Binary classification problems

Logistic regression from a neural networks perspective

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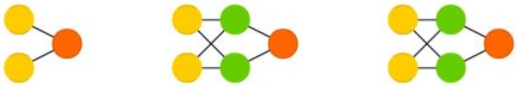

Binary classification problems

- 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** = **label** (a.k.a. target/dependent variable)
- **X** = matrix of **features** (continuous, categorical)



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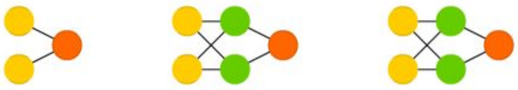
- we don’t model the response directly, rather its **probability**: **P(y=1|x)**
- probabilities lie in [0,1] (not +/- infinity)



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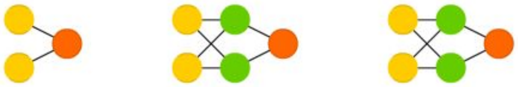
- **Q1: if you have *n* examples with *m* features X_{nm}, what would $f(X_{nm})$ look like? (shape of $\hat{y}$)**



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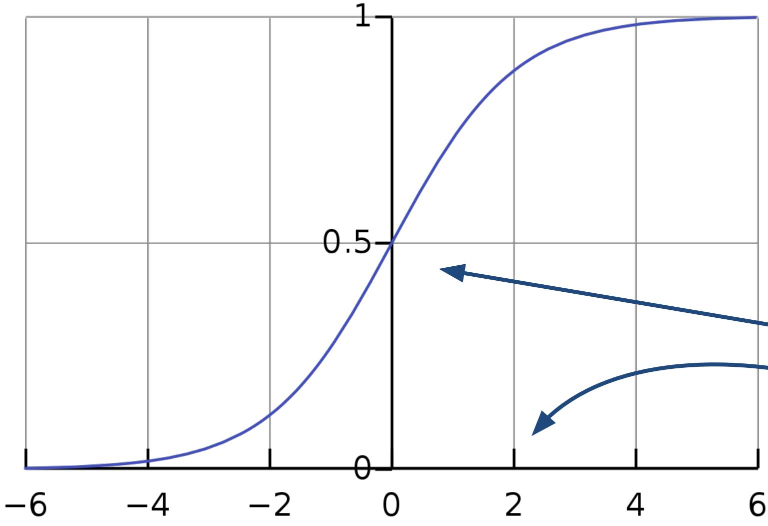
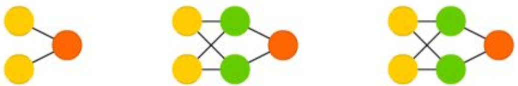


logistic function

probability (y)

predictor variable (z)

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

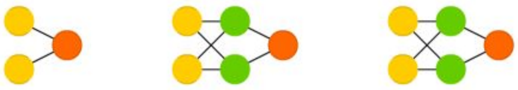


Logistic regression

- 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 <u>exponents</u>!)



Logistic regression

odds

- a little bit of algebra:

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

Logistic regression

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odds

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

log(odds): logit

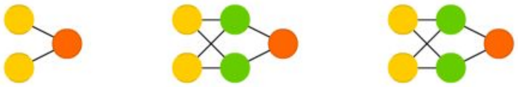
$$log\left(\frac{\sigma(z)}{1-\sigma(z)}\right) = logit(\sigma(z)) = \beta_0 + \beta_1 x$$

Logistic regression

- the **logit function** (log(odds)) is the **link function** between a linear expression of X and the probabilities of Y
- linear X expression (β_0+β_1x) → logit scale (continuous)
- logistic function: converts values on the logit scale back to probabilities

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

our objective!



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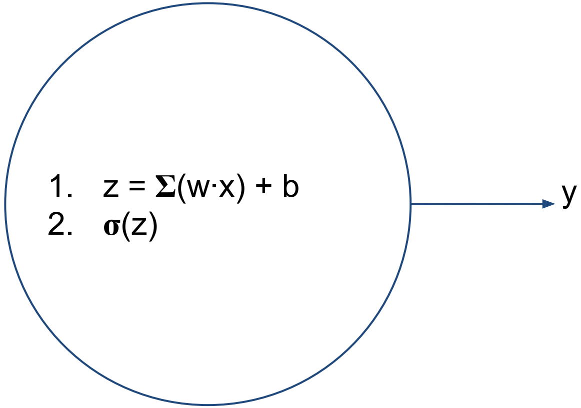
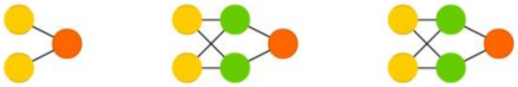
Looks familiar!





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?

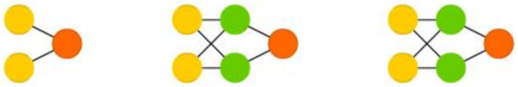
Estimating the coefficients

how do we obtain the model coefficients β?

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

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

difference between observed and
predicted values

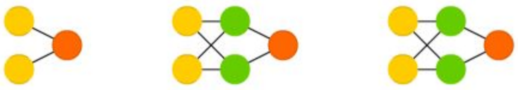


Estimating the coefficients

how do we obtain the model coefficients β?

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

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



Loss function for logistic regression

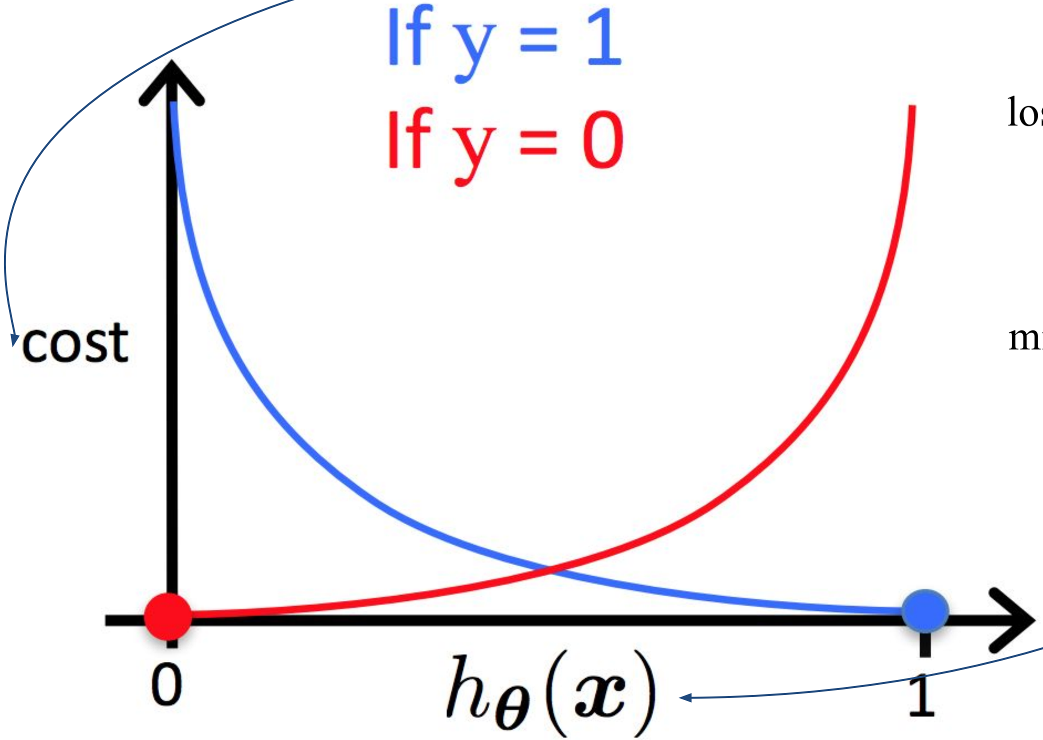
$$J(\beta) = \text{loss}(\hat{y}, y) =$$
$$-(y \cdot log(\hat{y}) + \cancel{(1-y) \cdot log(1-\hat{y})})$$

<u>if y = 1</u>

- y_hat → 1, loss → 0
- y_hat → 0 (but y = 1!), loss → infinity

the opposite holds if y = 0

Cost/loss function for logistic regression



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

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

$$\underset{\beta}{\text{minimize}}\, J(\beta)$$

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

Minimising the cost function

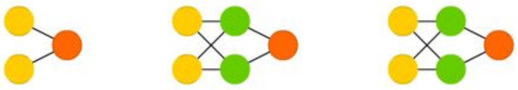
$$\begin{cases} J(\beta) = -\left(y \cdot log(\hat{y}) + (1-y) \cdot log(1-\hat{y})\right) \\ \underset{\beta}{\text{minimize}}\, J(\beta) \end{cases}$$

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

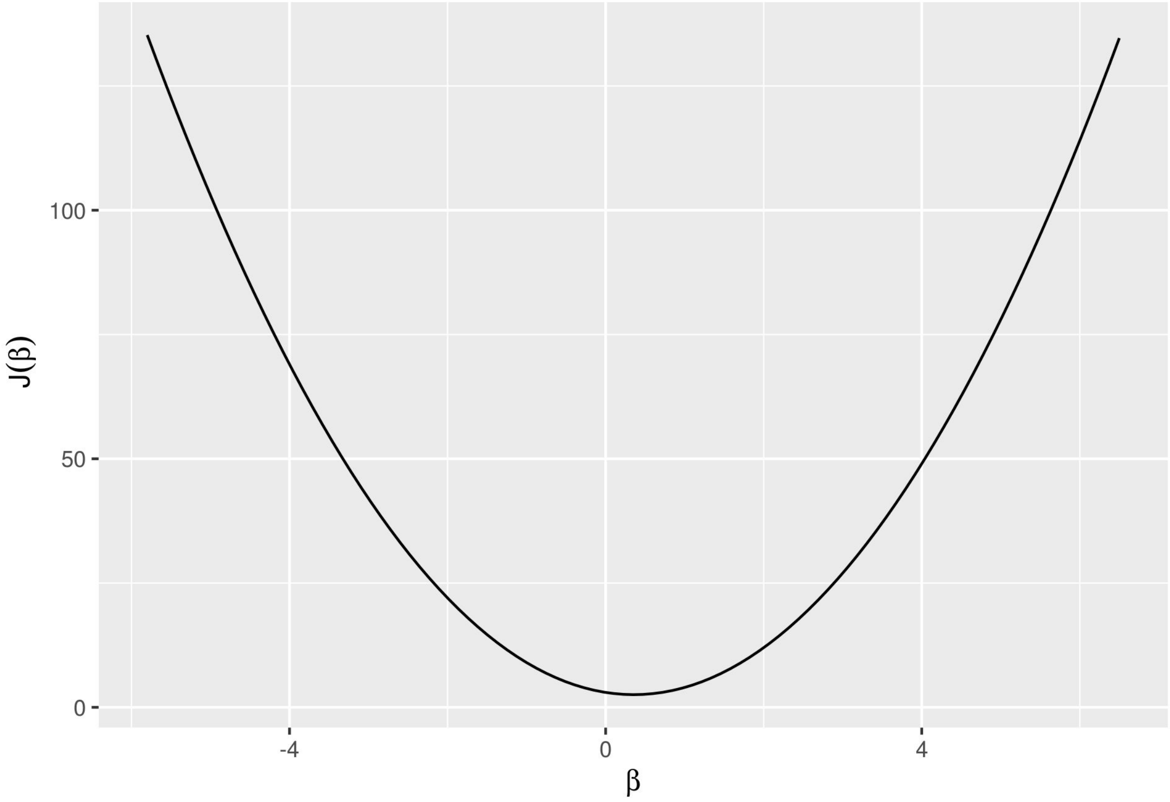
How do we minimise the cost function?
Any ideas?

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

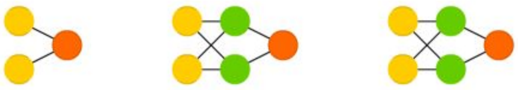


Minimise the cost function

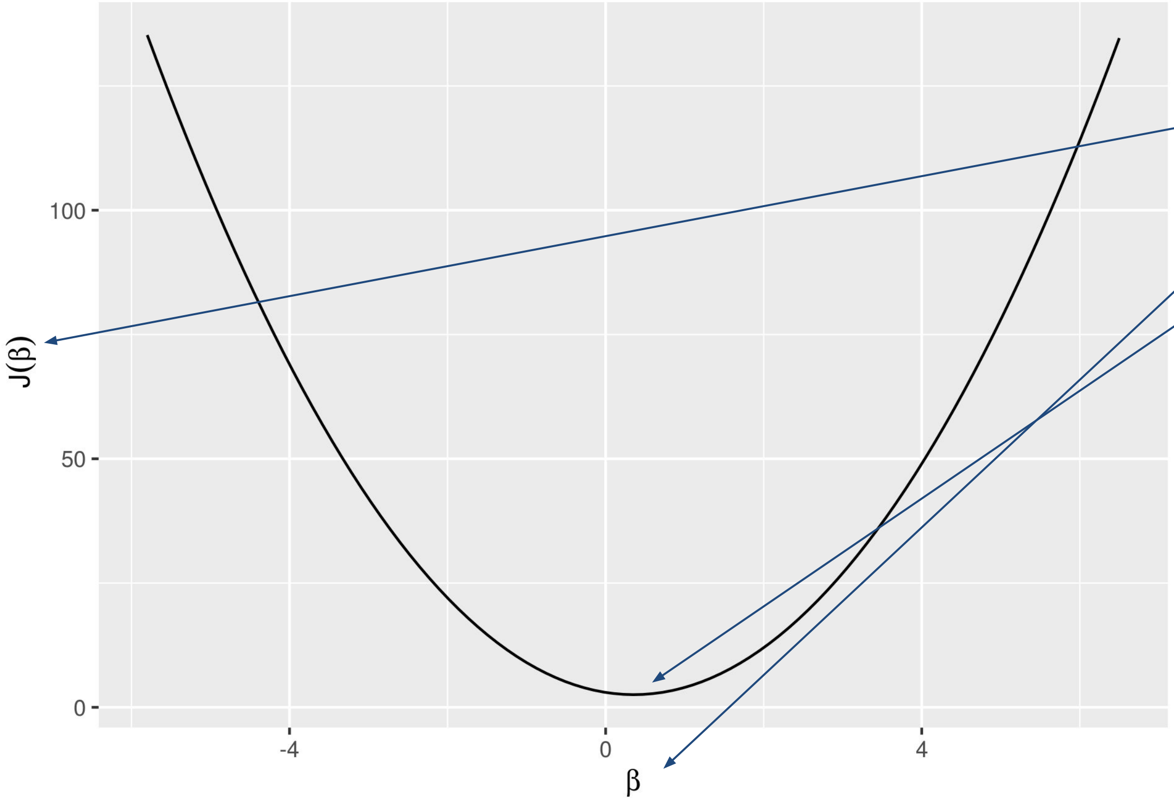


Simple logistic regression (1 parameter):

$$z = \beta \cdot x$$



Minimise the cost function



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

Simple logistic regression (1 parameter):

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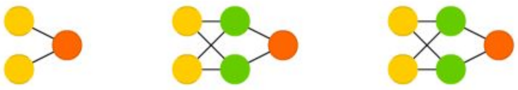
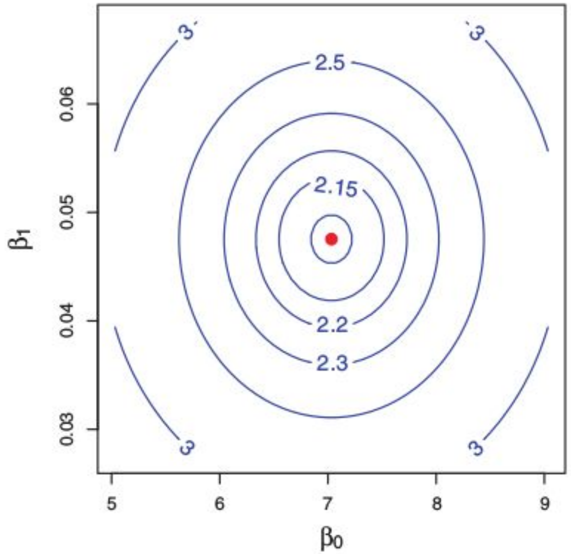
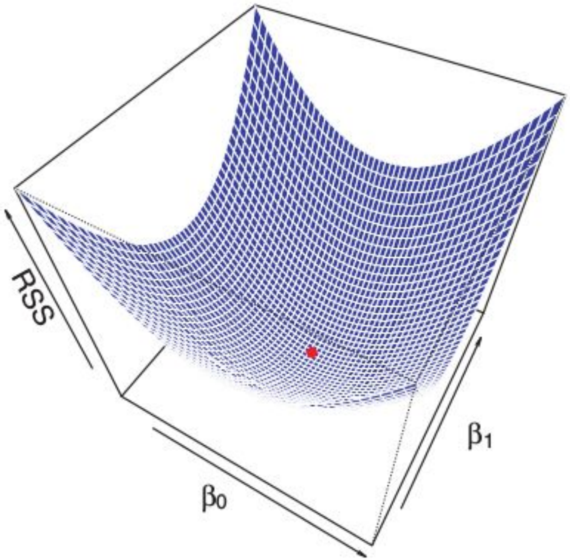


Minimise the cost function





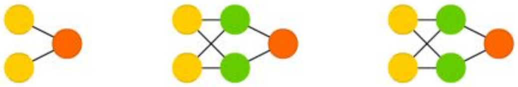
Multiple logistic regression

(e.g. 2 parameters):

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

Multiple logistic regression (> 2 parameters):

→ m-dimensional hyperspace

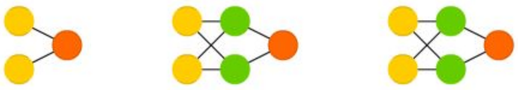


Cost function: finding the minimum?

<u>Gradient Descent</u>:

$$\underset{\beta}{\text{minimize}}\, J(\beta)$$

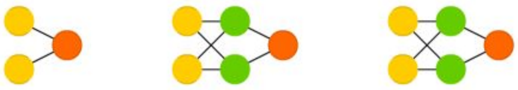
1. Start with initial values for β : (initialisation)
2. Change β in the direction of reducing J(β) : (descent)
3. Stop when the minimum is reached : (minimisation)



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 ~ $O(N^3)$); stepwise algorithm is more efficient
- algorithms are easier to program than analytical calculations
- etc.



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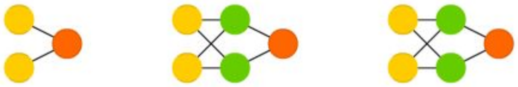
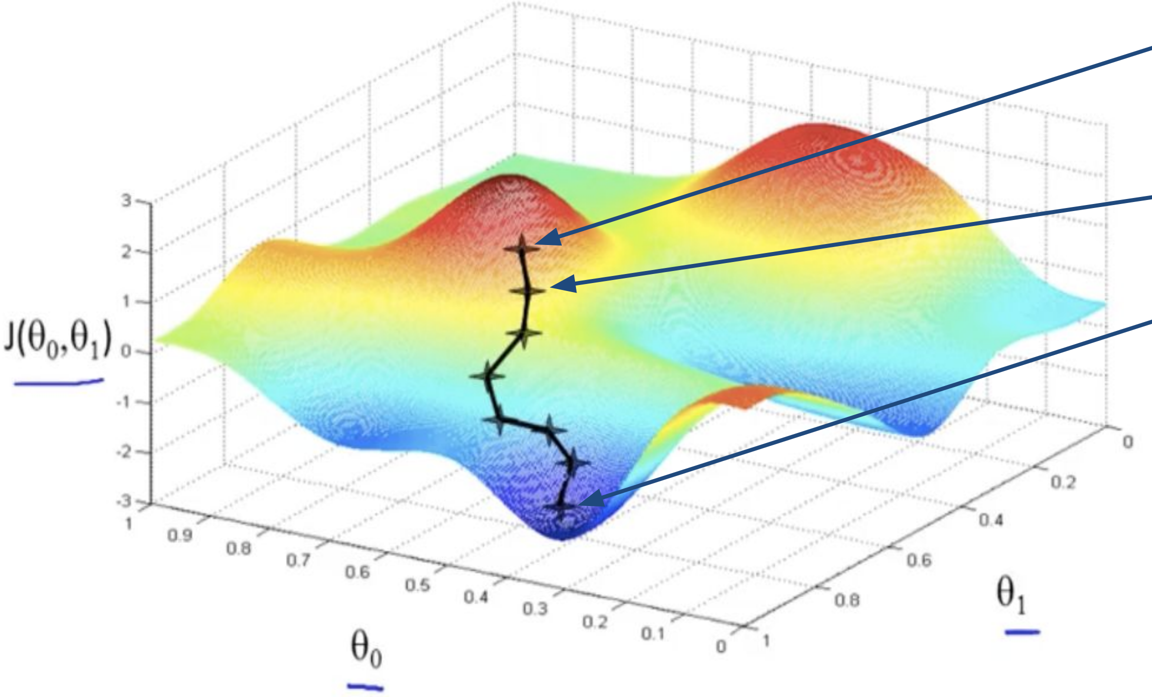
Mind you: in the algorithmic solution (gradient descent & co.) you will still need to take derivatives (but partial derivatives at specific data points)



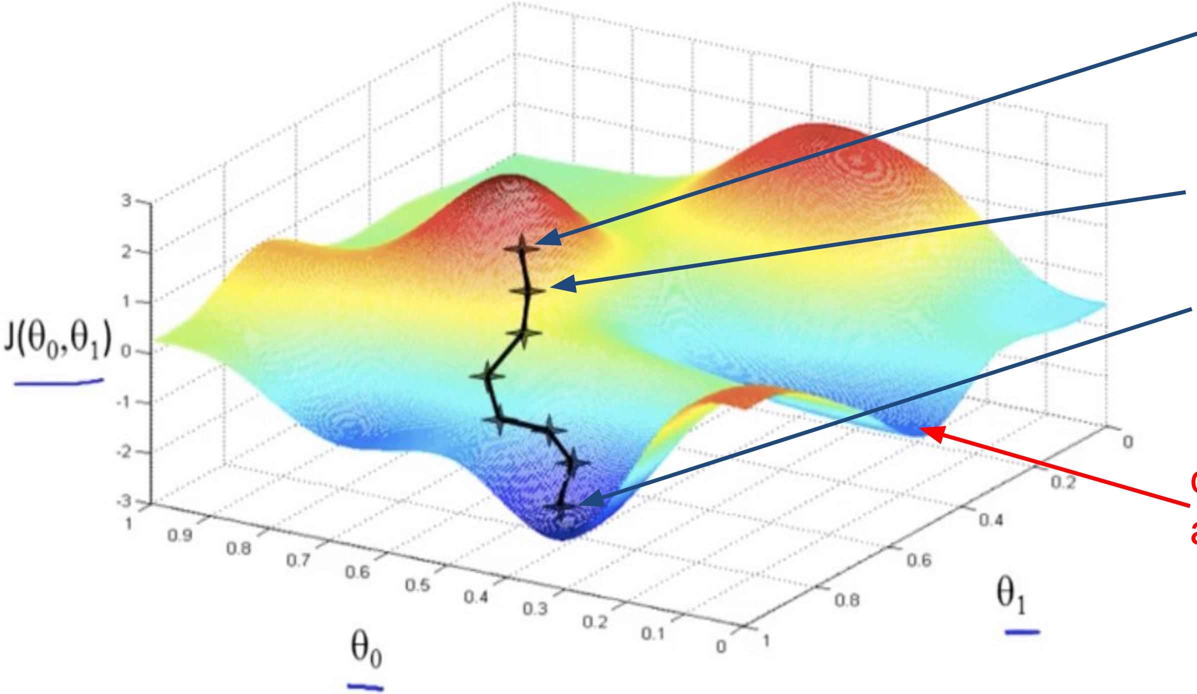
Gradient descent



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

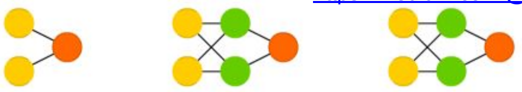
Gradient descent



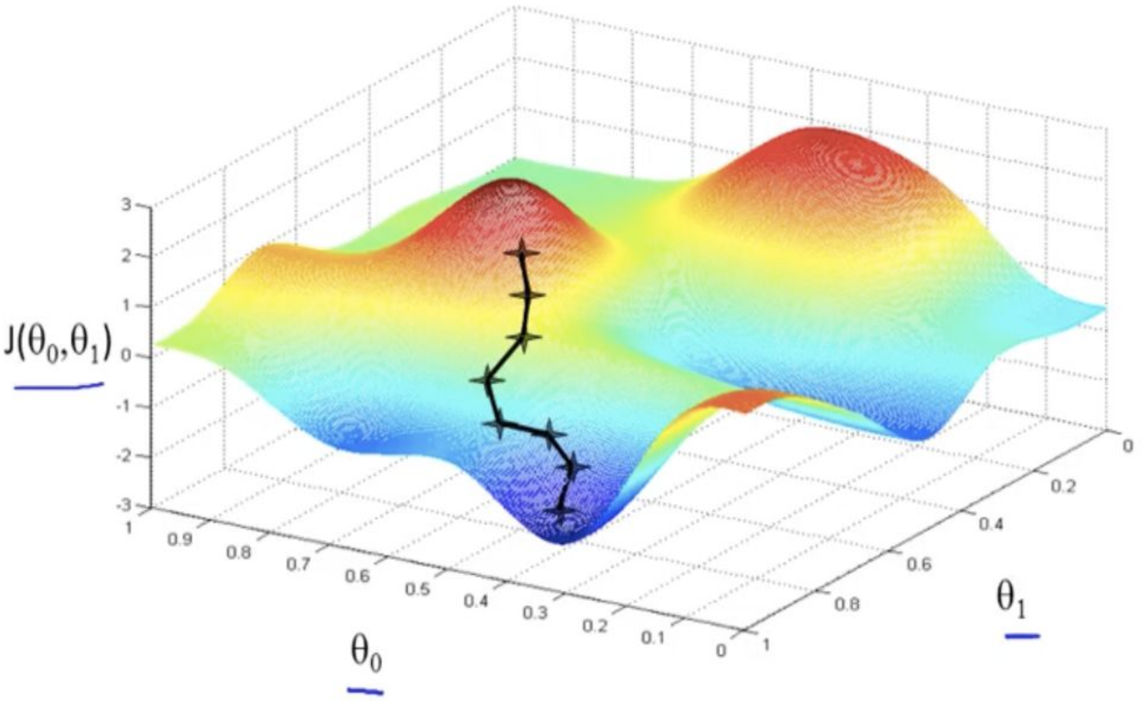
1. starting point (initialisation)
2. find the steepest direction around the starting point
3. take one step in this direction
4. repeat until convergence (local minimum)

changing initialisation may lead to a different local minimum!

Source: Andrew Ng
https://medium.com/@DBCerigo/on-why-gradient-descent-is-even-needed-25160197a635



Gradient descent



How do we find the steepest direction?

Source: Andrew Ng
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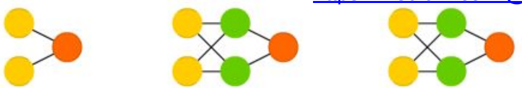


Gradient descent

new value for βj

old value for βj

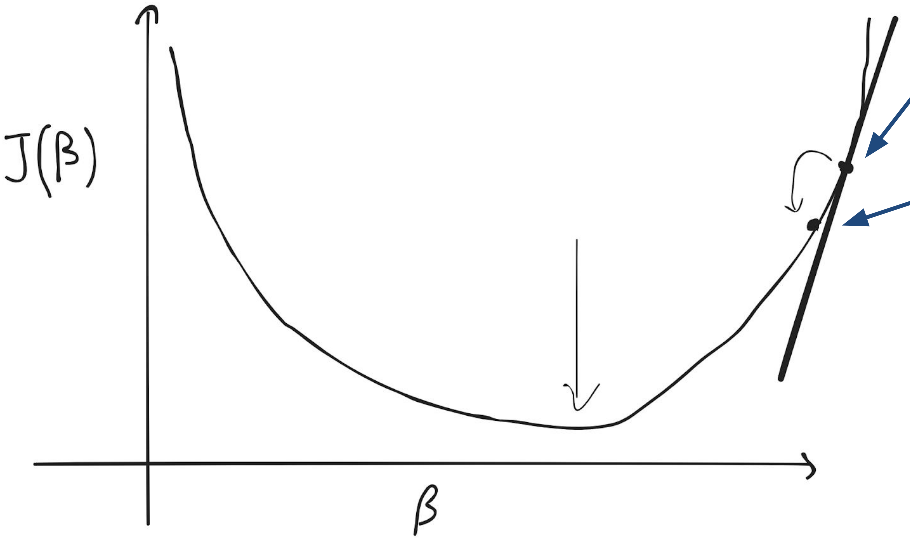
$$\beta_j := \beta_j - \alpha \frac{\partial}{\partial \beta_j} J(\beta)$$

assignment operator

learning rate (size of the steps)

Partial derivative of $J(\boldsymbol{\beta})$ with respect to $\boldsymbol{\beta}_j$

Gradient descent



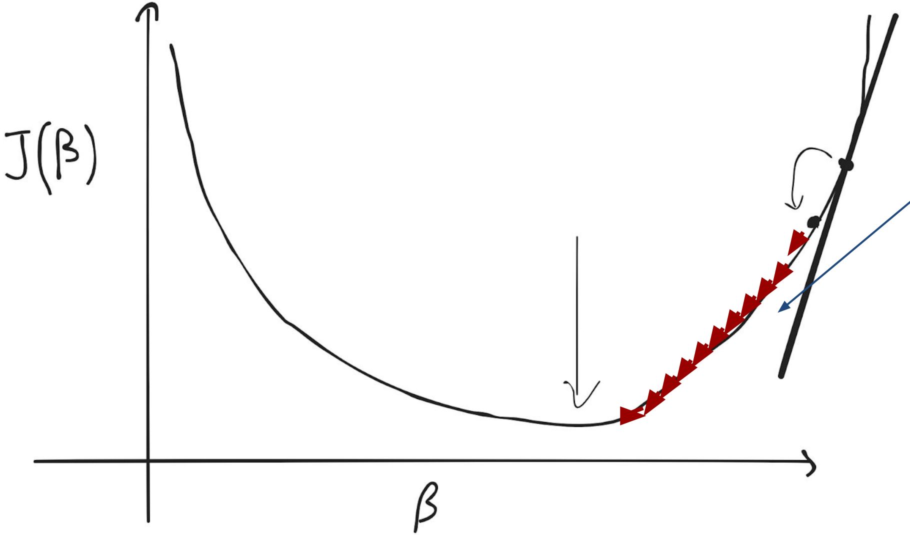
- starting point (initial value for β)
- calculate the (partial) derivative in that point
- → positive slope
- **update** the value for β
- repeat

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

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

made with ZITEBOARD

Gradient descent

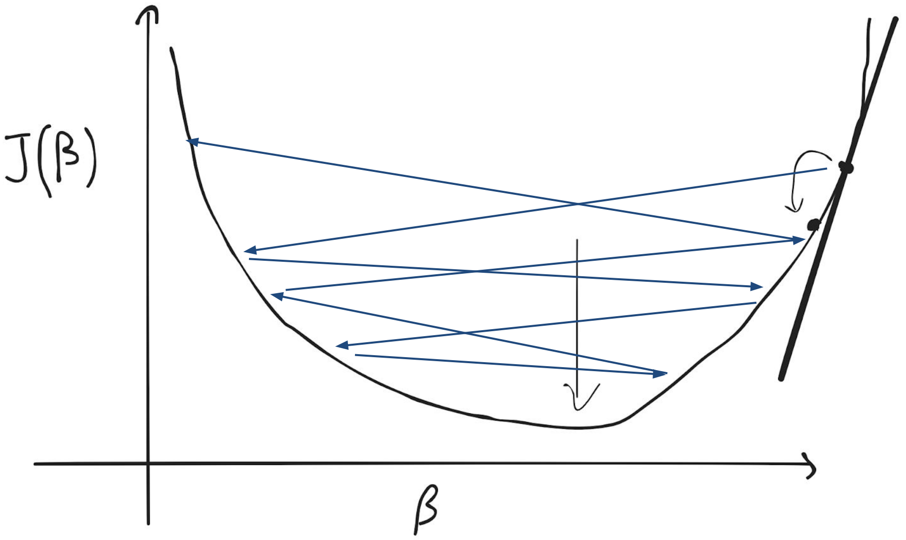


- $\boldsymbol{\alpha}$ controls the size of the updating step
- small $\boldsymbol{\alpha}$ → slow descent

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

MADE WITH ZITEBOARD

Gradient descent



- $\boldsymbol{\alpha}$ controls the size of the updating step
- large $\boldsymbol{\alpha}$ → overshooting: failure to converge

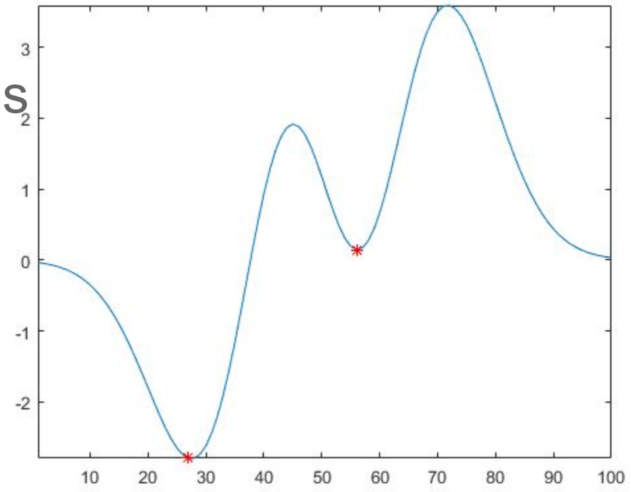
$$\beta_j := \beta_j - \alpha \frac{\partial}{\partial \beta_j} J(\beta)$$

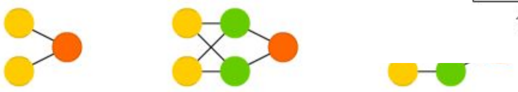
made with ziteboard

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





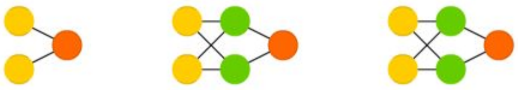
Logistic regression - recap

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

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

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

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



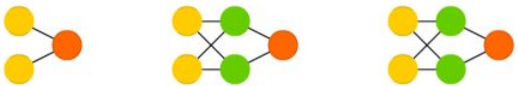
Logistic regression - recap

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

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

3) $J(w)$

forward propagation



Logistic regression - recap

backward propagation

$$\frac{\partial \hat{y}}{\partial z}$$

$$\frac{\partial J}{\partial \hat{y}}$$

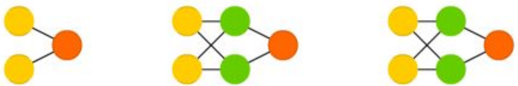
$$z = w \cdot x + b$$

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

$$J(w)$$

forward propagation

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



Logistic regression - recap

backward propagation

$$\frac{\partial \hat{y}}{\partial z} \qquad \frac{\partial J}{\partial \hat{y}}$$

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

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

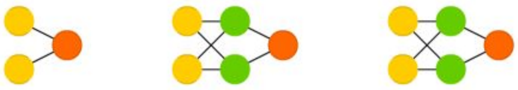
$$J(w)$$

forward propagation

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

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

chain rule



Logistic regression - recap

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

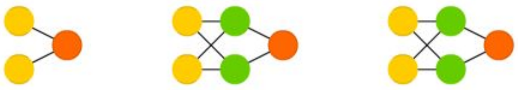
our objective!

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

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

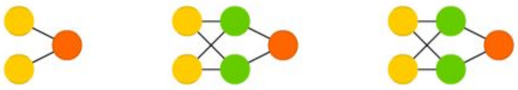
$$\frac{\partial J}{\partial b} = \frac{\partial J}{\partial z}$$

$$\left.\begin{aligned} w_1 &:= w_1 - \alpha \frac{\partial J}{\partial w_1} \\ w_2 &:= w_2 - \alpha \frac{\partial J}{\partial w_2} \\ b &:= b - \alpha \frac{\partial J}{\partial b} \end{aligned}\right\} \text{updating step}$$



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

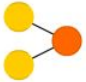


Binary classification metrics

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!

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

Logistic regression

- lab 4

→ day2_code01 logistic regression iris.ipynb