Machine learning: a hands-on introduction

Filippo Biscarini (CNR, Milan, Italy)

filippo.biscarini@cnr.it

Supervised learning

What is learning?

- building a statistical model for **predicting** an **output** based on one or more **inputs**
- statistical learning model is **trained** rather than explicitly programmed

What is learning?

- building a statistical model for **predicting** an **output** based on one or more **inputs**
- statistical learning model is **trained** rather than explicitly programmed
- **ML models do not learn by trying to understand what goes on, rather by trial and error through a vast number of examples (not like a university student but like a little child)**

What is learning?

1. <u>Input data</u> (e.g. genome variants, metabolites)
2. <u>Output examples</u> (e.g. disease status, biological characteristics)
3. <u>Performance measure</u>: how well is the algorithm working → adjustment steps

   → **learning**

You can do (statistical) learning in your head!

- The current price of an electric Tesla is $100,000
- The price of an electric Tesla next year will be $90,000
- The price of an electric Tesla in two years will be $81,000
- The price of an electric Tesla in three years will be $72,900
- How much will an electric Tesla cost in five years?

You can do (statistical) learning in your head!

TRAINING DATA

- The current price of an electric Tesla is $100,000
- The price of an electric Tesla next year will be $90,000
- The price of an electric Tesla in two years will be $81,000
- The price of an electric Tesla in three years will be $72900
- How much will an electric Tesla cost in five years?

NEW, UNKNOWN DATA

PRICE = PRICE_0*(1-0.10)^YEARS

PRICE IN FIVE YEARS= $59,049

MATHEMATICAL MODEL

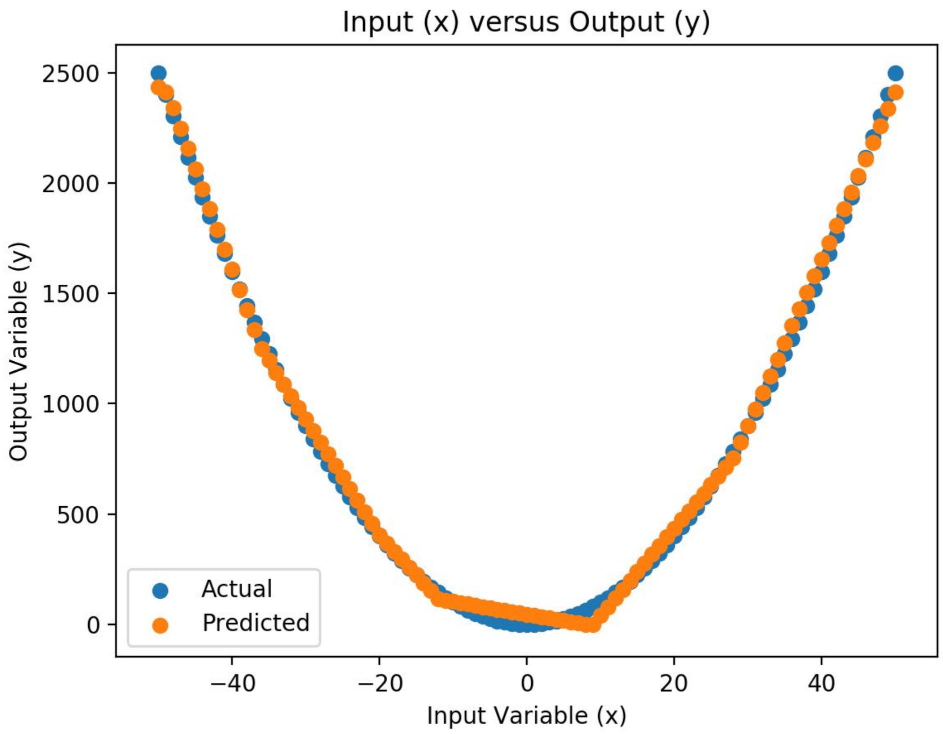
PREDICTION

The truth about learning

- Yesterday: **n. of cases = $2^{(days-1)}$**
- Today: **price = price_0 * $(1-0.10)^{years}$**

Is this what ML is learning?

The truth about learning



[From: https://machinelearningmastery.com/neural-networks-are-function-approximators/]

- (known) **quadratic function** (blue line)
- approximated with **machine learning** (orange line)

!! ML is not learning $y = x^2$!!

Why supervised?

Training examples

measured variables / features
on *n* examples

$$\begin{bmatrix} 1 \\ 0 \\ \vdots \\ 1 \end{bmatrix} = \begin{bmatrix} 0.12 & 1.5 & \dots & 0.9 \\ 2.05 & 0.95 & \dots & 1.1 \\ \vdots & \vdots & \ddots & \vdots \\ 3.5 & 0.88 & \dots & 1.75 \end{bmatrix}$$

labels / target variables (e.g. phenotypes) on n examples

Unsupervised learning

measured variables / features
on *n* examples

$$\cancel{\begin{bmatrix} 1 \\ 0 \\ \vdots \\ 1 \end{bmatrix}} = \begin{bmatrix} 0.12 & 1.5 & \dots & 0.9 \\ 2.05 & 0.95 & \dots & 1.1 \\ \vdots & \vdots & \ddots & \vdots \\ 3.5 & 0.88 & \dots & 1.75 \end{bmatrix}$$

The steps of a supervised learning problem

1. Collect the data
2. EDA and data preparation
3. Training a model on the data
4. Evaluate model performance
5. Improve model performance

80% of the time!

rinse and repeat!

model deployment

A little ML jargon

- **example** (record, observation)
- **feature** (independent variable, factor)
- **label** (dependent variable)
- **method**: the statistical method used for a problem
- **model**: the modelling of the problem (e.g. which features to include and how)
- **algorithm**: the technique by which the method is applied to the model and solved
- **training data**: data on which the ML algorithm is trained

Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
5.0	2.0	3.5	1.0	versicolor
6.2	2.2	4.5	1.5	versicolor
6.0	2.2	4.0	1.0	versicolor
6.0	2.2	5.0	1.5	virginica
6.3	2.3	4.4	1.3	versicolor
5.5	2.3	4.0	1.3	versicolor
5.0	2.3	3.3	1.0	versicolor
4.5	2.3	1.3	0.3	setosa
5.5	2.4	3.8	1.1	versicolor
5.5	2.4	3.7	1.0	versicolor
4.9	2.4	3.3	1.0	versicolor
6.7	2.5	5.8	1.8	virginica
6.3	2.5	4.9	1.5	versicolor

Regression and classification

Supervised learning problems

- Regression (**predictive**) problems
  - target (continuous) variable, output
- Classification (**predictive**) problems
  - label, class (qualitative variable): binomial, multinomial, ordinal, nominal

"given a set of data, the learning algorithm attempts to optimize a function (the model) to find the combination of feature values that result in the target output"

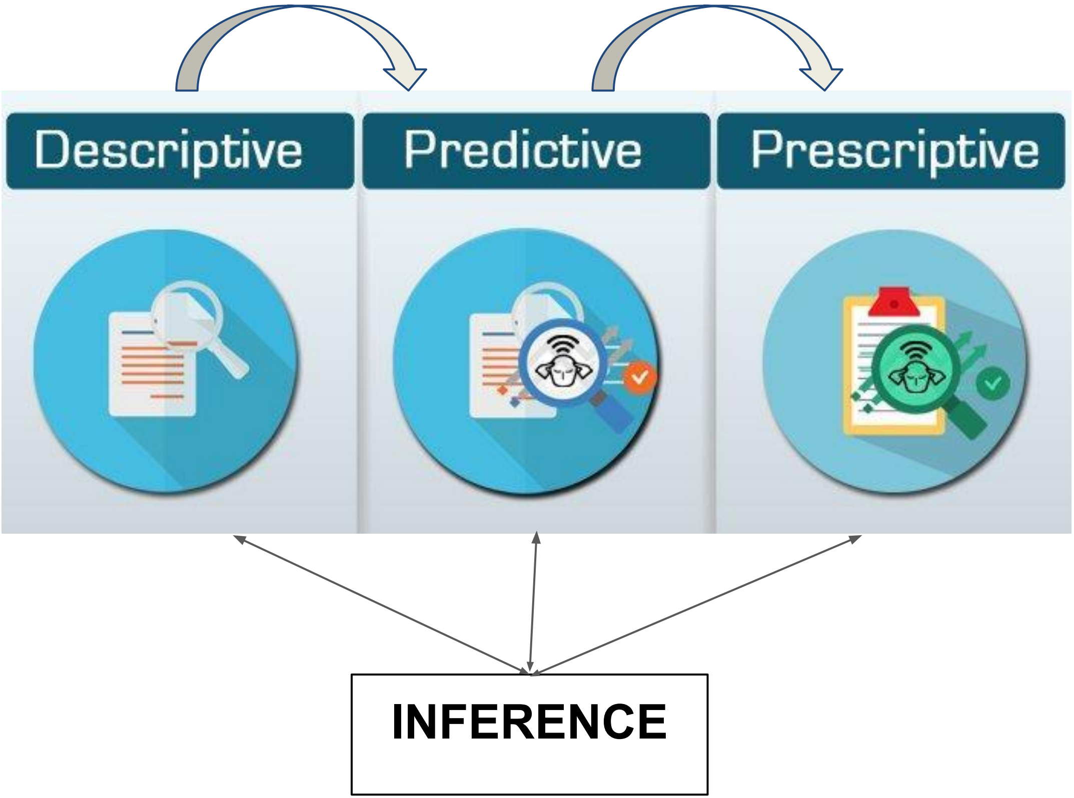
Supervised learning problems

- Regression (**predictive**) problems
  - target (continuous) variable, output
- Classification (**predictive**) problems
  - label, class (qualitative variable): binomial, multinomial, ordinal, nominal

Predict:

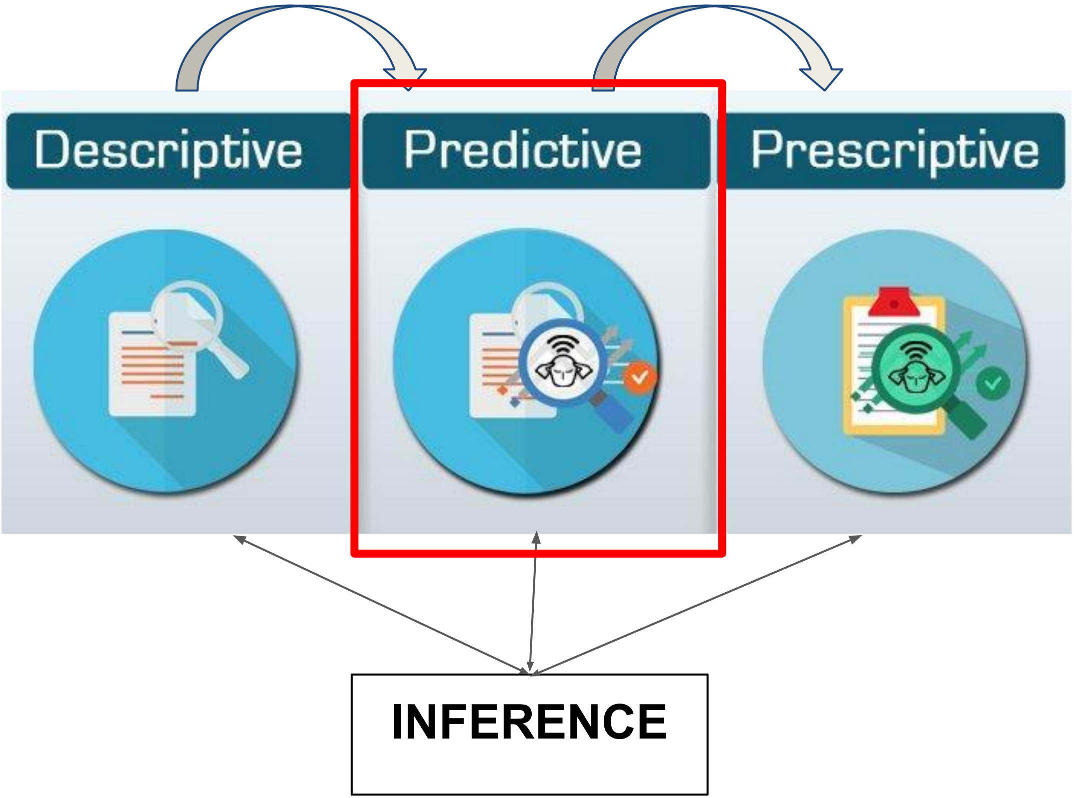
- the future (forecasting, prognosis)
- the unknown/unseen (e.g. sick/healthy, genetic predisposition etc.)
- real time (e.g. control traffic lights at rush hours)
- the past (e.g. when something happened, like conception date based on hormone levels)

Supervised learning problems



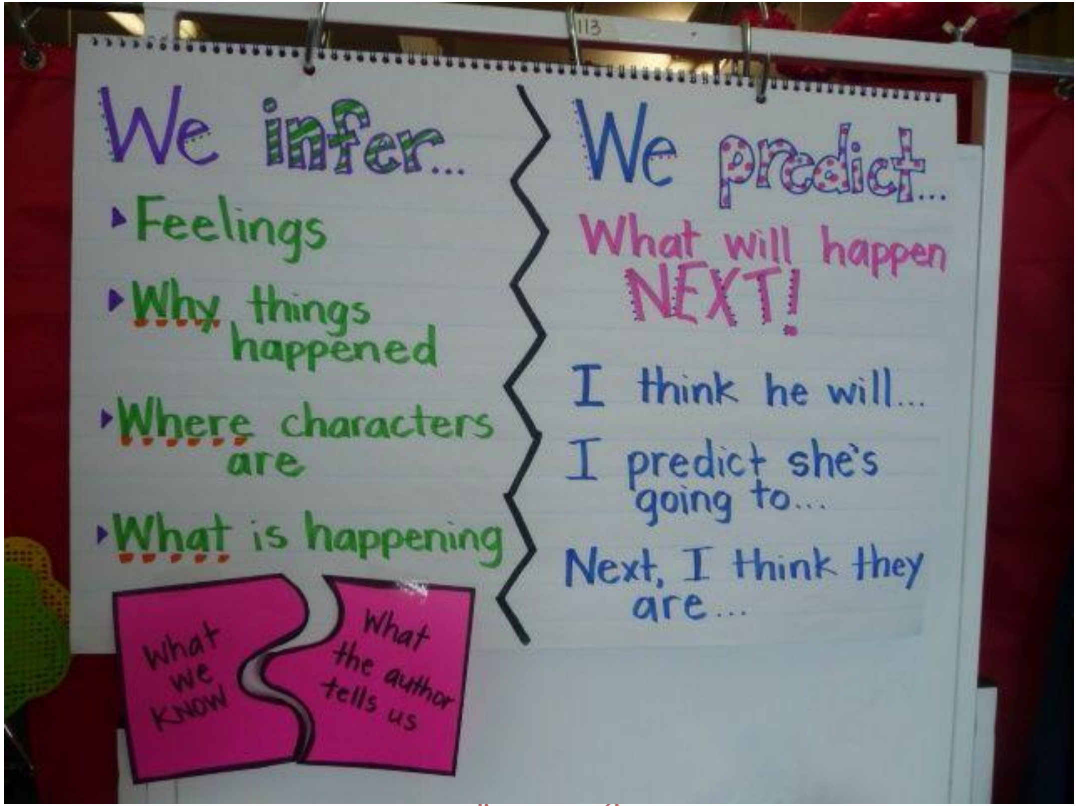
- Know the past
- Predict the future
- Act consequently

Supervised learning problems



- Know the past
- Predict the future
- Act consequently

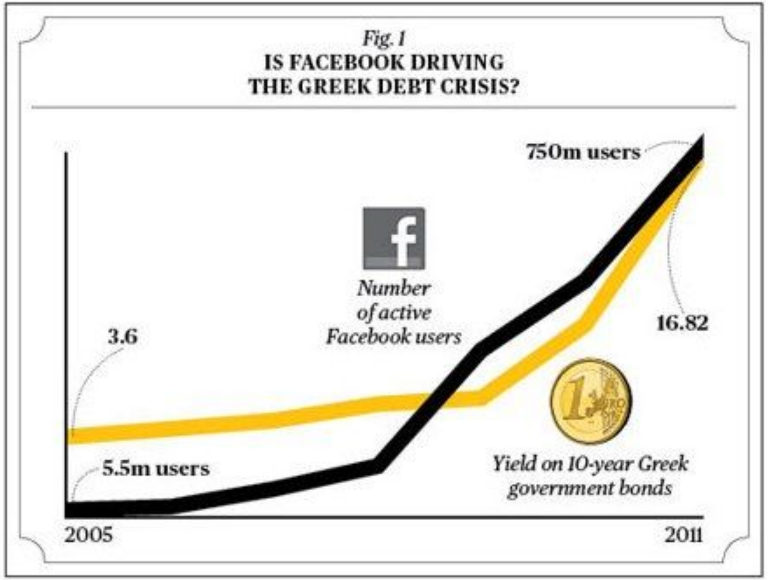
Inference vs Prediction



- different statistical problems
- different objectives, different rules … different ballparks
- inference is in general more difficult than prediction

What causes what?

- Typical inferential problem
- Correlation is not causation!
  - already since Pearson! (early 1900's)
  - spurious correlations generator
  - *apophenia* (from Greek, "to seem")



What causes what?

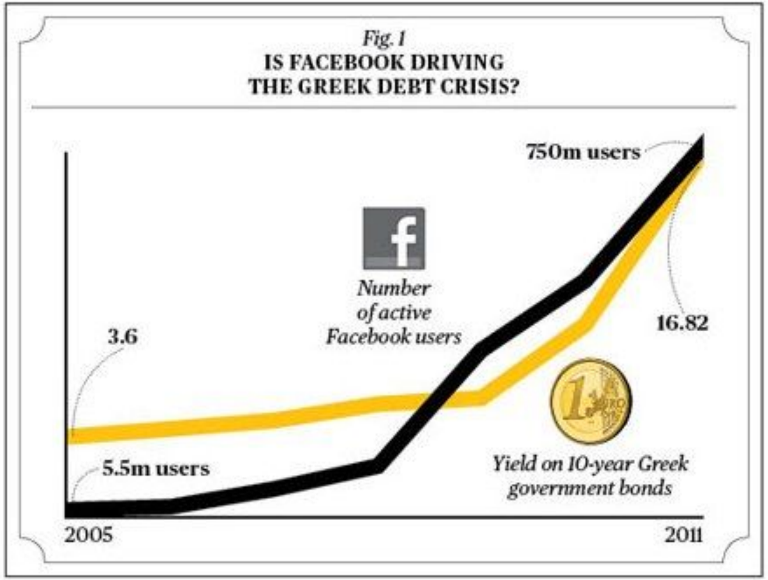
- Typical inferential problem
- Correlation is not causation!

Reverse causation

- n. of firemen←→size of the fire (the more the firemen, the bigger the fire?)
- smoking ← →depression (smoking causes depression?)

Missing variable

- ice cream consumption ← →n. of sunburn cases
- buying lighters ← →lung cancer



What causes what?

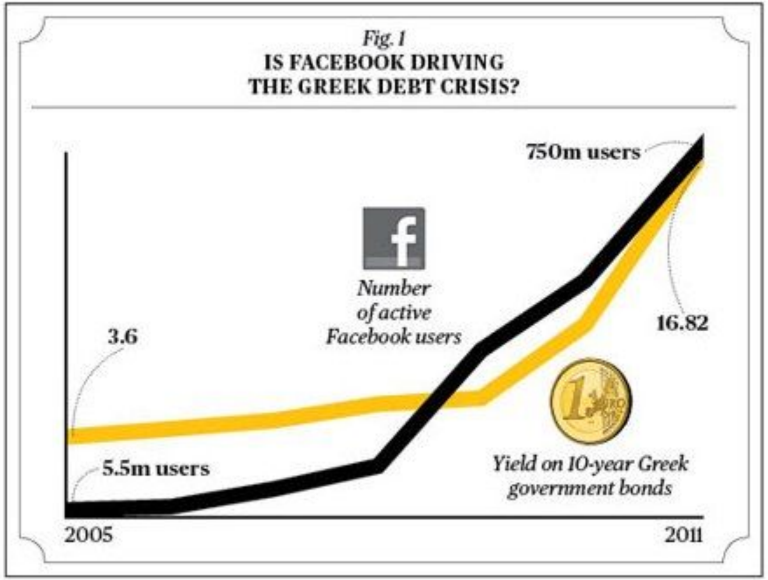
- Typical inferential problem
- Correlation is not causation!

Reverse causation

- n. of firemen←→size of the fire (the more the firemen, the bigger the fire?)
- smoking ← →depression (smoking causes depression?)

Missing variable

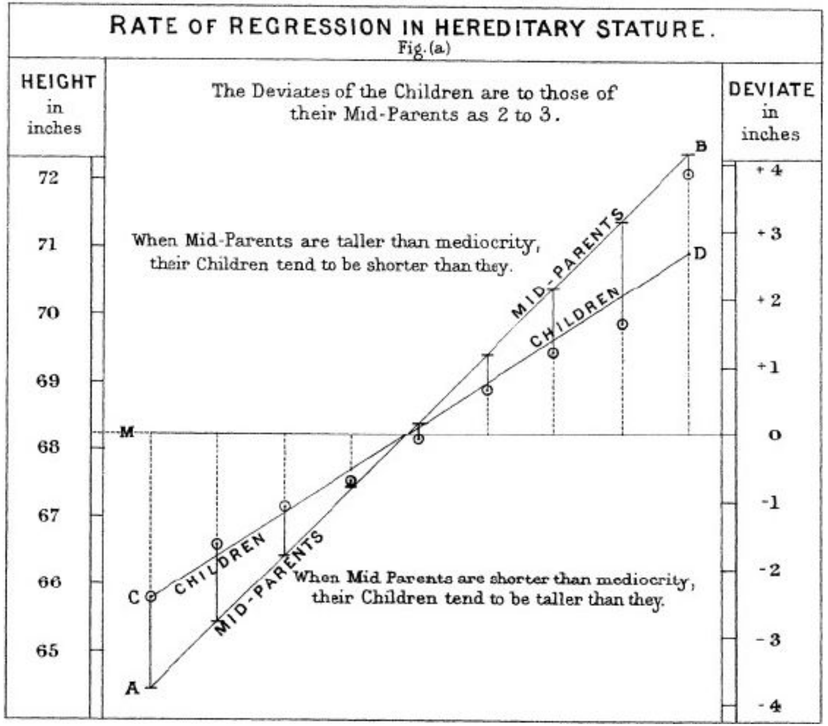
- ice cream consumption ← →n. of sunburn cases
- buying lighters ← →lung cancer



Q: reverse causation or missing variable?

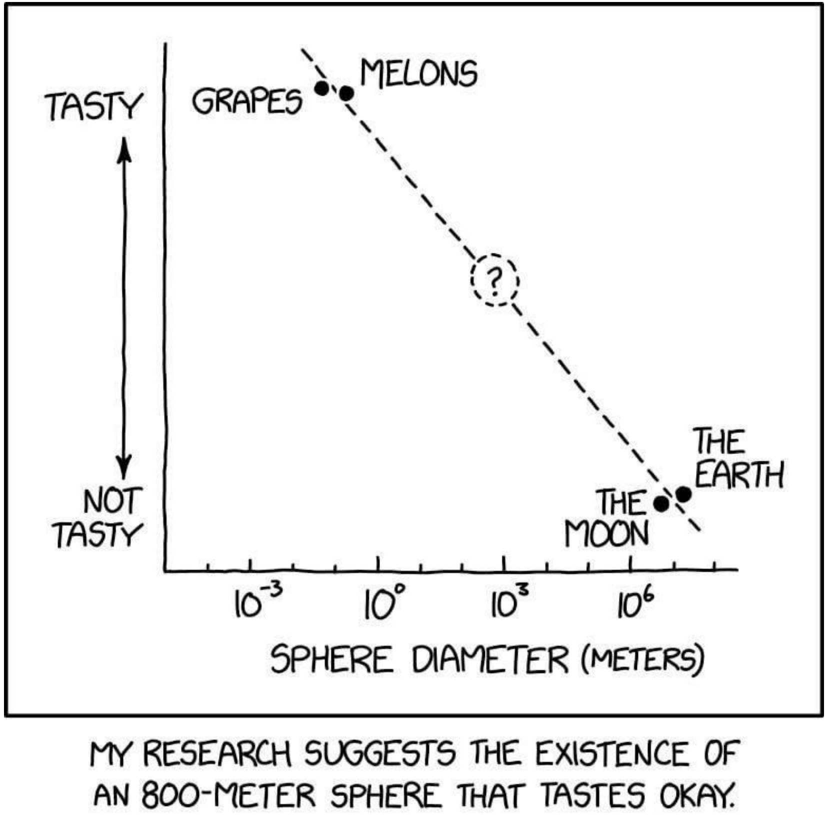
What causes what?

- Also regression!
  - **Galton**: predict the height of children from the height of their parents
  - But also the height of parents could be predicted from that of their children! (??)→no possible cause-effect relationship!



[Han, Ma, Zhu 2015]

What causes what?



<u>spurious regression</u>: can you spot the mistakes?

The probabilistic nature of cause (it gets trickier)

- you turn the key and the car engine starts: clear cause-effect link
- you take an ibuprofen pill and your headache goes away: how do you know it wouldn’t have gone anyway? → **counterfactual**
- smoking→lung cancer: my uncle always smoked and did not have lung cancer! my aunt never smoked and got lung cancer! →if you smoke it is **more likely** that you get lung cancer

X → Y: X increases/decreases the chances that Y happens

The probabilistic nature of cause (it gets trickier)

RCT: randomized (clinical) trial

	placebo %	statin %	relative risk reduction
heart attack	11.8	8.7	27%
stroke	5.7	4.3	25%
death from any cause	14.7	12.9	13%

[Heart Protection Study, 2002: https://www.thelancet.com/journals/lancet/article/PIIS0140-6736(02)09327-3/fulltext]

What causes what?

- **experiments** (RCT, A/B testing etc.)

without experiments

- post hoc, ergo propter hoc
- strength of correlation
- consistency (different datasets, studies etc.)
- dose-response relationship
- analysis “ceteris paribus” (controlling for confounders, stratifiers etc.)
- Bayesian Networks
- …

What causes what? ML perspective

“observational data alone does not provide causal insight” (Pearl and Mackenzie 2018*)

ML can help with causal questions:

- studying associations between variables: starting point for causal hypotheses
- estimating causal effects: quantify the dose-response relationship
- learning causal models: tools to reason about interventions and counterfactuals
- learning causal graphs: direction of causal relationships
- etc.

The gist of it: if you can predict y using x, then there probably is a causal relationship between x and y

*Pearl, J. and Mackenzie, D., 2018. The book of why: the new science of cause and effect. Basic books

Supervised learning problems

- Regression (**predictive**) problems
- Classification (**predictive**) problems

Predictive machines!

- Classifiers
- Predictors/Regressors

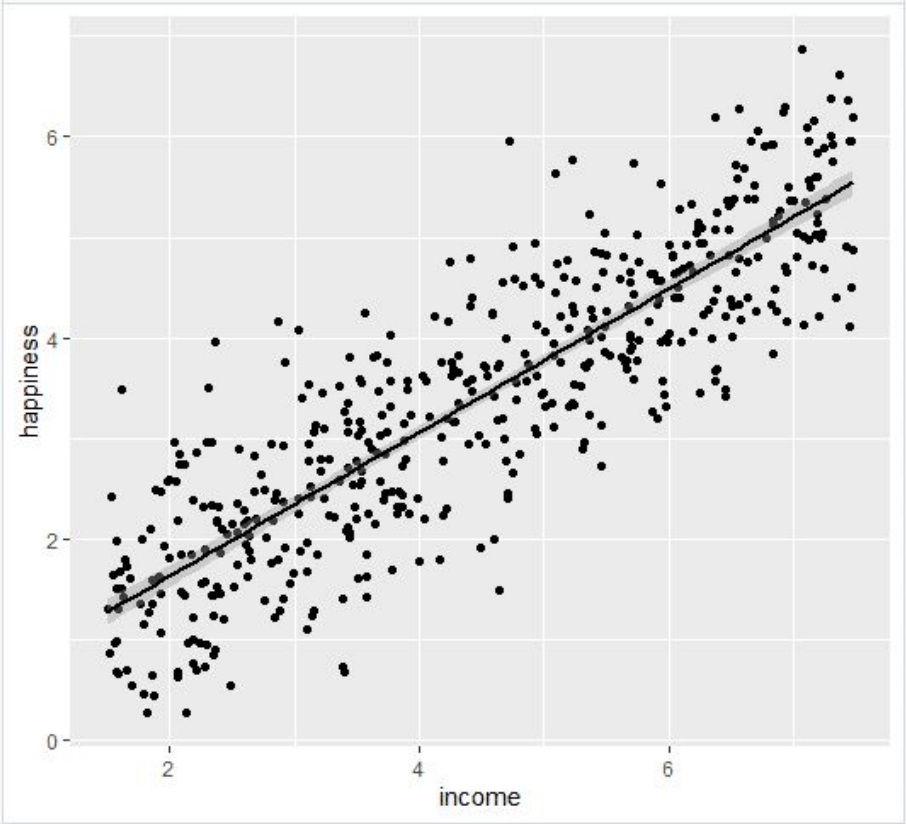
source:
https://blog.bigml.com/2013/03/12/machine-learning-from-streaming-data-two-problems-two-solutions-two-concerns-and-two-lessons/

Regression

Regression problems

- the response variable **y** is **quantitative**
- e.g.: *height*, *weight*, *yield* (milk, crops), *blood sugar concentration*
- **y** = **target** (dependent) variable (a.k.a. response, objective variable)
- **X** = matrix of **features** (continuous, categorical)
- **predictor**: y = f(x) = **P(X)** ← [predictive machine]

Regression problems - simple regression



happiness = (intercept) + beta*income

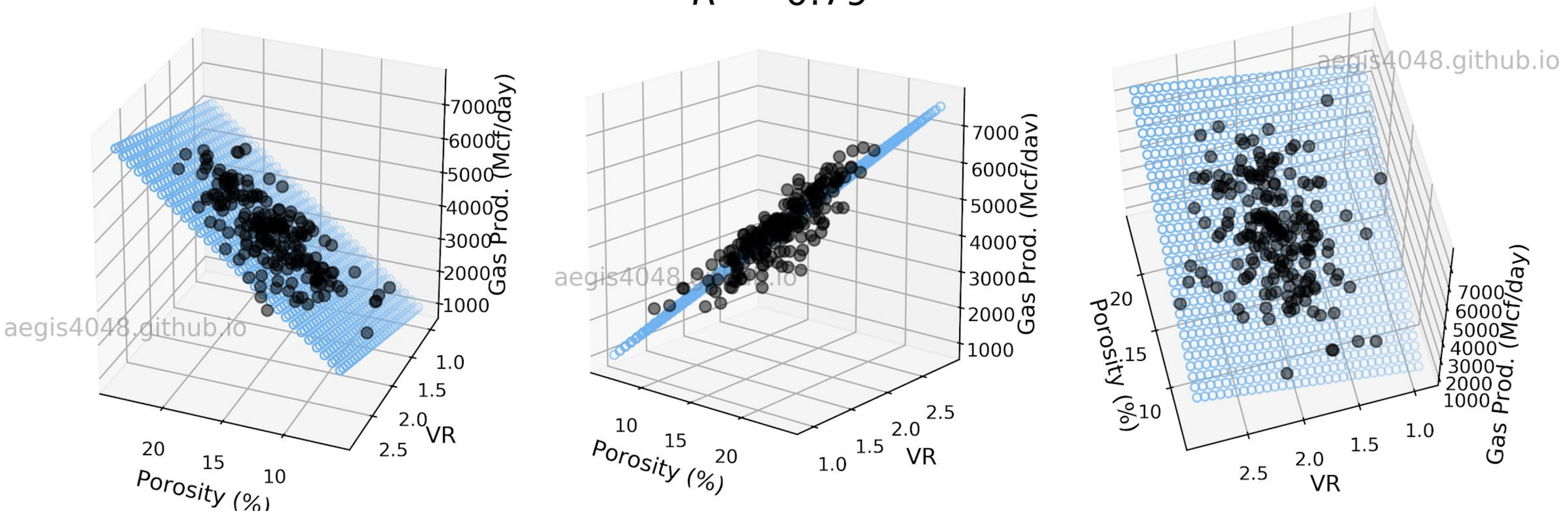
or

income = (intercept) + beta*happiness

Source: https://www.scribbr.com/statistics/linear-regression-in-r/

Regression problems - multiple regression

$R^2 = 0.79$



Source: https://aegis4048.github.io/mutiple_linear_regression_and_visualization_in_python

Multiple linear regression

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p + \epsilon$$

- y: target variable
- **β**'s: model coefficients
- X's: features (predictors, independent variables, factors)

Multiple linear regression

$$\mathbf{y} = \beta\mathbf{X} + \mathbf{e}$$

- matrix (compact) notation
- vectors of observations (**y**), coefficients (**β**) and residuals (**e**)
- matrix of features (**X**)

Multiple linear regression

$$\mathbf{y} = \beta\mathbf{X} + \mathbf{e}$$

estimation of coefficients

$$\hat{\mathbf{y}} = \hat{\beta}\mathbf{X}$$

→ **predictions!**

- matrix (compact) notation
- vectors of observations (**y**), coefficients (**β**) and residuals (**e**)
- matrix of features (**X**)

Predictions

$$\hat{y} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p$$

with the estimated coefficients $\boldsymbol{\beta}$ and the feature values **X** we obtain the predicted values $\hat{y}$

Predictions

$$\hat{y} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p$$

with the estimated coefficients $\boldsymbol{\beta}$ and the feature values **X** we obtain the predicted values $\hat{y}$

→ how do we obtain the model coefficients $\boldsymbol{\beta}$?

Estimation of model coefficients

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_p X_p + \epsilon$$

- define a **loss (cost) function**
- **minimise** the loss function

Estimation of model coefficients

- define a **loss (cost) function**

observations	**predictions**
$\mathbf{y}$	$\hat{\mathbf{y}} = \hat{\beta}\mathbf{X}$

difference between observed and predicted values

Estimation of model coefficients

- define a **loss (cost) function**

observations	predictions
y	$\hat{\mathbf{y}} = \hat{\beta}\mathbf{X}$

difference between observed and predicted values → **LEAST SQUARES**

Estimation of model coefficients

- minimise the **loss (cost) function**

$$RSS = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$RSS = \sum_{i=1}^{n} (y_i - \hat{\beta}_i X_i)^2$$

$$\underset{(\beta)}{\text{minimize}} \; (RSS)$$

LEAST SQUARES

Estimation of model coefficients

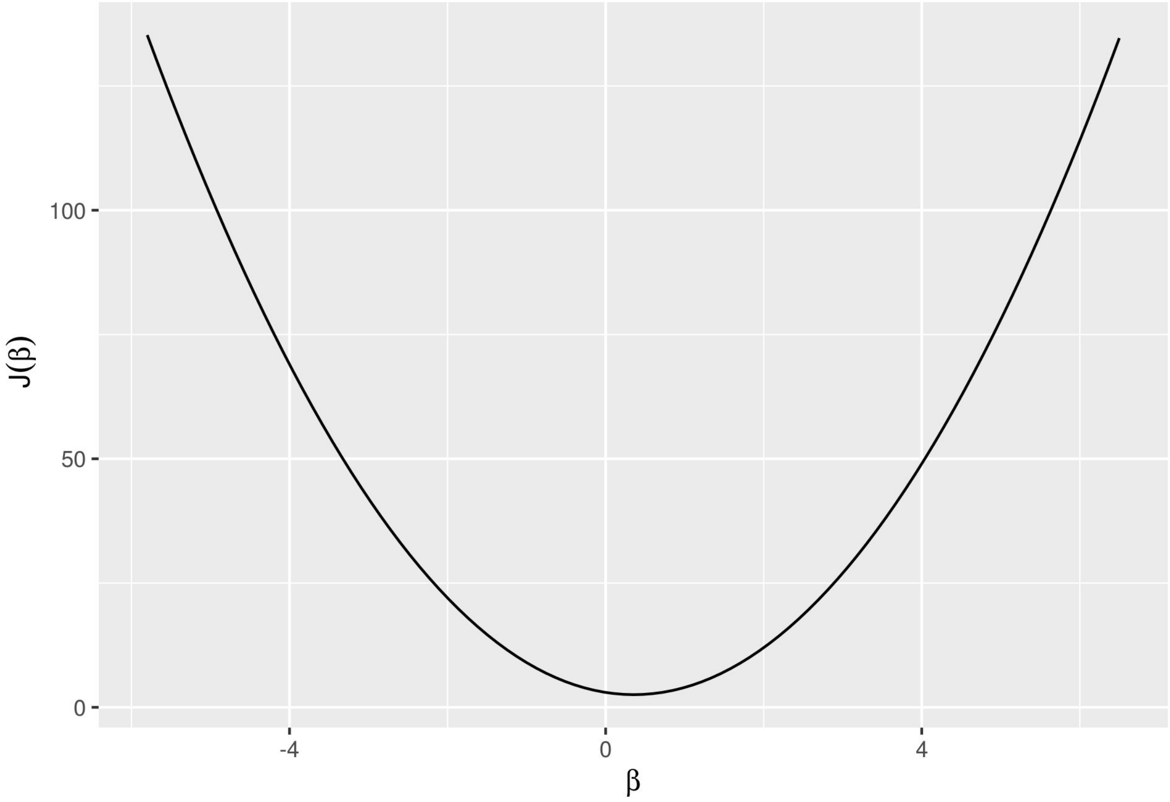
- minimise the **loss (cost) function**

$$J(\beta) = \frac{1}{2n} \sum_{i=1}^{n} \left(\beta_i X_i - y_i\right)^2$$

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

modified (normalized) RSS function

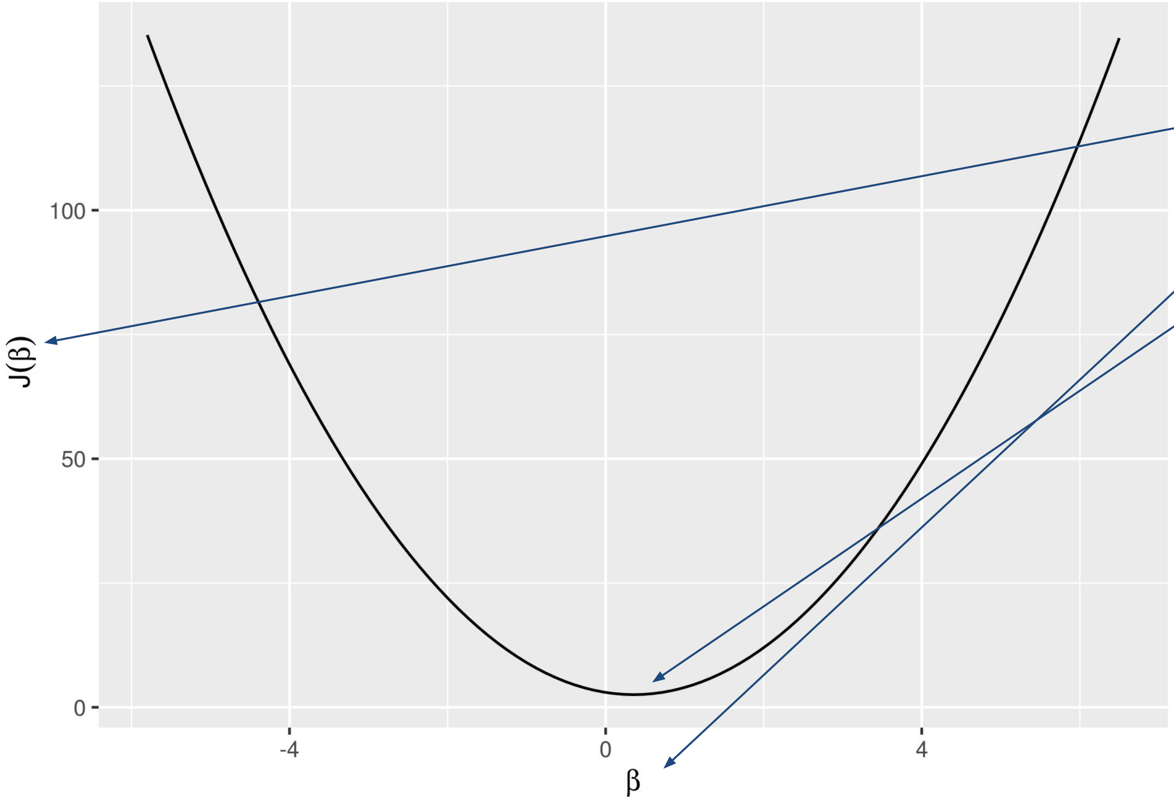
Minimise the loss function



Simple linear regression (1 parameter):

$$y = \beta \cdot x$$

Minimise the loss function

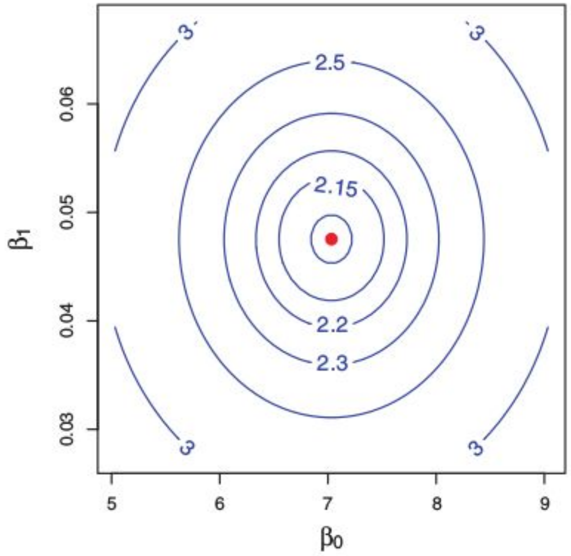


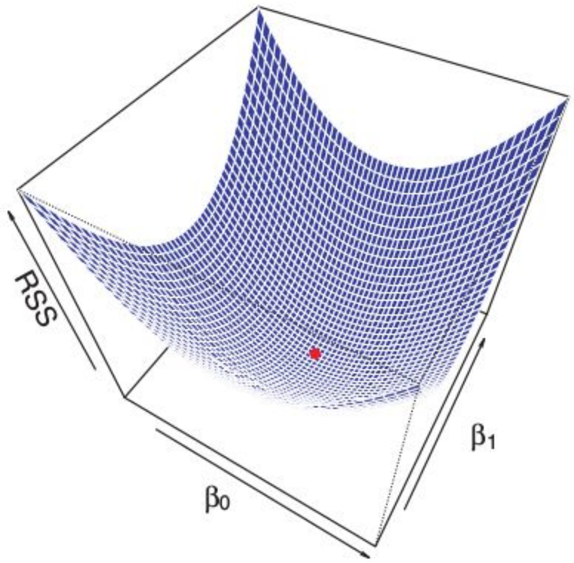
1. loss function
2. model parameters
3. minimum

Simple linear regression (1 parameter):

$$y = \beta \cdot x$$

Minimise the loss function

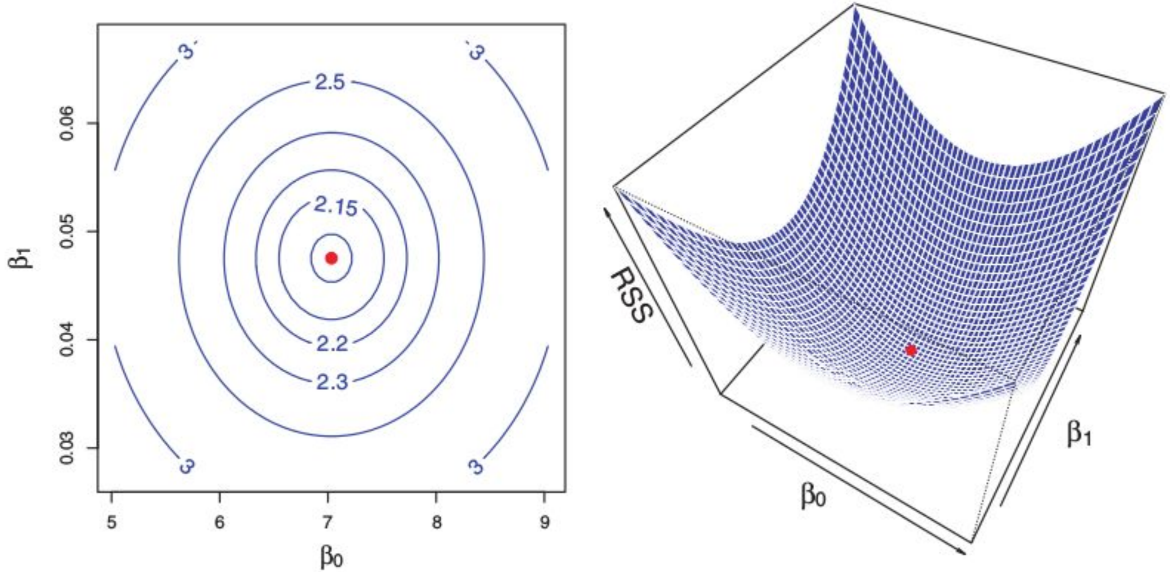




Multiple linear regression (e.g. 2 parameters):

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

Minimise the loss function



Multiple linear regression (e.g. 2 parameters):

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

Multiple linear regression (> 2 parameters):

→ m-dimensional hyperspace

Minimise the loss function

- Demonstration 1.1
- Exercise 1.1

→ 1.introduction_to_ml.Rmd

Minimising the cost function

- the defined cost function is **convex** (it has a minimum!)
- we saw an empirical approach to finding the minimum (manually try some values for the parameters) and the least squares approach

how do we minimise the cost function in machine learning?

Minimising the cost function

- 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

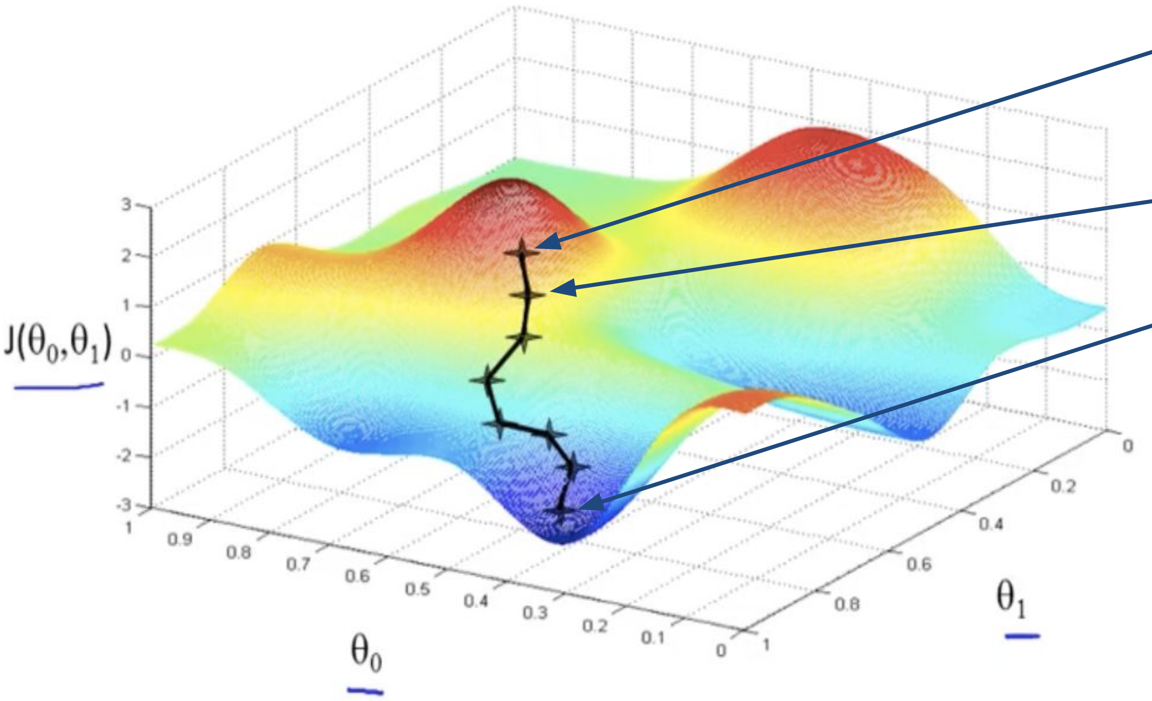
Loss function: finding the minimum?

Gradient Descent:

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

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)

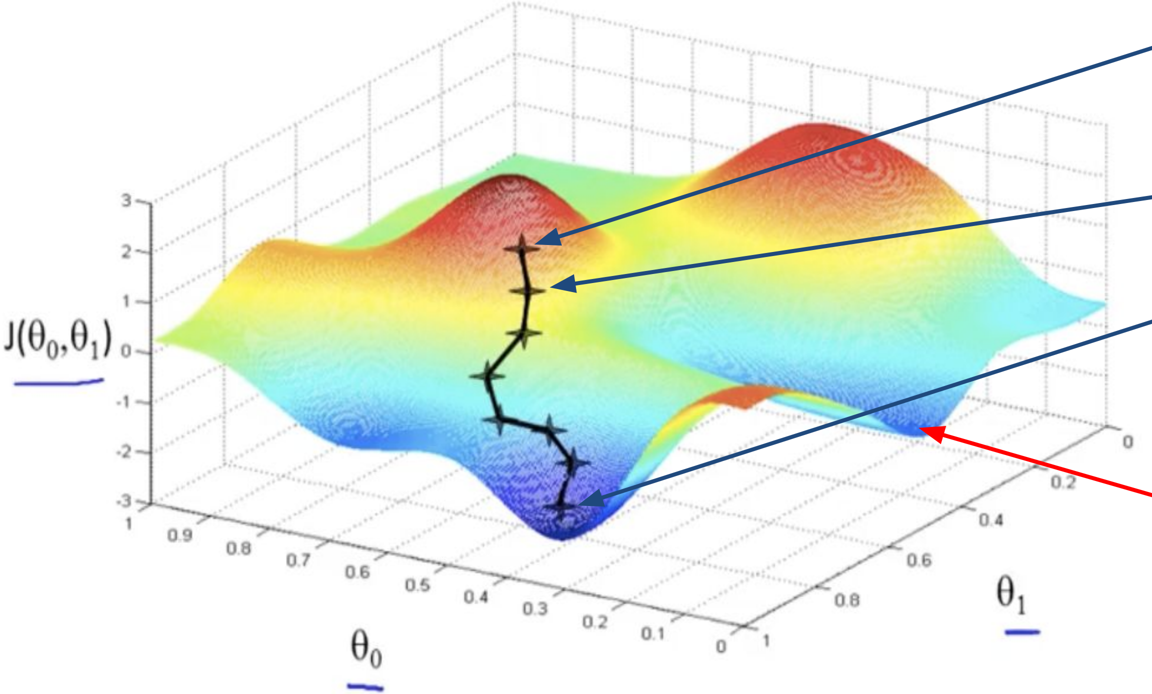
Gradient descent



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

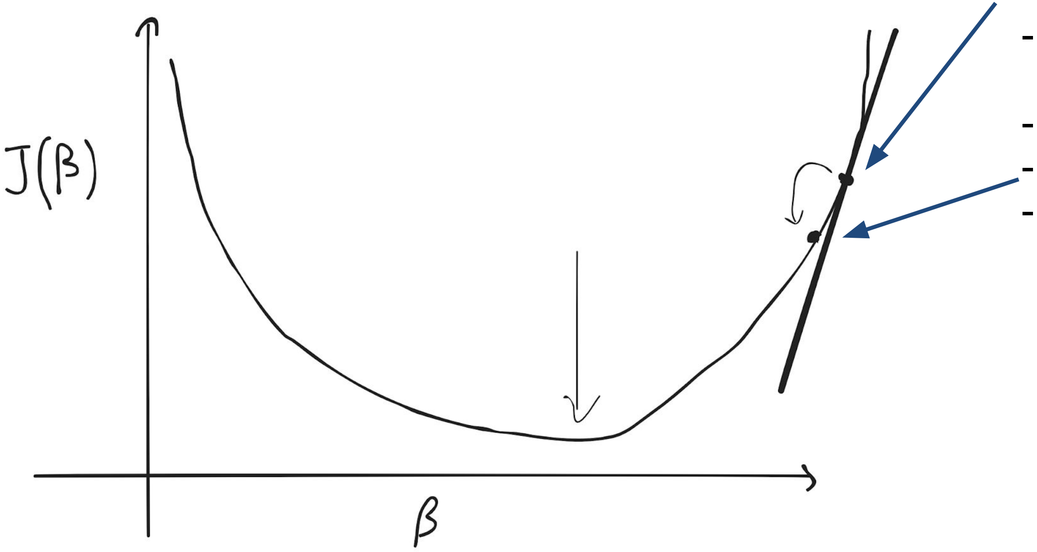
$$\beta_j := \beta_j - \alpha \frac{\partial}{\partial \beta_j} J(\beta)$$

assignment operator

learning rate (size of the steps)

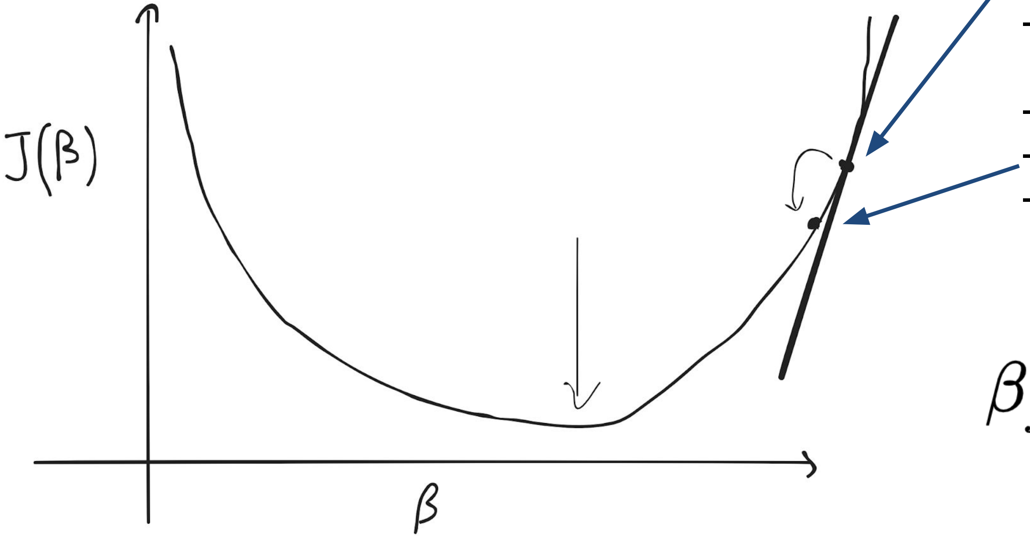
Partial derivative of J(**β**) with respect to $\boldsymbol{\beta}_j$

Gradient descent



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

Gradient descent

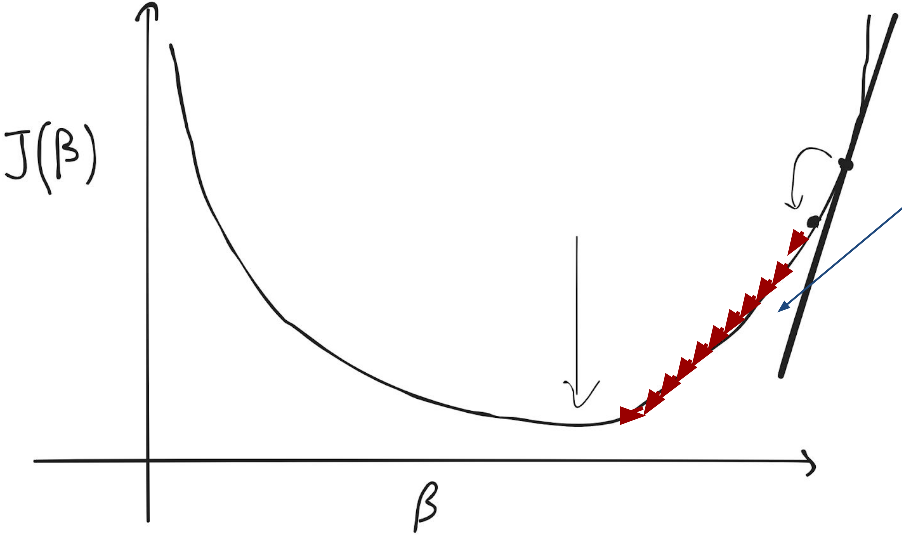


- starting point (initial value for β)
- calculate the (partial) derivative in that point
- → positive slope
- update the value for β
- repeat

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

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

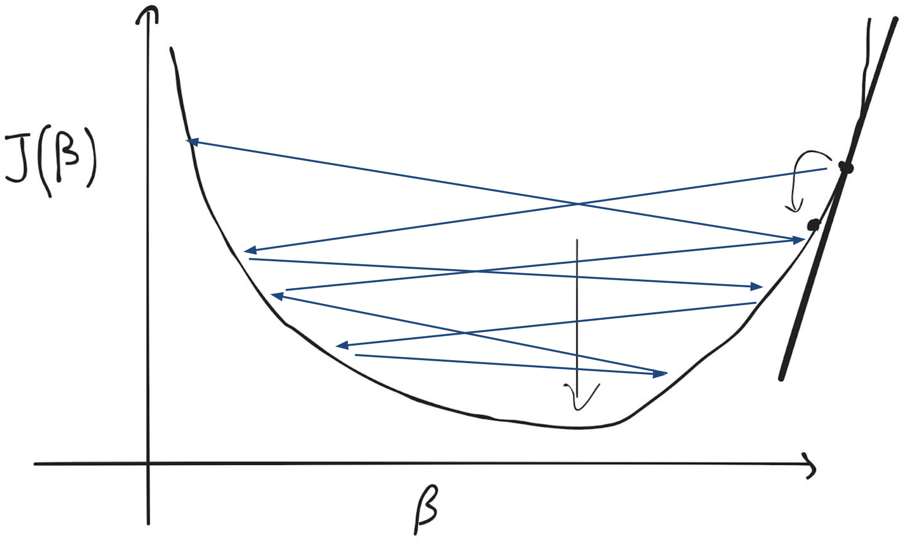
Gradient descent



- 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

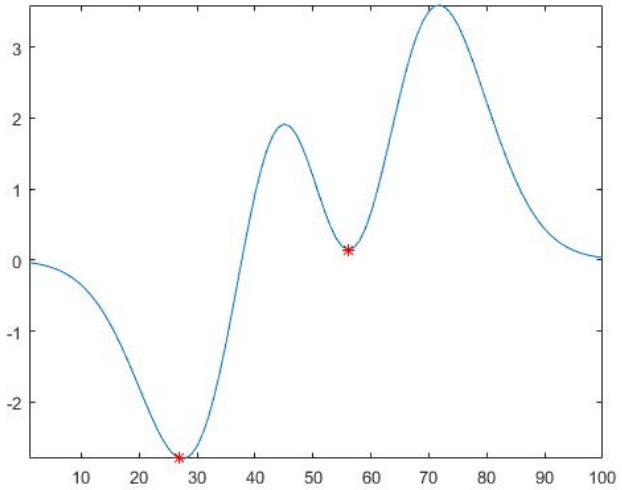


- **α** controls the size of the updating step
- large **α** → overshooting: failure to converge

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

Gradient descent - recap

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

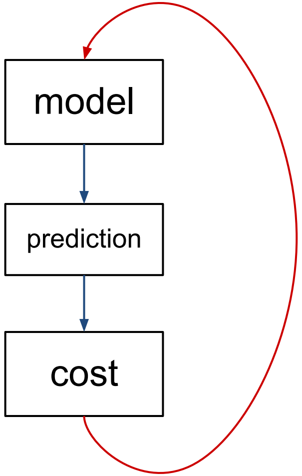


Linear regression - recap

1) $y = X \cdot \beta + e$

2) $\hat{y} = X\hat{\beta}$

3) $J(\beta) = \frac{1}{2n} \sum_{i=1}^{n} \left(y_i - \hat{\beta}_i X_i \right)^2$



[minimise J(B) - take derivatives - and update parameters]

Take away message

- **linear regression** from the machine learning perspective →a **predictive machine**
- to be able to make predictions, we first need to **estimate parameter coefficients**
- define a **loss function** and then use **gradient descent** to **minimize it**
- partial derivatives are used to **update** the values of the **parameters**
- **gradient descent** is a general method to minimise the loss (cost) function for a variety of machine learning models

Model evaluation

- we have our model
- we have estimated the parameters (coefficients) of the model
- we can now get predictions from our predictive machine

Model evaluation

- we have our model
- we have estimated the parameters (coefficients) of the model
- we can now get predictions from our predictive machine

→ how good is our model?

(root) Mean squared error (MSE)

$$MSE = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2$$

- average squared difference between predictions and observations

$$RMSE = \sqrt{MSE}$$

- on the same scale as the target variable

Mean absolute error (MAE)

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - f(x_i)|$$

- less sensitive to outliers

and the normalized version:

$$NMAE = \frac{MAE}{\bar{y}}$$

Correlations

- **Pearson's** linear correlation coefficient: $\rho_{y,\hat{y}}$

- **Spearman's** rank correlation coefficient: $\rho_{ry,r\hat{y}}$

rank variables!

Measuring performance

- Demonstration 1.2
- Exercise 1.2

→ introduction_to_ml.Rmd