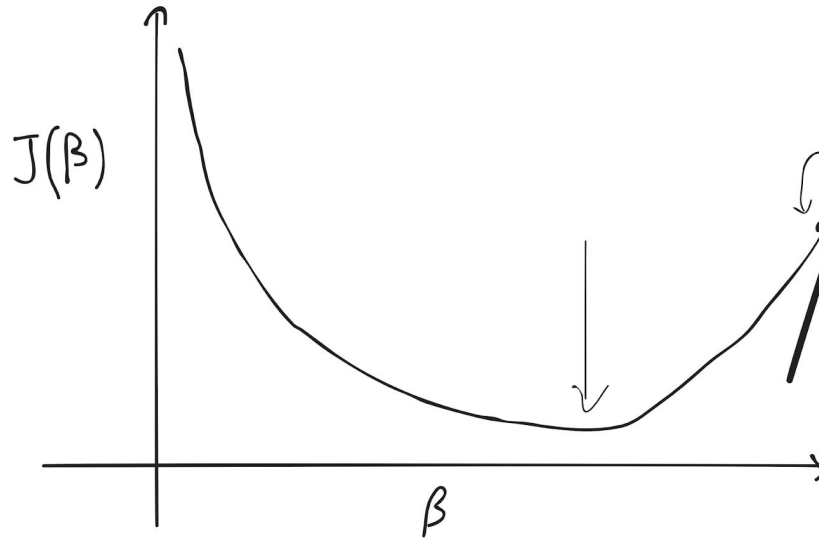
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Gradient descent



Gradient descent



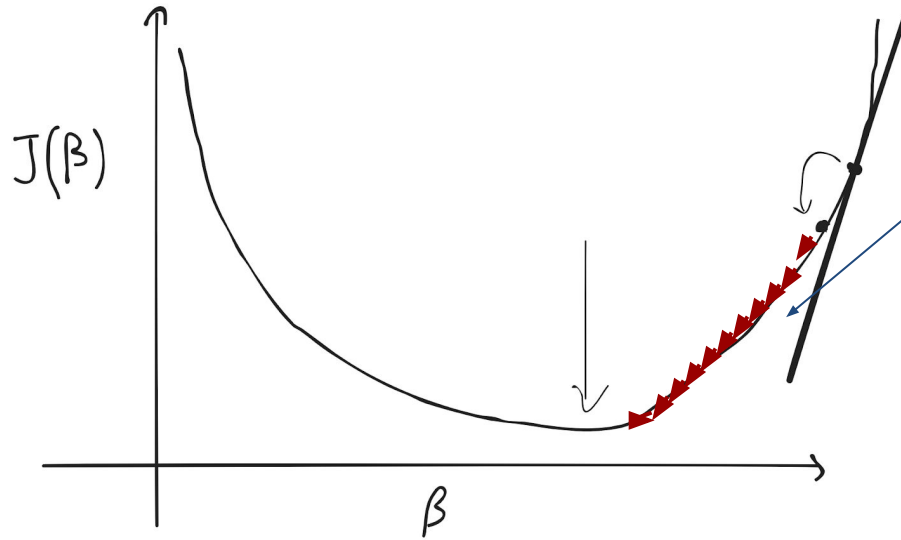
- starting point (initial value for β)
- calculate the (partial) derivative in that point
- \rightarrow positive slope
- **update** the value for β
- repeat

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

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



Gradient descent

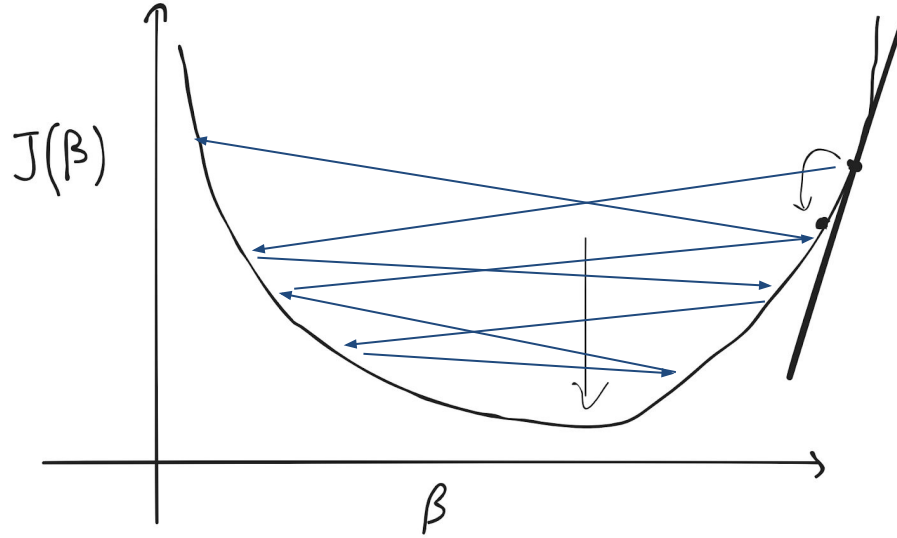


- α controls the size of the updating step
- small $\alpha \rightarrow$ slow descent

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



Gradient descent



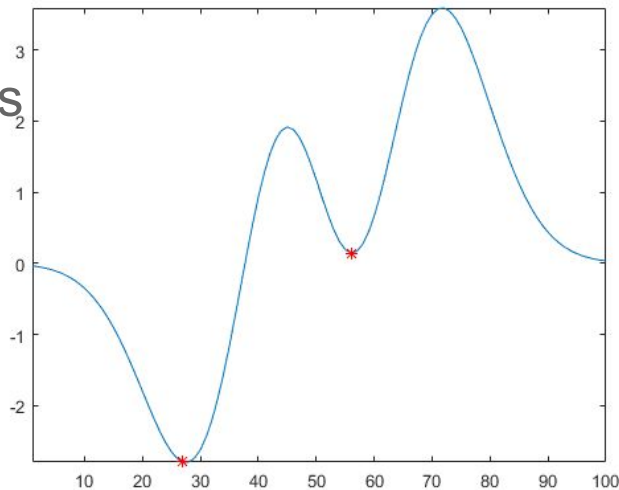
- α controls the size of the updating step
- large $\alpha \rightarrow$ overshooting: failure to converge

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



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** (intuition: the moving average of previous updates is weighed in into the calculations)
- **initialization** values



Logistic regression - recap

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

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

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

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

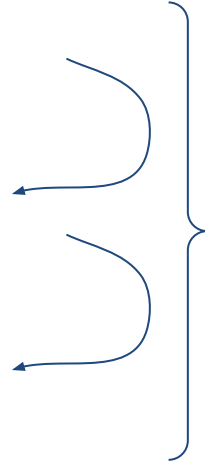


Logistic regression - recap

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

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

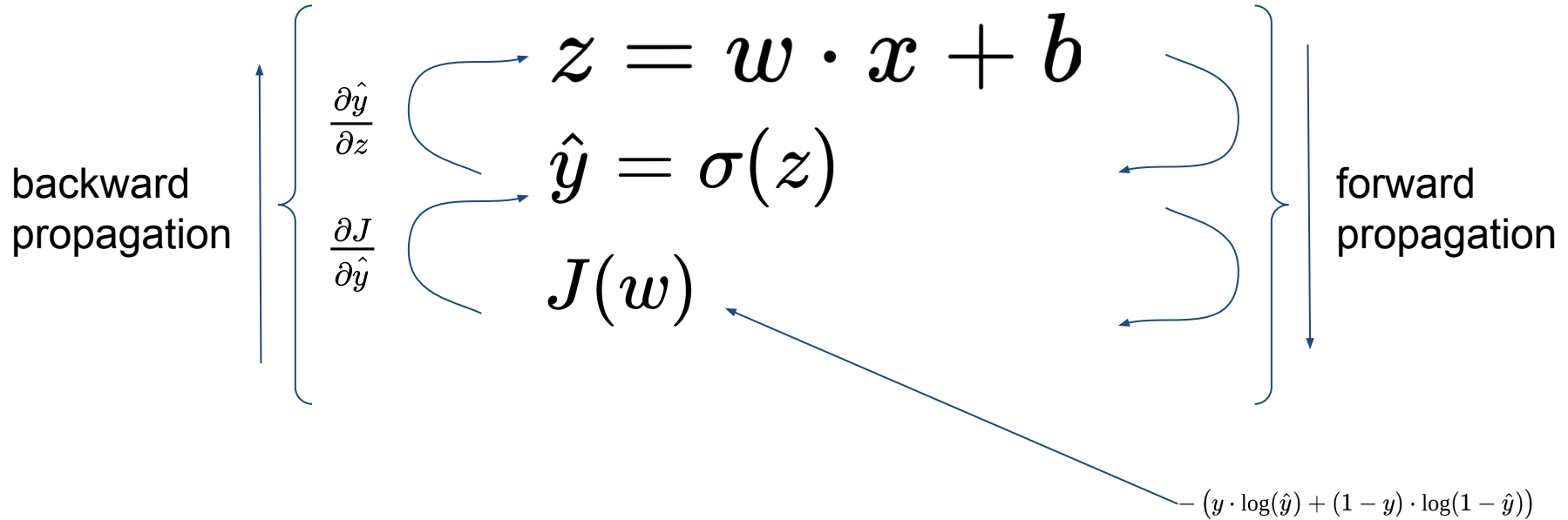
3) $J(w)$



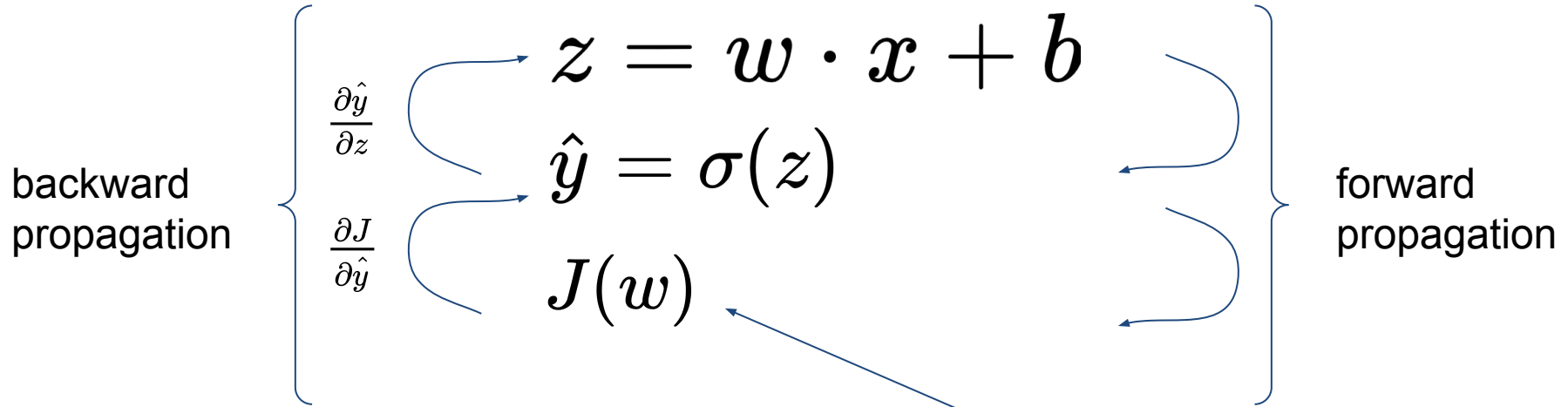
forward propagation



Logistic regression - recap



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
- detailed illustration of backpropagation: [in our blog](#)



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

