Datascience 3.0

Introduction to Machine learning in Python

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November 19, 2017

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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

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]
- Today we have 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)

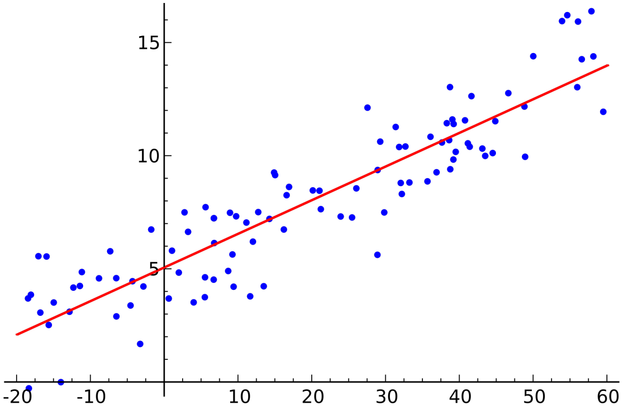

Figure: Linear regression (wikipedia)

Classification

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

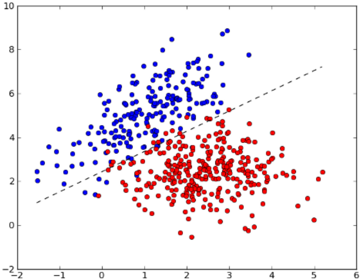

Figure: Classification example 1

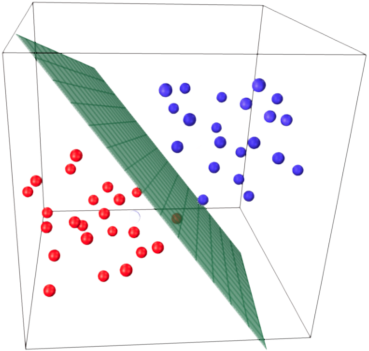

Figure: Classification example 2 (Sachin Joglekar's blog)

Linear regression

- We construct the model in the following form:

$$f_w(x) = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_n x_n$$

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

- We calculate model accuracy using the following formula[1]:

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

[1] 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*[2] one?
- Model that makes the smallest mistake on the data we have is *generally* great for us!
- But how do we find such model?

[2] 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[3] matrix $n \times m$ in memory: $O(nm)$

[3] 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?

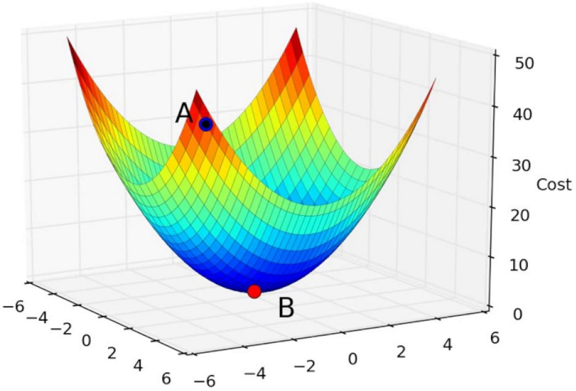

Figure: An example of the error function

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

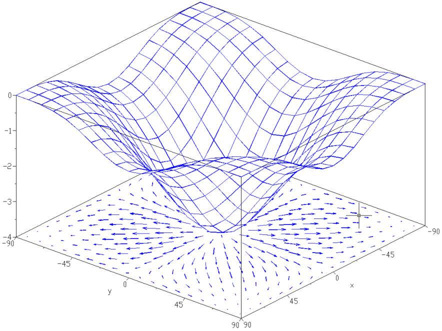

Figure: Blue arrows represent function gradients

Linear regression - gradient descent

Gradient descent algorithm:

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

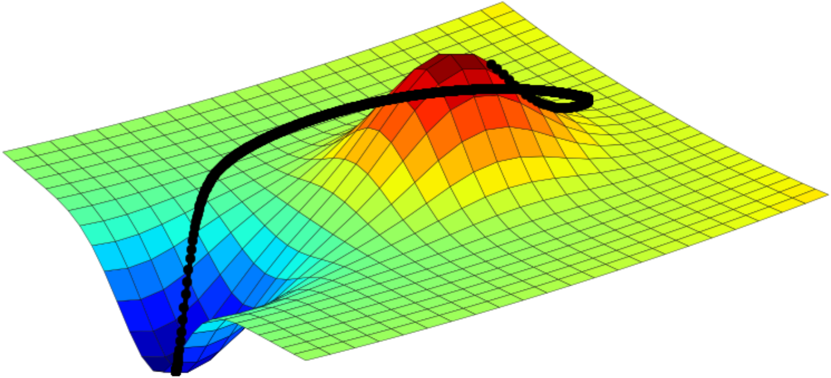

Figure: An example of the steps made by the gradient descent algorithm (github.com/joshdk)

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

- 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?

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

Linear regression - coding time

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

Linear regression - overfitting

- Analyze the following images[4]

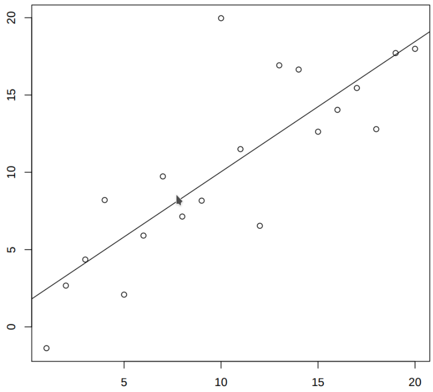

Figure: Linear regression 1

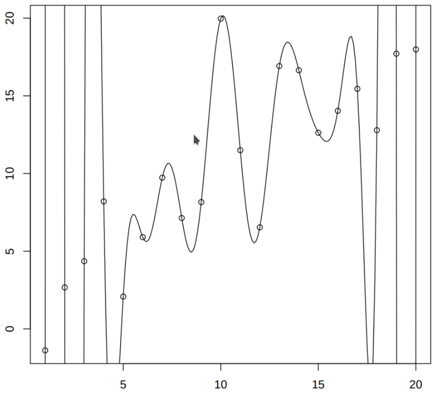

Figure: Linear regression 2

[4] 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)?

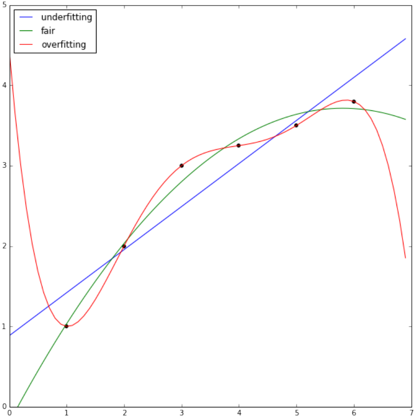

Figure: Examples of underfitting and overfitting

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?

Linear regression - underfitting and overfitting

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  - Indeed we are, if we have a decent representable test set

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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

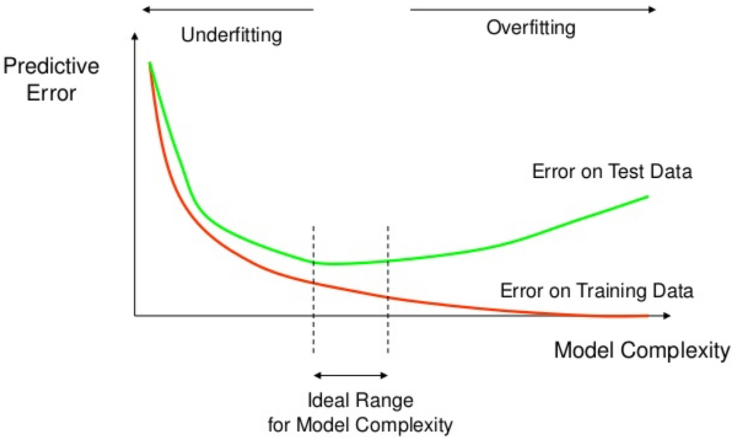


Figure: Graph showing the difference between underfitting and overfitting

Linear regression - How to battle underfitting?

- Take a more flexible model
- Instead of $f_w(x) = w_0 + w_1 x_1 + x_2 x_2$ take $g_w(x) = w_0 + w_1 w_2 x_1 + w_1^2 x1 + w_2^2 x2$
- Usually easier to solve then overfitting
- There is a wide variety of flexible models, and we can always complicate things[5]

[5] 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`

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?

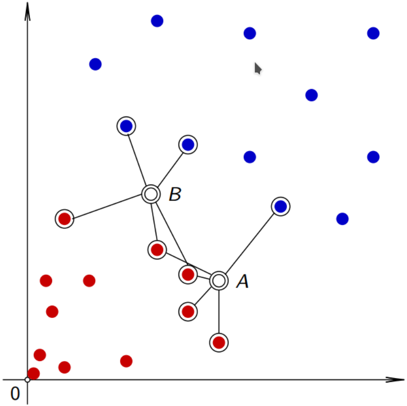


Figure: kNN example (image taken from [Janičić and Nikolić, 2017]

kNN

- How much is k?
  - 5

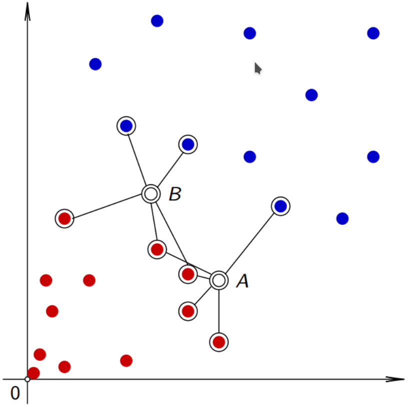


Figure: kNN example (image taken from [Janičić and Nikolić, 2017]

kNN

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

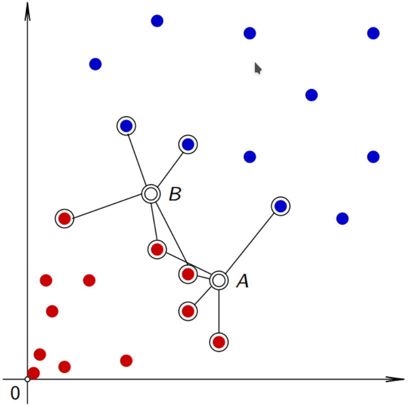


Figure: kNN example (image taken from [Janičić and Nikolić, 2017]

kNN

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

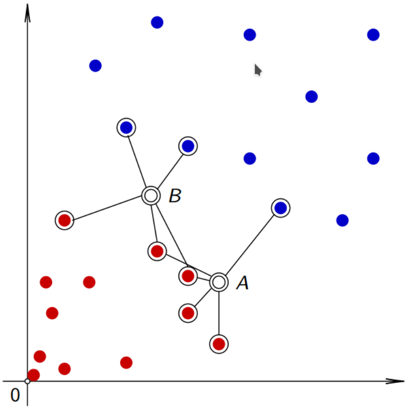


Figure: kNN example (image taken from [Janičić and Nikolić, 2017]

kNN

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

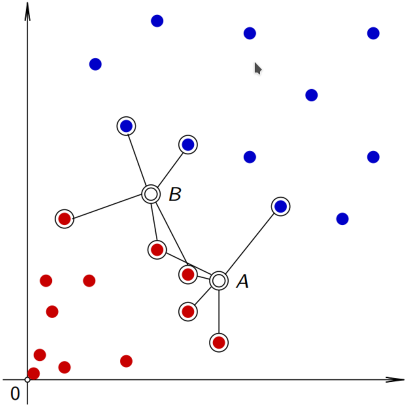
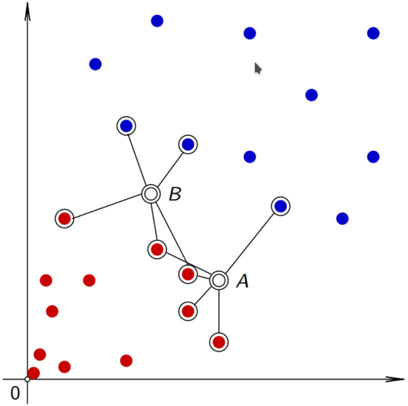


Figure: kNN example (image taken from [Janičić and Nikolić, 2017])

kNN

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



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kNN

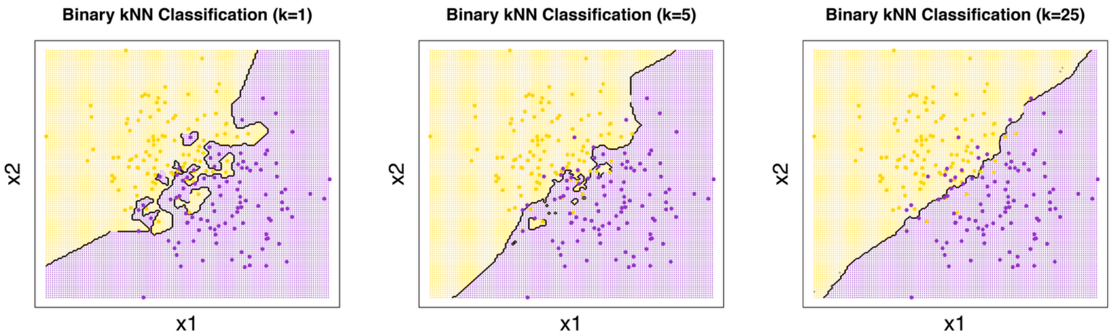

Figure: kNN example (image taken from Burton DeWilde's blog

kNN

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

kNN

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- What is the model in the kNN classifier?

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- How do we train the model?

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 $x = (x_1, \ldots, x_n)$ and $y = (y_1, \ldots, y_n)$
- Minkowski

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

- Manhattan (q = 1)

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

- Euclidean distance (q = 2)

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

kNN - Curse of dimensionality

- Our intuition is bad for high dimensionals spaces
- When dimensionality increases, the volume of space increases really fast
- This can make our dataset very sparse
- 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*
$$Acc = \frac{TP + TN}{TP + TN + FP + FN}$$
- *Precision*
$$Precision = \frac{TP}{TP + FP}$$
- *Recall* score
$$Recall = \frac{TP}{TP + FN}$$
- F_1 score
$$F_1 = \frac{2TP}{2TP + FP + FN}$$

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

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

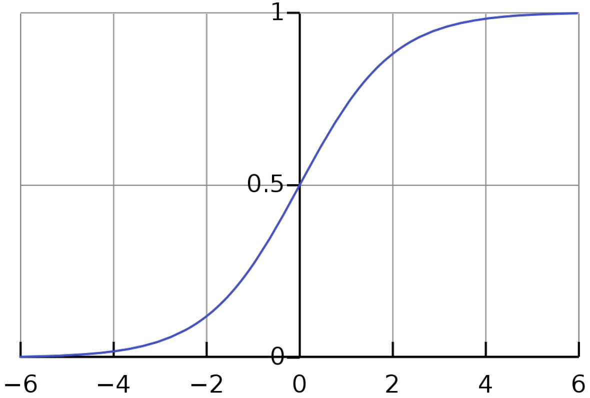

Figure: Graph of the sigmoid function

Logistic regression - loss function

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

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

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

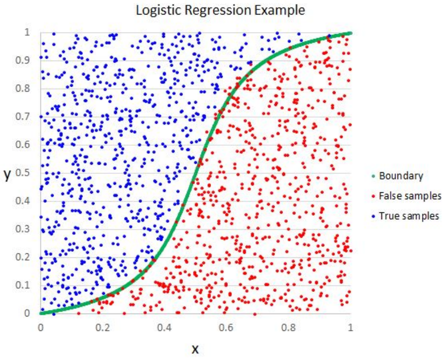

Figure: Example taken from www.helloacm.com

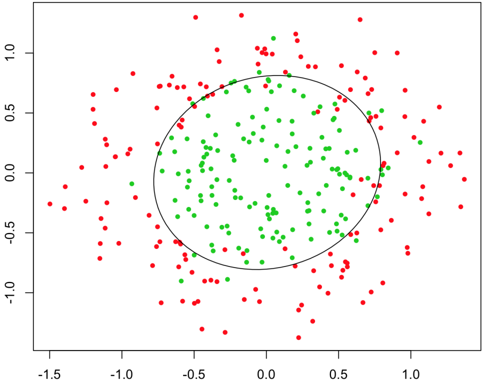

Figure: Example taken from statsblogs.com

Linear regression - coding time

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

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