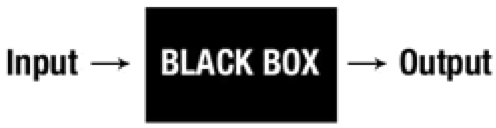
Material Summary: Regression Models

1. Problem Overview

1.1 Data Modelling

- As part of the data science process, we want to get a clear idea of what processes generate our data
    - **Scientific method**: Form a hypothesis and test it
    - Extension: Find a way to understand what's in the data
        - We already did this a lot of times: "mental models" captured our ideas
- A stricter way of modelling
    - Treat the data generating process as a function
        - "Black box"



    - Make some assumptions
    - Create a simplified version of reality under your assumptions
    - Check your model against reality
        - ⇒ Create better and more complex models

1.2 A Quick Peek at Machine Learning

- Machine learning is "**making computers learn with experience, without being explicitly programmed**"
    - Similar to how humans learn
- It's all about models
    - ML follows the same processes as we're going to do
    - ML algorithms are basically "function approximations"
        - Each algorithm does its own thing, i.e., has different assumptions, scope and performance
- It's also about selecting the best model
    - There are many "**helper algorithms**" to do so – either fully automated or semi-automated
        - Visualization algorithms
        - Fine-tuning algorithms
        - Model selection algorithms
- There are a lot of classes of problems
- The most used two
    - **Regression** – model a function which returns a number (i.e., returns a continuous variable)
        - Example: predict the temperature tomorrow
    - **Classification** – model a function which tries to differentiate between two (or more) predefined types of things
        - Example: predict if an image is of a cat or not
- The essence: once we assume a model, **we can make predictions** about function outputs
    - Thus, we can capture patterns in an otherwise unpredictable world

2. Linear Regression

1.1 Linear Regression Intuition

- Regression – predicting a continuous variable
- Problem statement
    - Given pairs of $(x; y)$ points, create a model
        - Under the assumption that y depends **linearly** on x (and nothinag else)

- Linear regression model
  - $y = ax + b$
    - a, b – unknown parameters
    - Example: $y = 2x + 3$
  - Real case: **we have many sources of error**
    - So, the relationship we observe, cannot be perfect
    - There is some noise added to our data
      - $y = ax + b + \varepsilon, \varepsilon$ – noise
    - We **don't want** to model the noise, only the "useful function"

1.2 Generating Data Points

- Generating a few "**ideal**" data points is easy

```
x = np.linspace(-3, 5, 10)
y = 2 * x + 3
plt.scatter(x, y)
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```

- Adding noise – draw from a random distribution

```
y_noise = np.random.normal(size = len(y))
y_with_noise = y + y_noise
plt.scatter(x, y_with_noise)
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```

- If we want, we can even configure the "**size**" of our noise
  - More noise = worse data = less accurate predictions

1.3 First Attempt at Modelling

- We know the process was linear
  - Why don't we simply guess a few functions?
    - Remember: what we need to know are the parameters a and b

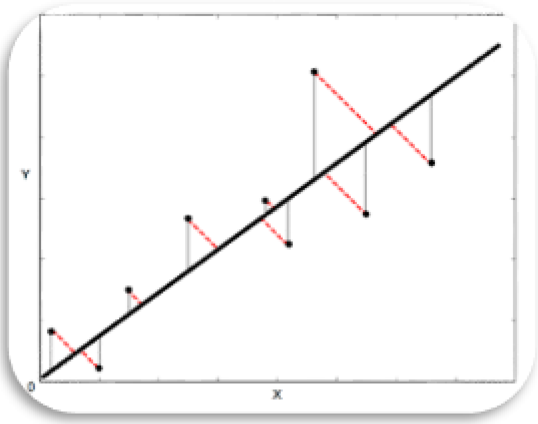
```
for y_guess in [3 * x + 8, 4 * x + 3, -2 * x]:
  plt.scatter(x, y_with_noise)
  plt.plot(x, y_guess)
  plt.show()
```

  - We can see that some functions perform much better than others
  - Idea: the best function lies "**closest**" to all points
  - Meaning
    - Try to measure the distances from all points to the line
    - See when these distances are smallest
      - This will be the best line

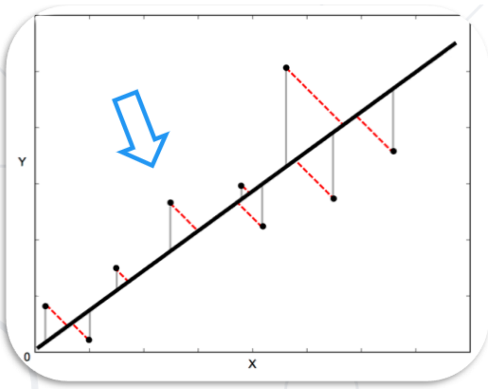
1.4 Distances

- By definition, the distance from a point A to the line l is measured on the perpendicular from A to l
  - Red dashed lines
  - This is correct but very computationally expensive
- Another approach: consider vertical distances
  - Gray solid lines
  - Equivalent measures (for our purposes)

- You can prove it to yourself



- Look at a point and its projection
  - x-coordinate: the same
  - y-coordinate
    - Point: we know it from the start
    - Projection: we can calculate it
- Calculating the projection $\tilde{y}$
  - It's whatever the model function produces for x
  - $\Rightarrow \tilde{y} = ax + b$
- Distance becomes a very simple difference
  - $d = y - \tilde{y}$
    - But… now distances can be negative



- To make distances positive, we can do a lot of things
- Simplest: take the absolute value
  - This is used sometimes
    - Mean absolute error, MAE
  - Although it works quite well, there are a few problems with it
  - E.g. $d = 0$ at the "**perfect**" line
- Better: square the distance
  - It's also non-negative everywhere but…
    - Is almost always > 0
    - Emphasizes bigger errors more (can be good or bad)
  - This is called mean square error (**MSE**)
- New definition of distance
  - $d = (y - \tilde{y})^2$

1.5 Cost Function

- We want to somehow account for all points

- We can simply sum all distances to get a measure of "the total distance" from all points to the line
- Since we can have 4, 10, 100 or 10^9 points, we also need to normalize the error

- The sum of distances now becomes
  - $J = \frac{1}{n}\sum_{i=1}^{n}(y_i - \tilde{y_i})^2$
  - This is what we call our **total cost function**
    - **Beware of confusing terms: d is usually called a "loss function", while J is the "(total) cost function"**
  - This is an estimation of the total distance
  - **Minimizing this function will produce the best line**

1.6 Calculating the Cost Function

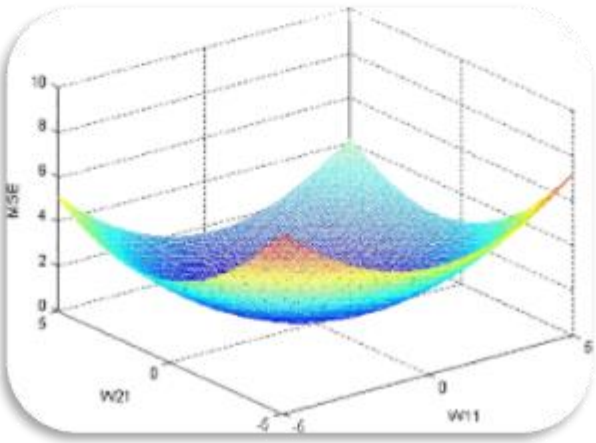
- The code is pretty simple
- Given points $x,\ y$ and a line with parameters a, b we can simply substitute in the formula above
  - First, for each x, compute $\tilde{y} = ax + b$
  - After that, compute the distances $(y - \tilde{y})^2$
  - Return the sum of all distances, divided by the number of points

```
def calculate_loss(x, y, a, b):
    y_predicted = a * x + b
    distances = (y - y_predicted) ** 2
    return np.sum(distances) / len(x)
```

  - Now that we have a quantifier, we can go back to our three guessed lines and calculate their loss functions
    - It will give us the intuition of what we're dealing with

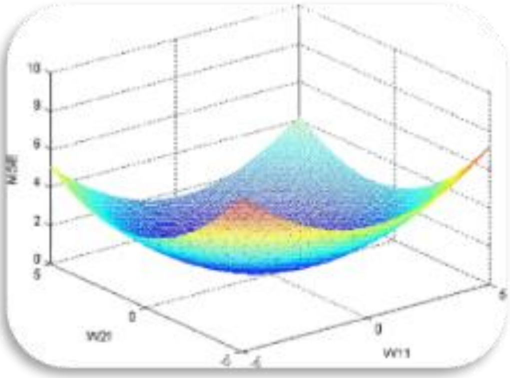
1.7 Inspecting the Cost Function

- Note that J does not depend on x and y
  - x and y are already fixed – we don't touch the data at all when we try to model it
  - $\Rightarrow J$ depends only on the line parameters $a,\ b$
    - In math jargon, J is a function of a and b: $J = f(a, b)$
- Also note the form of J: it's $(\cdots)^2$
  - This is a paraboloid (3D parabola)
  - See how varying a and b gives us a different output number for J
  - It has exactly one min value
    - And we can see it
  - Our task: find the parameters $a,\ b$ which make J as small as possible



1.8 Minimizing the Cost Function

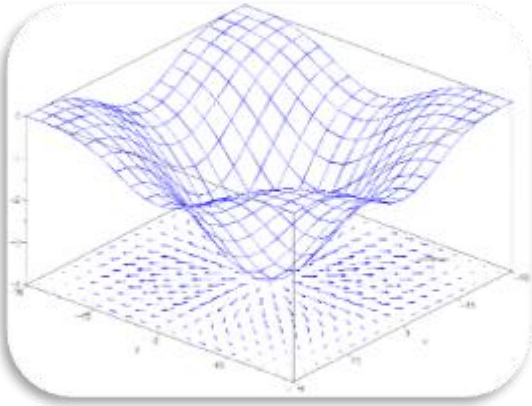
- Intuition
    - If the plot was a real object (say, a sheet of some sort), we could slide a ball bearing on it
    - After a while, the ball bearing will settle at the "**bottom**" due to gravity
    - We could measure the position of the ball and that's it :)
- More "nerd speak"
    - This is the same task – we have a gravity potential energy that the ball tries to minimize
        - When it's minimal, the ball remains in stable equilibrium



- Turns out, we can also do this using calculus
    - In many dimensions
- We can find the optimal parameters right away
    - Because the function is really simple
    - But we'll stick to another approach because this is what is useful for all other ML tasks
- We'll try to replicate the example with the ball
    - Basically, we'll try to slide (descend) over the function surface until we reach the minimum
    - This method is called **gradient descent**

1.9 Gradient Descent

- We know what **descent** is
    - How about **gradient**?
- The gradient (let's call it g for now) is a vector function
    - Like J, g accepts two values a and b
    - g returns a vector which shows where **the steepest ascent** is
    - g is all arrows on the picture
    - Interpretation
        - The length of the vector tells us how steep the maximum is
            - Long vector = very, very steep; short vector = relatively flat
        - The direction of the vector tells us where to go in order to get there
        - Gradients will almost work
        - Except they show us the highest point, and we're looking for the **lowest one**
        - Solution: just take the negative gradient $-g$
        - Ascending on $-g$ is the same as descending on g
        - This is good now, but how is the gradient defined?
        - We saw from the picture that it's related to a function
        - The gradient of a function $J(a, b)$ is a vector $g(a, b)$ with the following components
        - $g_a = \frac{\partial J}{\partial a}, \; g_b = \frac{\partial J}{\partial b}$



- The ∂ symbol means "**partial derivative**"
- If you don't understand this, you only need to know that partial derivatives are quite easy to calculate

- Remember that $J = \frac{1}{n}\sum(y_i - \widetilde{y_i})^2$
  - We can prove that
  - $\frac{\partial J}{\partial a} = -\frac{2}{n}\sum x_i(y_i - \widetilde{y_i}); \frac{\partial J}{\partial b} = -\frac{2}{n}\sum(y_i - \widetilde{y_i})$
- This can be implemented easily

```
a_gradient = -2 / len(x) * np.sum(x * (y - (a * x + b)))
b_gradient = -2 / len(y) * np.sum(y - (a * x + b))
```

  - Note how this code makes use of numpy and its extremely easy operations on arrays
- Now, if we know $x,\ y,\ a, b$ we can calculate the gradient vector
  - You'll also see the gradient of J being denoted as ∇J
    - This is simply math notation
- Let's now get to the real descent
- Iterative algorithm – perform as long as needed
  - Start from some point in the $(a; b)$ space: $(a_0; b_0)$
  - Decide how big steps to take: number α
    - Called "**learning rate**" in ML terminology
- Use the current a, b and x, y to compute ∇J
  - $-\nabla J_a$ tells us how much to move in the a direction in order to get to the minimum
  - Similar for $-\nabla J_b$
- Take a step with size α in each direction
  - $a_1 = a_0 - \nabla J_a; b_1 = b_0 - \nabla J_b$
  - $(a_1; b_1)$ are the new coordinates
- Repeat the two preceding steps as needed
  - Usually, we do this for a fixed number of iterations

1.10 Gradient Descent Code

- Gradient descent step

```
def perform_gradient_descent(x, y, a, b, learning_rate):
    a_gradient = -2 / len(x) * np.sum(x * (y - (a * x + b)))
    b_gradient = -2 / len(y) * np.sum(y - (a * x + b))
    new_a = a - a_gradient * learning_rate
    new_b = b - b_gradient * learning_rate
    return (new_a, new_b)
```

- Entire process: 1000 iterations

```
model_a, model_b = -10, 20 # Start points; can be anywhere
alpha = 0.01 # Learning rate
for step in range(1001):
    model_a, model_b = perform_gradient_descent(
        data_x, data_y, model_a, model_b, alpha)
    if step % 100 == 0:
        error = calculate_loss(data_x, data_y, model_a, model_b)
        print("Step {}: a = {}, b = {}, J = {}".format(
            step, model_a, model_b, error))
print("Final line: {} * x + {}".format(model_a, model_b))
```

1.11 Results and Interpretation

- Going through the entire process, we now have a line $y = ax + b$ which describes our data in the best way
  - We could plot the evolution of J to see that it always decreases
    - If it doesn't, this indicates a problem with our algorithm
- This was a lot of work
  - Thankfully, there are libraries that hide away all that complexity for us
  - scikit-learn is the most popular of them
    - Arguably, the most popular of the scikits as well
  - Also, generalizes trivially to more dimensions

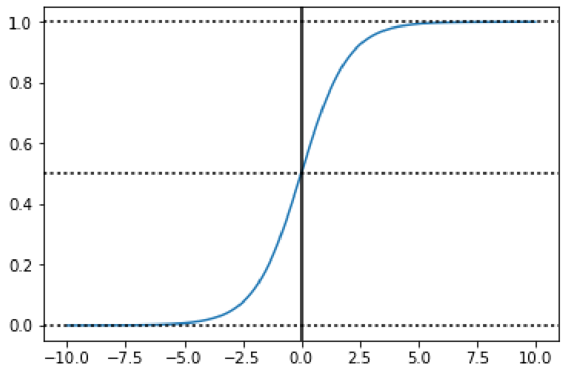
```
from sklearn.linear_model import LinearRegression

model = LinearRegression()
model.fit(data_x.reshape(-1, 1), data_y)
print(model.coef_, model.intercept_)
```

3. Logistic Regression

1.1 Logistic Regression

- The name is a bit misleading
  - This is used for classification
- Two classes, 0 and 1
  - Can generalize to more classes using a "trick"
- A function to discriminate: **sigmoid**
  - $x < 0 \Rightarrow y = 0; x > 0 \Rightarrow y = 1$
  - We'll look at the implementation later
- Loss function
  - Similar to the linear regression cost function
- Gradient descent
- Usage in scikit-learn



```python
from sklearn.linear_model import LogisticRegression
```

1.2 Overview of the Process

- We dealt mainly with the modelling part
  - It's only a piece of the puzzle
- Many algorithms to choose from
  - Each with its own features and drawbacks
- Many ways to test that we're on a correct path
- The end result depends mainly on
  - The person working on the dataset
  - The data quality
  - Less prominent but also worth mentioning
    - Data size (bigger is usually better)
    - Data acquisition and sampling processes