Datascience 4.0

Introduction to Machine learning in Python

contact info on next slide

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Before we start.. Who we are?

- Last year Nemanja Micovic
  `nemanja_micovic@matf.bg.ac.rs`
- This year me, Milan Cugurovic
  `milan_cugurovic@matf.bg.ac.rs`
- There are a lot of as at:

Faculty of Mathematics Machine Learning Group

- Based at Faculty of Mathematics
- Includes researchers, students and particioners from various research institutions and leading IT companies
- Led by proffessor Mladen Nikolic [1]
- Lectures/talks and practical sessions are held on every 2 weeks
- MATF Machine Learning Group: `machinelearning.math.rs`
    - Feel free to visit our sessions and join in!

[1] web: poincare.matf.bg.ac.rs/∼ *nikolic*, *email* : *nikolic@matf.bg.ac.rs*

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About Machine learning

- Field of Artificial Intelligence
- Very active research field today
- Has acomplished amazing results
- Built on multiple mathematical disciplines

About Machine learning

Famous definition by Tom M. Mitchell

- A computer program is said to learn from **experience E** with respect to some class of **tasks T** and **performance measure P** if its performance at tasks in T, as measured by P, improves with experience E

What is the goal of Machine learning?

- To create models able to generalize
- To give a theoretical base of generalization
- To solve a whole class of problems difficult for deterministic algorithms

Some result of Machine learning

- 1992 - TD-Gammon, computer program develoepd by Gerald Tesauro able to play backgammon
- 2011 - IBM's Watson wins in quiz *Jeopardy!*
- 2012 - Google X creates system able to recognize cats on video recordings
- 2015 - Classification error for images reduced to 3.6% (5-10% is the error made by humans)
- 2016 - Google creates AlphaGo, agent able to play Go who beats the world champion 4:1
- 2017 - AlphaGo plays against its 2016 version and wins 100/100 games
- October 2017 - AlphaGo Zero learnt to play the game of Go simply by playing games against itself, starting from scratch (40 days)

Applications of Machine learning

- Autonomous driving
- Bioinformatics
- Social networks
- Algorithm porfolio
- Playing video games
- Image classification
- Recognizing handwritting
- Natural language processing
- Generating optimization algorithms [Andrychowicz et al., 2016]
- Generating images

- Computer vision
- Detecting credit card frauds
- Data mining
- Medical assistance and assesment
- Marketing
- Targeted marketing
- Controlling robots
- Economy
- Speach recognition
- Recommendation systems

But why is it so successful and popular today?

- There is serious amount of mathematics behind [Murphy, 2012, Bishop, 2006, Hastie et al., 2001, Shalev-Shwartz and Ben-David, 2014, Vapnik, 1995]

$$
\begin{gathered}
P(\sup_{f\in\mathcal{F}}(R(f)-E(f))>\varepsilon) \leq \\
2P(\sup_{f\in\mathcal{F}}(E'(f)-E(f))>\varepsilon/2) = \\
2P\left(\sup_{l\in\mathcal{L}_{z_1,\dots z_N,z'_1,\dots,z'_N}}\left(\frac{1}{N}\sum_{i=N+1}^{2N} l_i-\frac{1}{N}\sum_{i=1}^{N} l_i\right)>\varepsilon/2\right) \leq \\
2\sum_{l\in\mathcal{L}_{z_1,\dots z_N,z'_1,\dots,z'_N}} P\left(\frac{1}{N}\sum_{i=N+1}^{2N} l_i-\frac{1}{N}\sum_{i=1}^{N} l_i>\varepsilon/2\right) = \\
2\sum_{l\in\mathcal{L}_{z_1,\dots z_N,z'_1,\dots,z'_N}} P\left(\frac{1}{N}\sum_{i=N+1}^{2N} l_i-R(f)+R(f)-\frac{1}{N}\sum_{i=1}^{N} l_i>\varepsilon/2\right) \leq \\
2\sum_{l\in\mathcal{L}_{z_1,\dots z_N,z'_1,\dots,z'_N}}\left(P\left(\frac{1}{N}\sum_{i=N+1}^{2N} l_i-R(f)>\varepsilon/2\right)+P\left(R(f)-\frac{1}{N}\sum_{i=1}^{N} l_i>\varepsilon/2\right)\right) \leq \\
2\sum_{l\in\mathcal{L}_{z_1,\dots z_N,z'_1,\dots,z'_N}}(\exp(-N\varepsilon^2/2)+\exp(-N\varepsilon^2/2)) = \\
4\sum_{l\in\mathcal{L}_{z_1,\dots z_N,z'_1,\dots,z'_N}}\exp(-N\varepsilon^2/2) =
\end{gathered}
$$

Figure: *M. Nikolic, Machine learning*

But why is it so successful and popular today?

- Don't be afraid, today we talk ML introduction without so much math stuff
- Big amounts of data
- We also have graphical cards with thousands of processors
  - They allow us to get extremely high levels of parallelization
- Industry and academia complement each other
  - Our meeting here today is the evidence of that :)

Types of machine learning

- Supervised learning
- Unsupervised learning
- Reinforcement learning

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Supervised learning

- Our main focus today
- We are given attributes $x_1, x_2, ...x_n$
- Using them, we need to predict target variable y
- We want to create a model that will approximate $f(x_1, x_2, ..., x_n) = y$
- So we need to create a function $f' \approx f$

Regression

- Target variable y is continuous
- Trying to predict temperature (y) using pressure (x)

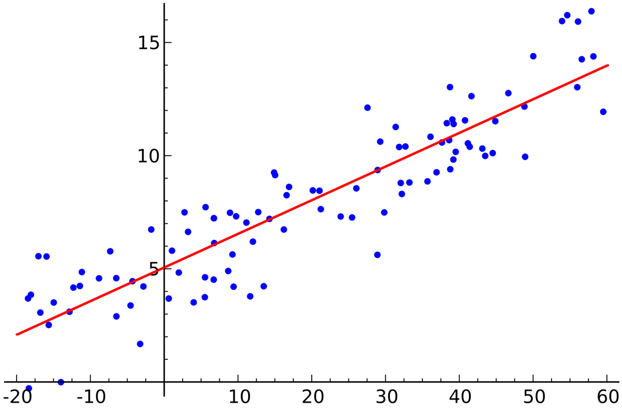

Figure: Linear regression (wikipedia)

Classification

- Target variable y is discreete
- Trying to predict gender (y) using weight (x_1) and height (x_2)

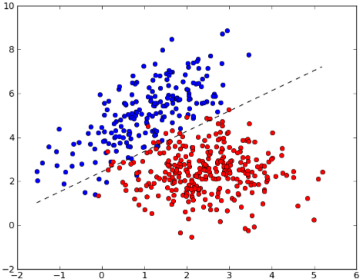

Figure: Classification example 1

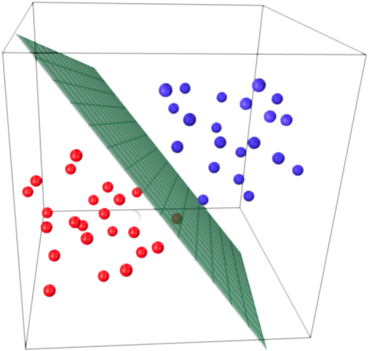

Figure: Classification example 2 (Sachin Joglekar's blog)

Linear regression

- We construct the model in the following form:

$$f_w(x) = w_0 + w_1x_1 + w_2x_2 + \ldots + w_nx_n$$

$$f_w(x) = w_0 + \sum_{i=1}^{n} w_ix_i$$

- We calculate model accuracy using the following formula[2]:

$$Loss(w) = \frac{1}{N}\sum_{i=1}^{N}(Y_i - f_w(X_i))^2$$

[2] Which is usually called *Mean squared error*

Linear regression - minimization problem

- We have lots of different models
- Every tuple $(w_0, w_1, \ldots, w_n)$ defines a different model
- What is the *best*[3] one?
- Model that makes the smallest mistake on the data we have is *generally* great for us!
- But how do we find such model?

[3] Using term *best* is tricky here, but let's stick with it for now.

Linear regression - minimization problem

- Actually, that's not so difficult to do, we can derive the following equation with a bit of algebra
- Let's assume for simplicity that we have only one attribute x
- x_i is the i-th dataset element
- y_i is the target value for i-th dataset element

$$w = (X^\top X)^{-1} X^\top Y$$

$$X = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \dots & \\ 1 & x_N \end{bmatrix} \quad Y = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_N \end{bmatrix}$$

Linear regression - minimization problem

So what's the problem then?

- Matrix multiplication - lowest complexity so far $O(n^{2.373})$ [Gall, 2014]
- Matrix inverse - lowest complexity so far $O(n^{2.373})$
- Storing big[4] matrix $n \times m$ in memory: $O(nm)$

[4] non sparse, we can store sparse matrices more efficiently

Linear regression - gradient descent

- How does our error function generally look?
- Which point has the smaller error, A or B?

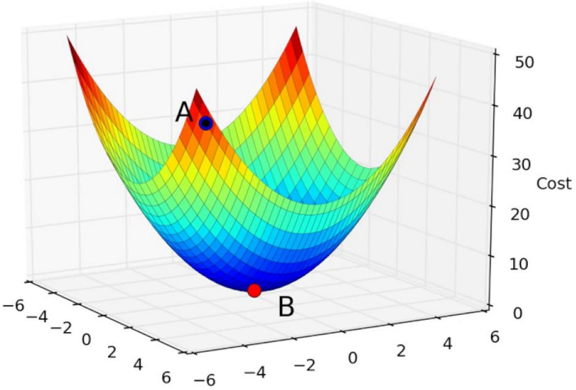

Figure: An example of the error function

Linear regression - gradient descent

Can we somehow *descend* into the function minimum?

- Yes!

But how?

- Calculate gradient of the error function with respect to w
- This vector *points* into the direction of the fastest function growth

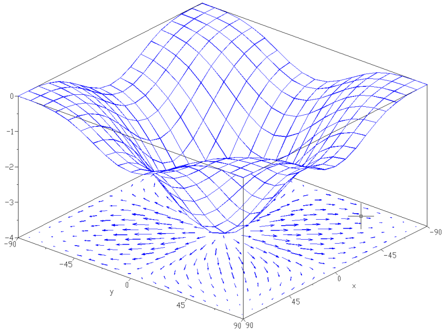

Figure: Blue arrows represent function gradients

Linear regression - gradient descent

Gradient descent algorithm:

- Repeat until convergence
  - $w_j := w_j - \mu \frac{\partial}{\partial w_j} Loss(w), \ j \in \{1, 2, ..., n\}$

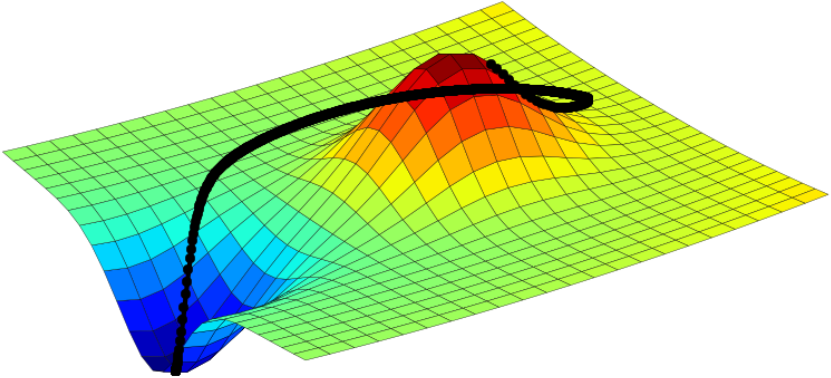

Figure: An example of the steps made by the gradient descent algorithm (github.com/joshdk)

Linear regression - (R)MSE

- Mean

$$\bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i$$

- Mean squared error (MSE)

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - f_w(x_i))^2$$

- Root mean squared error (RMSE)

$$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - f_w(x_i))^2}$$

Linear regression - R^2

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(f_w(x_i) - y_i)^2}{\sum_{i=1}^{N}(\bar{y} - y_i)^2}$$

- It could be interpreted as change in the target value y which our model is failed to explain by changing the variable x.
- Errors on which we define variance and R^2:

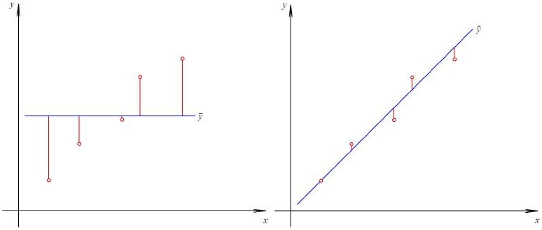

Figure: M. Nikolic, Machine learning

Linear regression - R^2

- Coefficient of determination, mostly called R^2
- It is the **proportion of the variation** in the **dependent** variable that is predictable from the **independent** variable(s)
- We can say that it determines how much of variability has our model **managed to explain**
- What is the minimum of R^2?
- What is the maximum of R^2?

Linear regression - coding time

- Let's code linear regression in `scikit-learn`

Linear regression - overfitting

- Analyze the following images[5]

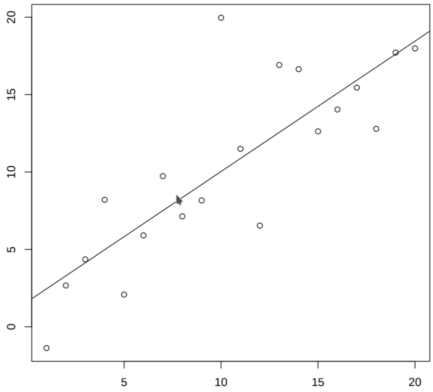

Figure: Linear regression 1

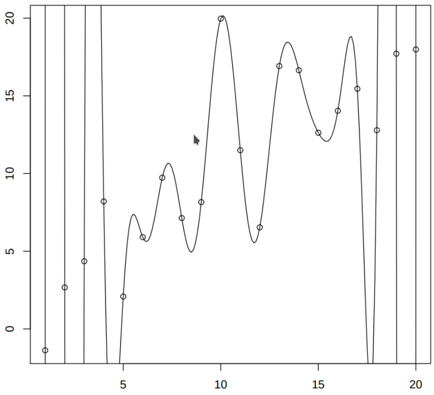

Figure: Linear regression 2

[5]Images taken from book *P. Janičić, M. Nikolić, Artificial Intelligence*

Linear regression - underfitting and overfitting

- Given 3 models, which one do you prefer in respect to black points (dataset samples)?

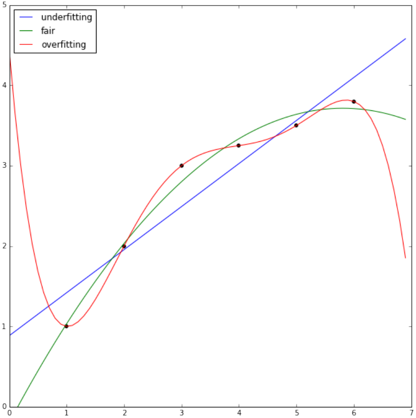

Figure: Examples of underfitting and overfitting

Linear regression - underfitting and overfitting

Underfitting

- A situation in which our model is not flexible enough in order to capture the essence of a phenomena

Overfitting

- A situation in which our model is too flexible and it fits too well towards the training data we feed it

Linear regression - underfitting and overfitting

- If $MSE_{train} = 0$, are we *always* happy?

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- If we have overfitting, which one will be bigger, MSE_{train} or MSE_{test}?
  - $MSE_{test} > MSE_{train}$

Linear regression - underfitting and overfitting

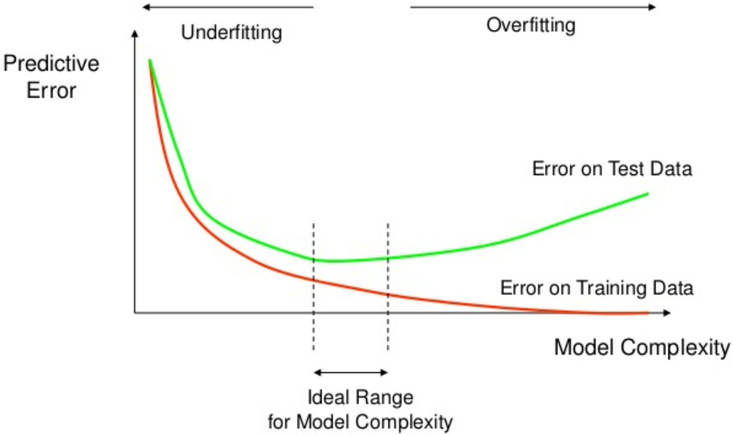


Figure: Graph showing the difference between underfitting and overfitting

Linear regression - How to battle underfitting?

- Take a more flexible model
- Instead of $f_w(x) = w_0 + w_1x_1 + w_2x_2$ take $g_w(x) = w_0 + w_1w_2x_1 + w_1^2x_1 + w_2^2x_2$
- Usually easier to solve then overfitting
- There is a wide variety of flexible models, and we can always complicate things[6]

[6] As in life and mathematics...

Linear regression - How to battle overfitting?

Regularization

- It allows us to control model complexity
- Term λ controls the *intensity* of regularization
- There are multiple options to pick from for function Ω
- Interesting tutorial: https://www.analyticsvidhya.com/blog/2016/01/complete-tutorial-ridge-lasso-regression-python/
- We modify the minimization problem into:

$$\min_{w} \frac{1}{N} \sum_{i=1}^{N} (y_i - f_w(x_i))^2 + \lambda \Omega(w)$$

Linear regression - Ridge regularization

- Very commong regularization function
- It forces optimization algorithms not to increase model coefficients too much
- If coefficients get increased, then the sum of their squares rise a lot

$$\Omega(w) = \|w\|_2^2 = \sum_{i=1}^{n} w_i^2$$

- Using ridge, we obtain the following minimization problem

$$\min_w \frac{1}{N} \sum_{i=1}^{N} (y_i - f_w(x_i))^2 + \lambda \sum_{i=1}^{n} w_i^2$$

Linear regression - coding time

- Let's code ridge regression in `scikit-learn` [7]

[7] Challenge: code Lasso Regression, which performs L1 regularization, i.e. adds penalty equivalent to absolute value of the magnitude of coefficients

K-Nearest neighbours (kNN)

kNN

- Simple yet sometimes powerful classification algorithm
- `K` inside name comes from parameter k
- k determines the number of neighbours we check when classifying an instance

kNN

- How much is k?

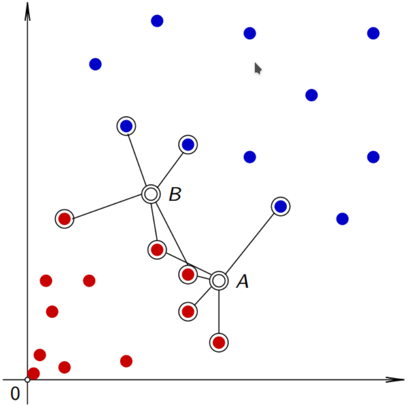
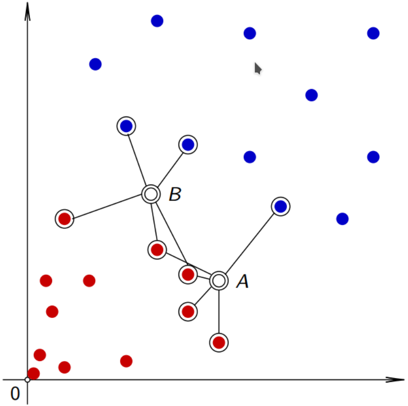


Figure: kNN example (image taken from [Janičić and Nikolić, 2017])

kNN

- How much is k?
  - 5



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kNN

- How much is k?
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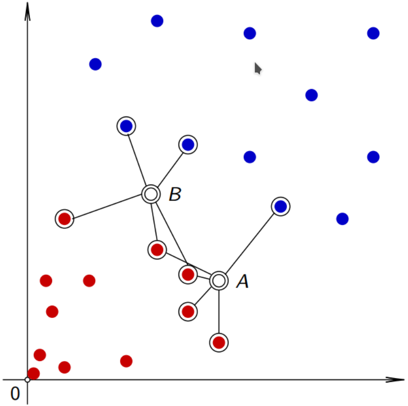
- What is the class of A?



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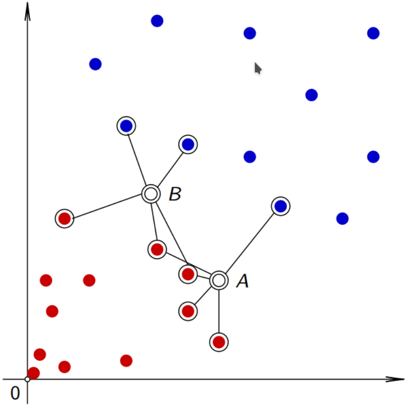
kNN

- How much is k?
  - 5
- What is the class of A?
  - Red



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kNN

- How much is k?
  - 5
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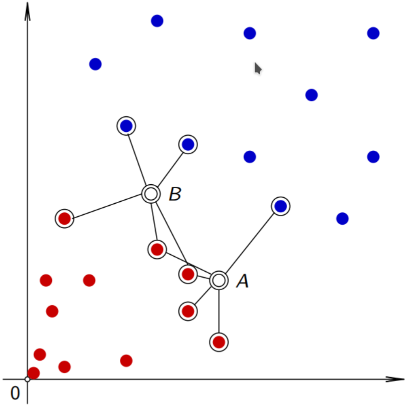
  - Red
- What is the class of B?



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kNN

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  - 5
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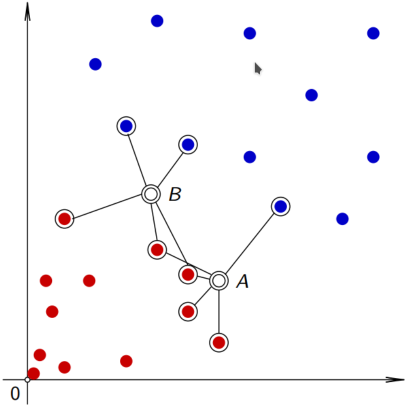

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kNN

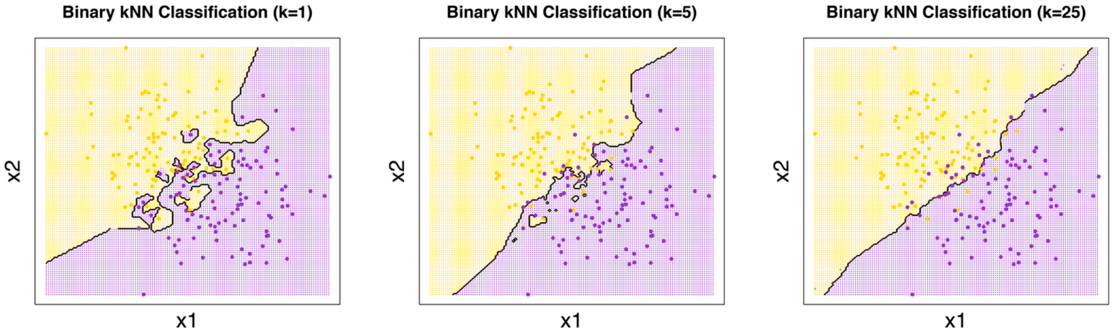

Figure: kNN example (image taken from Burton DeWilde's blog)

kNN

- In linear regression, we represented our model with coefficients w

kNN

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kNN

- In linear regression, we represented our model with coefficients w
- What is the model in the kNN classifier?
  - There is no such thing, we only need to know k
- How do we train the model?
  - We don't, but every time we must calculate neighbours for a new instance

kNN - distances

- There are multiple functions we can use to calculate distances
- Assume we are given points $x = (x_1, ..., x_n)$ and $y = (y_1, ..., y_n)$
- Minkowski

$$\left(\sum_{i=1}^{n}(|x_i - y_i|)^q\right)^{\frac{1}{q}}$$

- Manhattan (q = 1) [8]

$$\sum_{i=1}^{n}|x_i - y_i|$$

- Euclidean distance (q = 2)

$$\sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$$

[8] Taxi metrics :)

kNN - Curse of dimensionality

- Our intuition is bad for high dimensionals spaces
  - $lim_{n \to \infty} \frac{V_{0.99}^n}{V_1^n} = lim_{n \to \infty} \frac{0.99^n}{1^n} = 0$
  - In hd spaces, all dots are far away from center of ball
  - if a point is classified on the basis of close neighbors, close neighbors are expected
- When dimensionality increases, the volume of space increases really fast
- This can make our dataset very sparse (even if it isn't sparse, then our algorithm is very computationally expensive)
- Essentially, we number of dataset instances required increases exponentially with the dimensionality
- This is very bad for kNN

Classification - important metrics

- TP (true positive): those that are positive and our model was correct
- TN (true negative): those that are negative and our model was correct
- FP (false positive): those that are negative and our model was wrong
- FN (false negative): those that are negative and our model was wrong
- *Accuracy*

$$Acc = \frac{TP + TN}{TP + TN + FP + FN}$$

  - Example: only two classes, in one class, 99 instances, in the other only 1 instance. We can achieve impressive score 0.99 just by saying that all instances are from the first class.
    (Credit card detection, tumor detection etc.)

Classification - important metrics

- *Precision*

$$Precision = \frac{TP}{TP + FP}$$

  - The proportion of positive instances in all instances that were declared positive
- *Recall* score

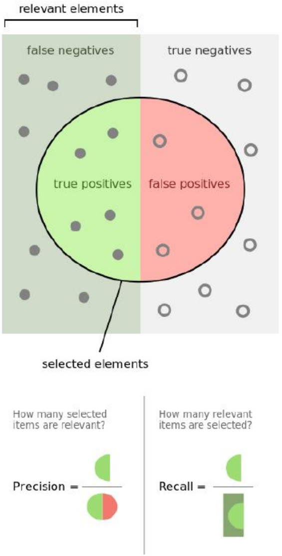
$$Recall = \frac{TP}{TP + FN}$$

  - The proportion of found positive instances in all positive instances
- F_1 score

$$F_1 = 2 * \frac{Precision * Recall}{Precision + Recall}$$

  - If all instances is positive - Recall is max
    If no positive instances - Precision is max

Classifcation - Precision/Recall ilustration



kNN - coding time

- Let's code kNN Classifier in `scikit-learn` [9]

[9] Any idea for kNN Regression?

Logistic regression

Logistic regression

- Classification algorithm
- By design, similar to linear regression
- We want to approximate $p(y|x)$

$$f_w(x) = w_0 + \sum_{i=1}^{n} w_i x_i$$

- $f_w(x)$ is not in interval $[0, 1]$

Logistic regression - sigmoid function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

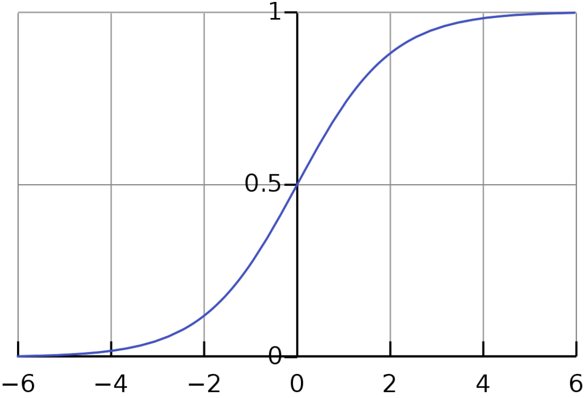


Figure: Graph of the sigmoid function

Logistic regression - loss function

- We define the loss function as following (check [Bishop, 2006, Murphy, 2012] for details)

$$Loss(w) = -\sum_{i=1}^{N} \log p_w(y_i|x_i) = -\sum_{i=1}^{N} [y_i \log f_w(x_i) + (1 - y_i) \log(1 - f_w(x_i))]$$

- Function defined as: $L(u, v) = -u \log v - (1 - u) \log(1 - v)$ is a loss function![10] Why?

[10] Her name is binary crossentropy!

Logistic regression - minimization problem

- We end up with the following minimization problem

$$\min_{w} - \sum_{i=1}^{N} [y_i \log f_w(x_i) + (1 - y_i) \log(1 - f_w(x_i))]$$

- Which is a convex function with a global minimum

Logistic regression - examples

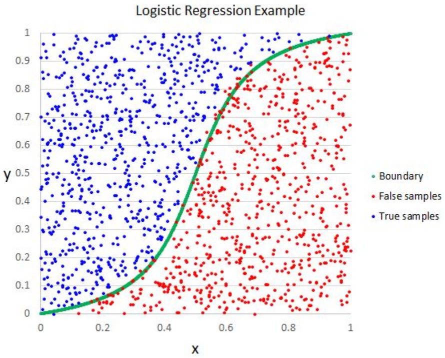


Figure: Example taken from www.helloacm.com

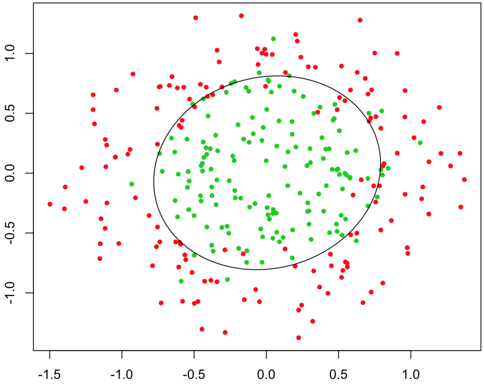


Figure: Example taken from statsblogs.com

Linear regression - coding time

- Let's code logistic regression in `scikit-learn`

Table of contents

Neural Networks - First Look

- Most popular and most appropriate machine learning methods
- As I said before:
  - Medical diagnostic
  - Image recognition and Object detection
  - Autonomous driving
  - NLP (Natural Language Processing)
  - Go, FlappyBird ...
- Five main types:
  - Feed Forward neural network (basic)
  - Convolutional neural network (images)
  - Recurent neural network (memory)
  - Recursive neural network (tree)
  - Graph neural network (graph)
- The reason for their re-popularity (computational power!)

Before we dive in...

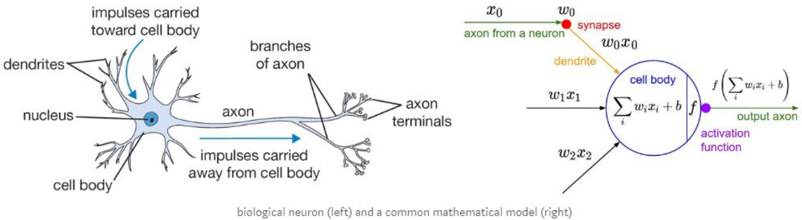
- Biological motivation and connection
  - Neuron - the basic computational unit of the brain
  - Around 86 billion neurons can be found in the human nervous system
  - They are connected with approximately $10^{14} - 10^{15}$ synapses
  - Human 'training process' - a couple of years :) (AlphaGo 40 days right now)
- Mathematical strength
  - Universal approximation theorem
  - Let $\phi(\cdot)$ be a nonconstant, bounded, and monotonically-increasing continuous function. Let I_m denote he m-dimensional unit hypercube $[0,1]^m$.The space of continuous functions on I_m is denoted by $C(I_m)$. Then, given any $\epsilon > 0$ and any function $f \in C(I_m)$, there exists an integer N, real constants v_i, b_i in and real vectors $w_i \in {}^m$, where $i = 1, 2, ..., N$, such that we may define:

    $$F(x) = \sum_{i=1}^{N} v_i \phi(w_i^T x + b_i)$$

    as an approximate realization of the function f, where f is independent of ϕ; That is $|F(x) - f(x)| < \epsilon$, for all $x \in I_m$.
  - **I am apologize for previous theorem**, in other words...

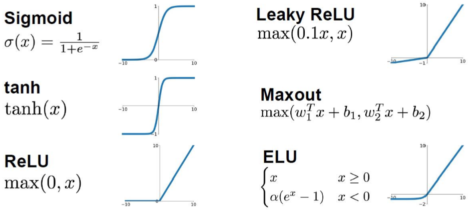
Main parts of Feed Forward Neural Network

- Neuron:



biological neuron (left) and a common mathematical model (right)

- You see f, f is an activation function:



Layers

- Neurons (with its activation functions) are stored in layers[11]
- Input layer - No computation is done here within this layer, they just pass the information to the next layer
- Hidden layer**s** - they perform computations and then transfer the weights (signals or information) from the input layer to the following layer (another hidden layer or to the output layer)
- Output layer - Here we finally use an activation function that maps to the desired output format (e.g. softmax for classification)

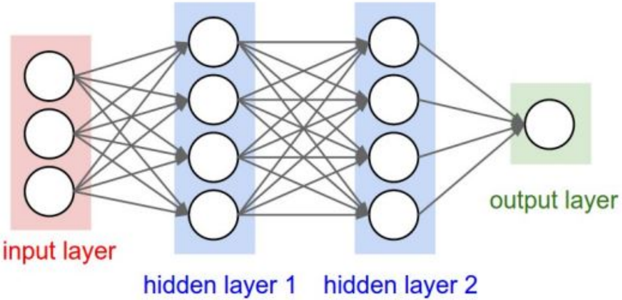
$$softmax((x_1, \dots, x_C)) = \left(\frac{e^{x_1}}{\sum_{i=1}^{C} e^{x_i}}, \dots, \frac{e^{x_C}}{\sum_{i=1}^{C} e^{x_i}} \right)^{12}$$

[11] A block of nodes

[12] MNIST interpretation, choose one out of ten digits

Fully image

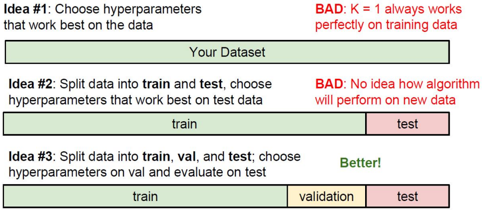
- Feed Forward Neural Network



- Idea of Dropuot

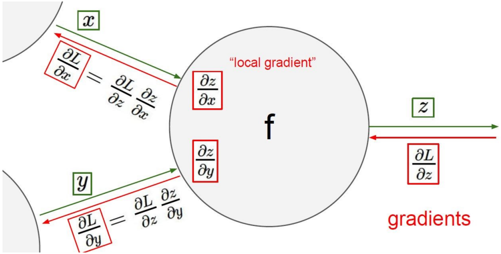
Should I learn something?

- Give me the data!



[13]

- Ok, when I have the data, I learn via backprop.



[13] Check on the internet the term 'cross-validation'

Feed Forward Neural Network - coding time

- Let's code MNIST[14] Feed Forward Neural Network in `keras`[15] [16]

[14]The MNIST database (Modified National Institute of Standards and Technology database) is a large database of handwritten digits

[15]https://keras.io/

[16]Search for the Colvolutional Neural Network on the internet! Can you solve MNIST problem using CNN?

Questions?

Thank you for your attention!

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