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April 27th, 2020

Introduction to Machine Learning

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Objectives of the Day

- Present the main objectives of Machine Learning
- Introduce Supervised vs Unsupervised Learning
- Opportunity to introduce basic definitions and notations
- Linear and Logistic Regression as a starting point for Supervised Learning
- k-Means and Principal Component Analysis (PCA) as a starting point for Unsupervised Learning

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Introduction to Machine Learning

1. What is Machine Learning
2. Unsupervised vs Supervised Learning
3. Linear Regression
4. Logistic Regression
5. K-Means and PCA

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Machine Learning Examples

- ***Finance:*** *Identify patterns preceding a significant financial event*
- ***Health:*** *Make a diagnostic from an X-ray or another kind of image*
- ***Retail:*** *Offer personal recommendations based on recent choices of products*
- ***Marketing:*** *Organize customers into classes based on their past behavior*

But also…

- ***Automotive :*** *Interpret traffic images for automated vehicles*
- ***Media/Avertising:*** *Generate images of non-existing people for synthetic scenes*
- ***Art:*** *Generate synthetic music, text or paintings in the "style" of an existing artist*

What is common between all these examples?

Availability of large Datasets used to "Train" the Machine Learning algorithm!

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The Data Explosion behind Machine Learning

- 90% of the world's data was created in the last five years.
- 10^{18} bytes of data are created on the Internet every day.
- In 2 days, as many data are created as from the beginning of history to 2003.

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Machine Learning Definition

- *A computer program is said to learn from experience E with respect to some task T and some performance measure P if its performance on T, as measured by P, improves with experience E.*

(Toni Mitchell, 1997)

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Classical Machine Learning Example

Extract from the MNIST dataset

Machine Learning Problem:

*Based on a Training Set of 60,000 labelled digit images (**the experience E**), learn an algorithm that, given a new pixellized input image, automatically recognizes which digit it represents (**the Task T**). **Performance P** measure will quantify the accuracy of the algorithm on a Test Set of 10,000 images.*

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Some Definitions of Artificial Intelligence

- *Machines that can perform tasks that are characteristics of human intelligence (Chess/Go games are an example)*

Turing Test for Human Intelligence

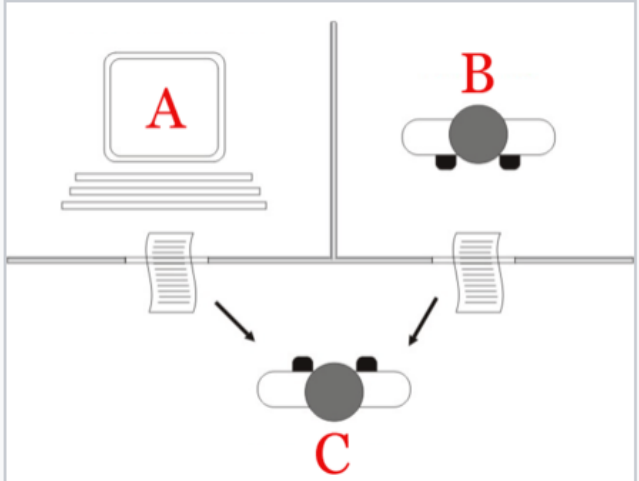
Turing, A.M. (1950). Computing machinery and intelligence. Mind, 59, 433-460.

COMPUTING MACHINERY AND INTELLIGENCE

By A. M. Turing

1. The Imitation Game

I propose to consider the question, "Can machines think?" This should begin with definitions of the meaning of the terms "machine" and "think." The



The "standard interpretation" of the Turing test, in which player C, the interrogator, is given the task of trying to determine which player – A or B – is a computer and which is a human. The interrogator is limited to using the responses to written questions to make the determination.[1] (Wikipedia)

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Supervised vs Unsupervised Learning

- **Supervised Learning:** the task T is specified by the user. T is clearly defined because the data are labelled and the computer has to predict the labels of new data.

- **Unsupervised Learning:** the computer is given some unlabeled data and the task T is to organize them based on the recognition of similar patterns in some groups of data. Let the numbers speak for themselves!

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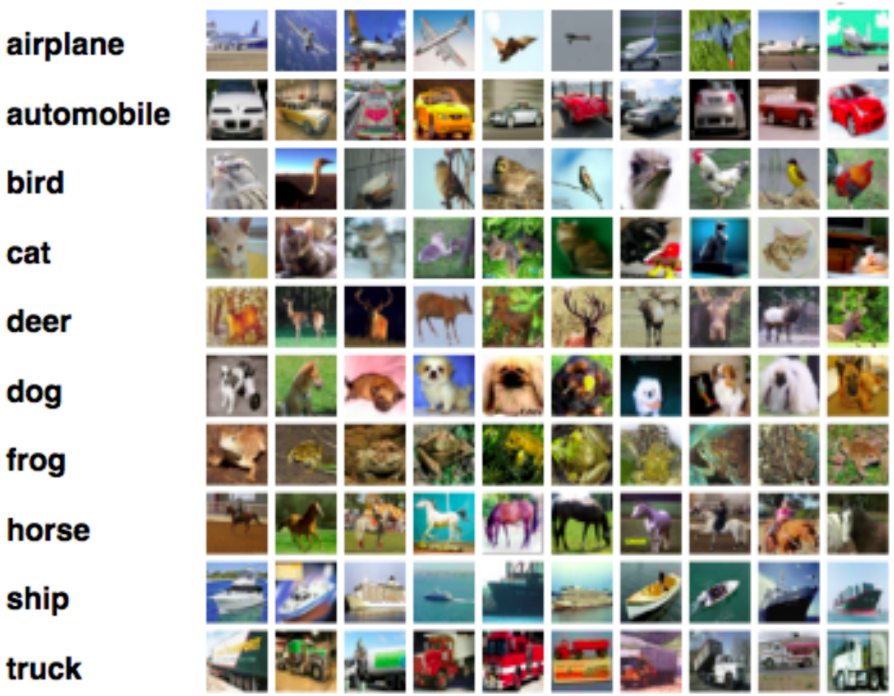
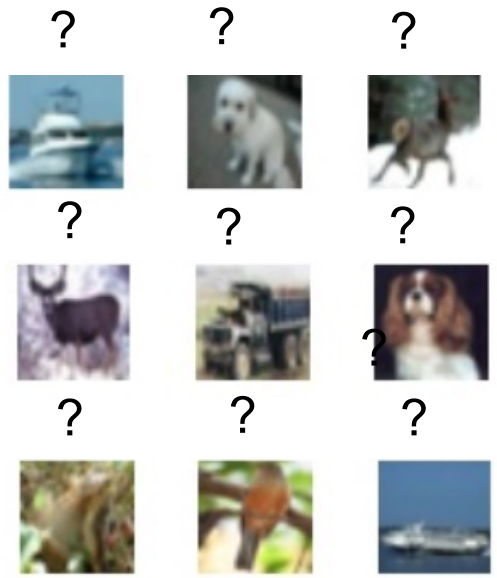
Supervised Learning: Classification

Data : (x,y) where x is image and y is label



Excerpt of the CIFAR-10 dataset, Source: https://www.cs.toronto.edu/~kriz/cifar.html

Task: Learn a function to find y when only x is known.



The CIFAR-10 dataset consists of 60000 32x32 colour images labelled in 10 classes, with 6000 images per class.

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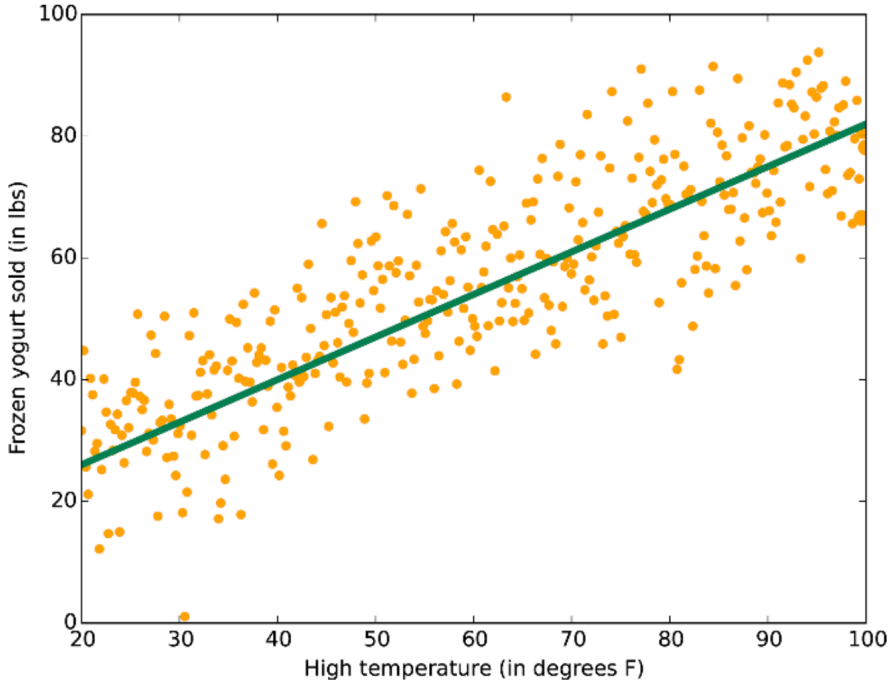
Supervised Learning Example: Regression



Task T: from the Training Set of pairs (Temperature, Yoghurt Sold) **(the Experience**) establish a formula for predicting Yoghurt Sold when only the Temperature is known (**the Task**) such that the averaged squared error is minimized (**the Performance).**

https://docs.microsoft.com/en-us/azure/machine-learning/studio/algorithm-choice

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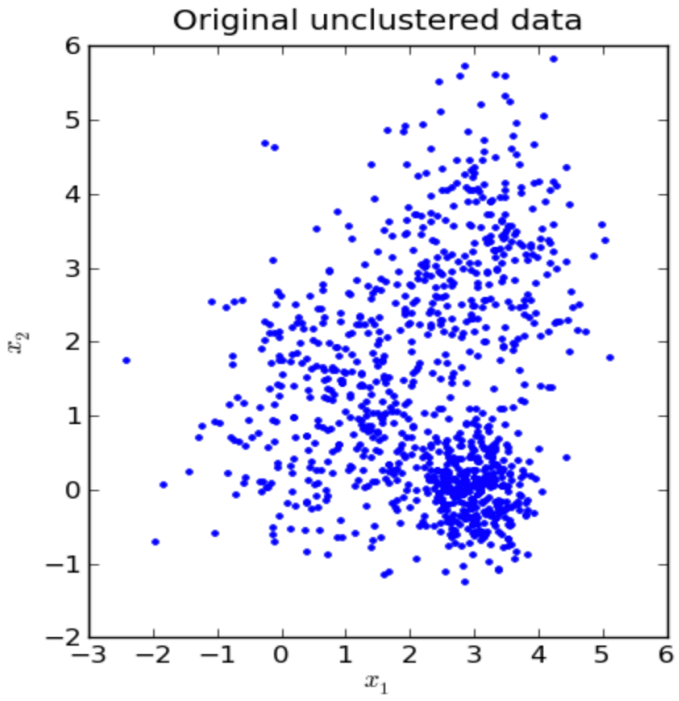
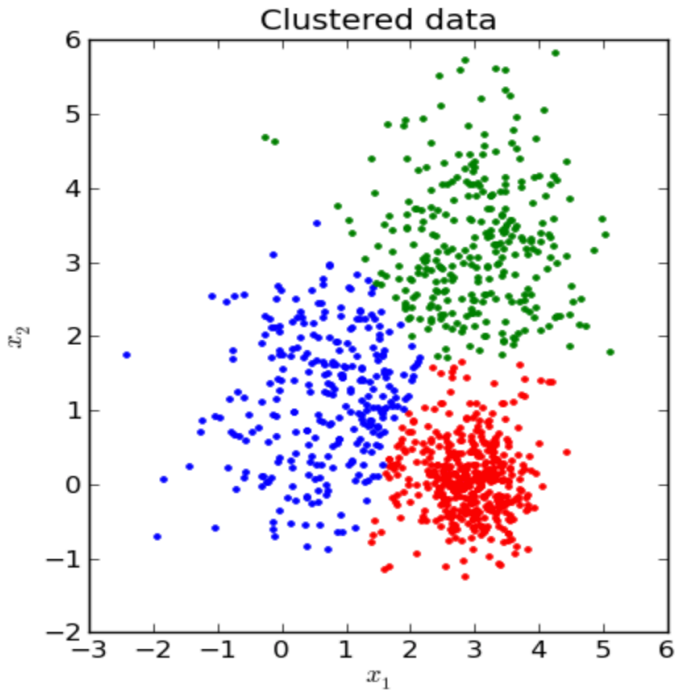
Unsupervised Learning: Clustering

Data : x only, no label y



Task : Organize the x's into clusters in which a new x can be classified



Let the data speak for themselves!

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Clustering Examples

- Sort costumers into different categories in order to target them by marketing
- Among many press articles, identify those which deal with the same story
- From a satellite image, identify classes of regions where the data seem to behave in a “similar” fashion

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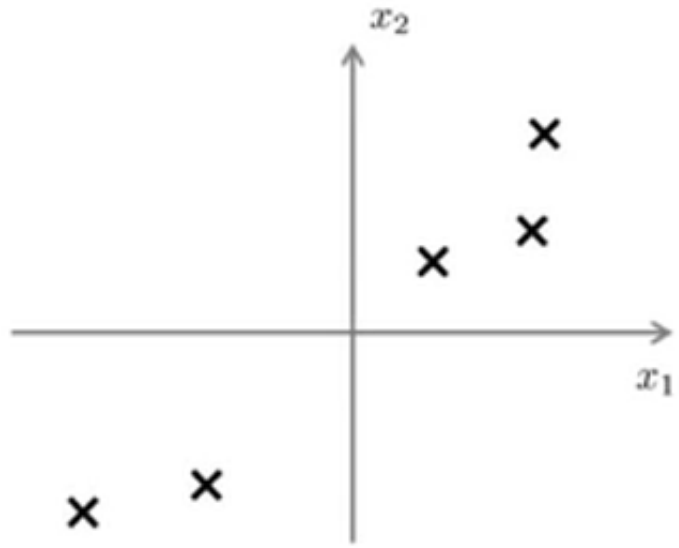
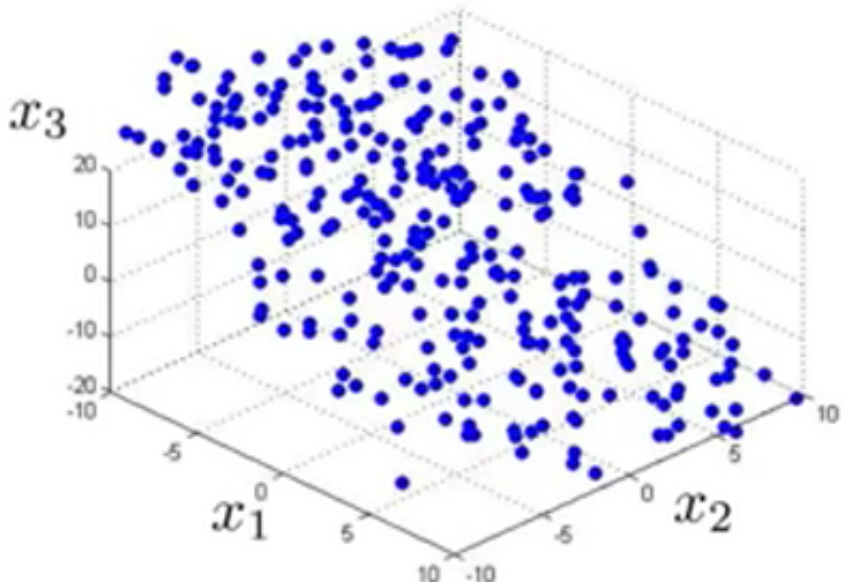
Unsupervised Learning: the PCA approach



Opportunity to Project 2-D Data into 1-D space



Opportunity to Project 3-D Data into 2-D space

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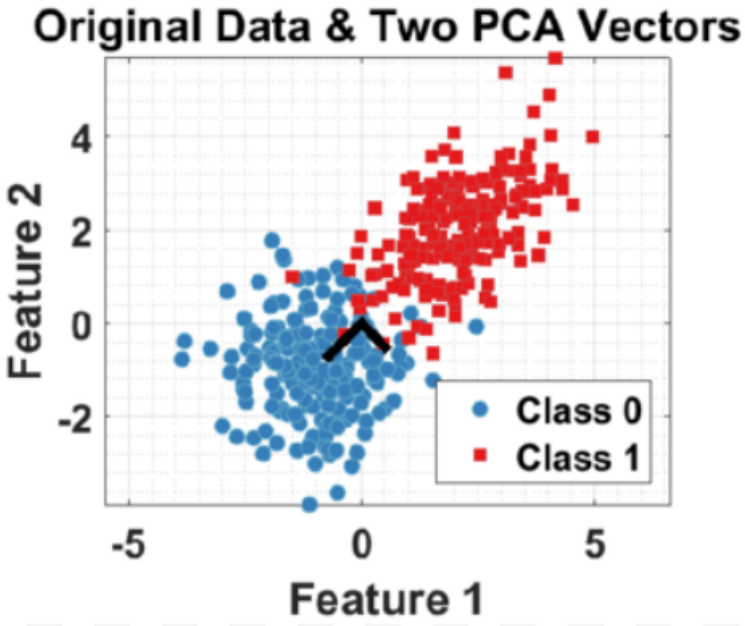
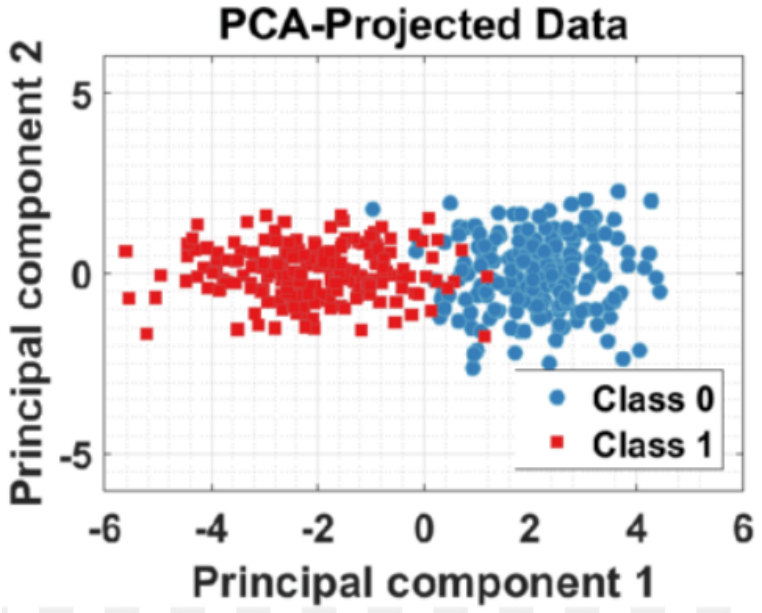
Unsupervised Learning with PCA (1)





Task: identify lower dimension spaces where data can be easily classified

"Unsupervised" because the labels are not used in the PCA calculations

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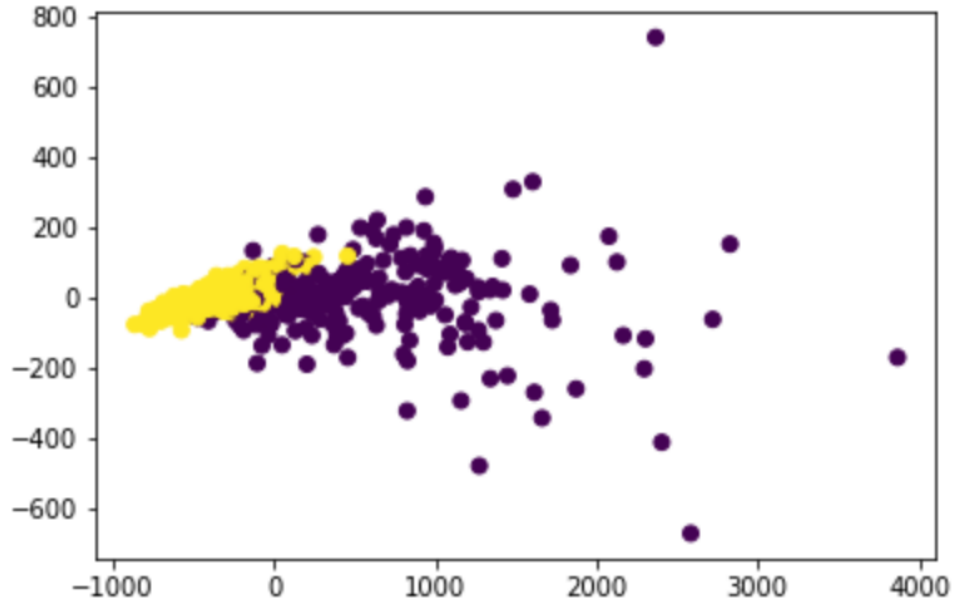
Unsupervised Learning with PCA (2)

Breast Cancer Data (original dataset is in 30 dimensions)



Task: identify lower dimension spaces where data can be easily classified

Dimensionality Reduction often used as a First Step before Clustering!

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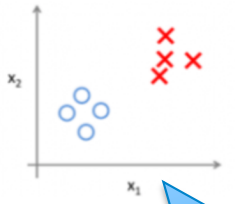
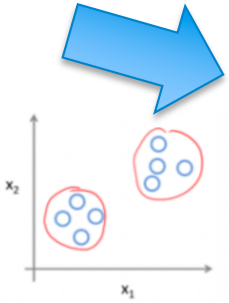
Supervised vs Unsupervised Learning

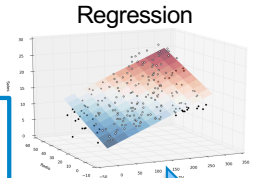
MACHINE LEARNING

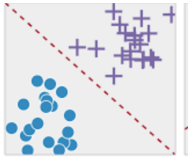


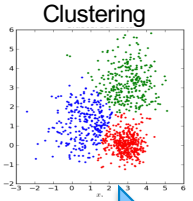
SUPERVISED LEARNING
Training Set:
Data x with labels y

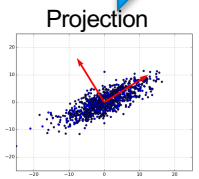


UNSUPERVISED LEARNING
Training Set:
Just Data x









Regression
(y is real number/vector)

Classification
(y is class or integer number/vector)

Clustering
(group x's in clusters)

Dimensionality Reduction
(compress x's)

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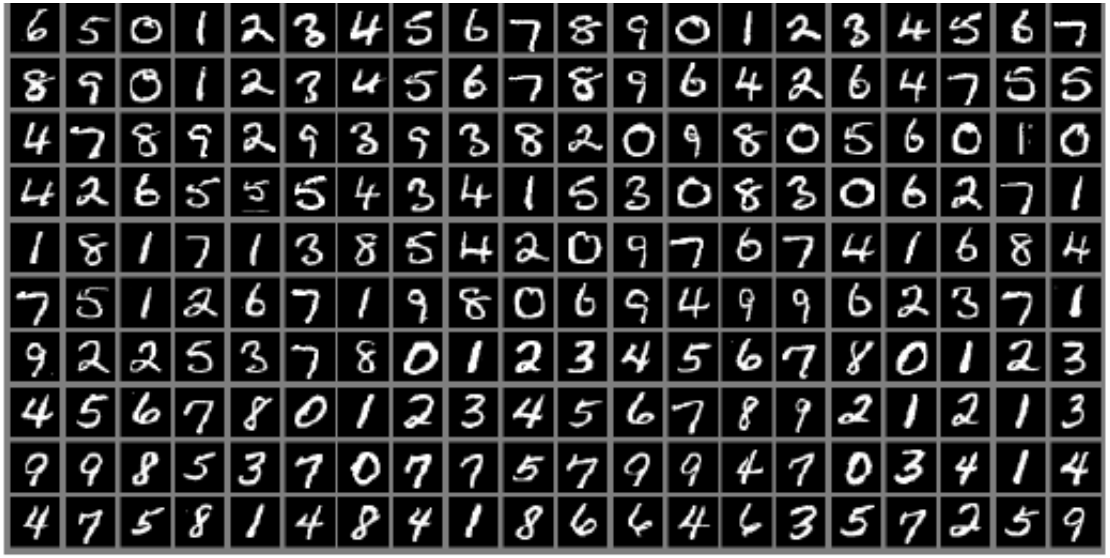
When data are labelled, the same problem can be addressed as a Supervised or an Unsupervised one



Extract from the MNIST dataset

Supervised approach: each image is labelled by the digit it represents

Unsupervised approach: ignore the labels and try to sort all the images into classes

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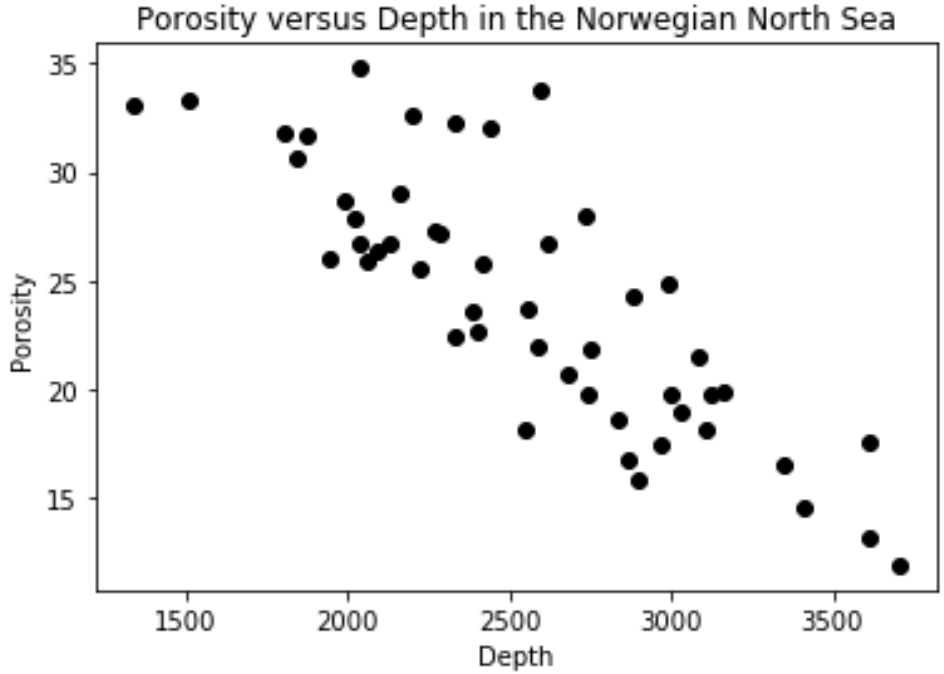
Standard Machine Learning Terminology and Notation



m = number of training examples (here we have m=50 pairs of data)
x's= input variables/**features** (here x is just depth)
y's= output variables/**target** variables (here y is porosity)
$\left(x^{(i)}, y^{(i)}\right)$ is the i^{th} training example

Data derived from Ramm and Bjorlykke, 1994

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What does Linear Regression do?

Fit a linear function to the data. In Machine Learning terminology, this function is called the « **Hypothesis** » $\boldsymbol{h_\theta(x)}$

$$\boldsymbol{h_\theta(x) = \theta_0 + \theta_1 x}$$

θ_0 and θ_1 are called the **parameters** (or the weights) of the model.

For each value of the feature $x^{(i)}$ in the Training Set , we want $h_\theta\left(x^{(i)}\right)$ to be close to the target $y^{(i)}$. In other words, we wish to minimize the **Cost Function** $\boldsymbol{J\left(\theta_0, \theta_1\right)}$ (also called **Loss Function**).

$$\boldsymbol{J\left(\theta_0, \theta_1\right) = \frac{1}{2m}\sum_{i=1}^{m}\left(y^{(i)} - h_\theta\left(x^{(i)}\right)\right)^2 = \frac{1}{2m}\sum_{i=1}^{m}\left(y^{(i)} - \theta_0 - \theta_1 x^{(i)}\right)^2}$$

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Minimizing the Cost Function for Linear Regression

To simplify , assume that the **« Bias »** term θ_0 in the hypothesis is zero

$$h_\theta(x) = \theta_1 x$$

The cost function $J(\theta_0, \theta_1)$ becomes

$$\boldsymbol{J(\theta_1)} = \frac{1}{2m}\sum_{i=1}^{m}\left(y^{(i)} - \theta_1 x^{(i)}\right)^2 = \boldsymbol{\theta_1^2}\left(\frac{1}{2m}\sum_{i=1}^{m} x^{(i)2}\right) - \boldsymbol{2\theta_1}\left(\frac{1}{2m}\sum_{i=1}^{m} x^{(i)}y^{(i)}\right) + \left(\frac{1}{2m}\sum_{i=1}^{m} y^{(i)2}\right)$$

The cost function is simply a **second degree polynomial in $\boldsymbol{\theta_1}$**, minimum for

$$\theta_1^* = \frac{\sum_{i=1}^{m} x^{(i)}y^{(i)}}{\sum_{i=1}^{m} x^{(i)2}}$$ (this is called the normal equation)

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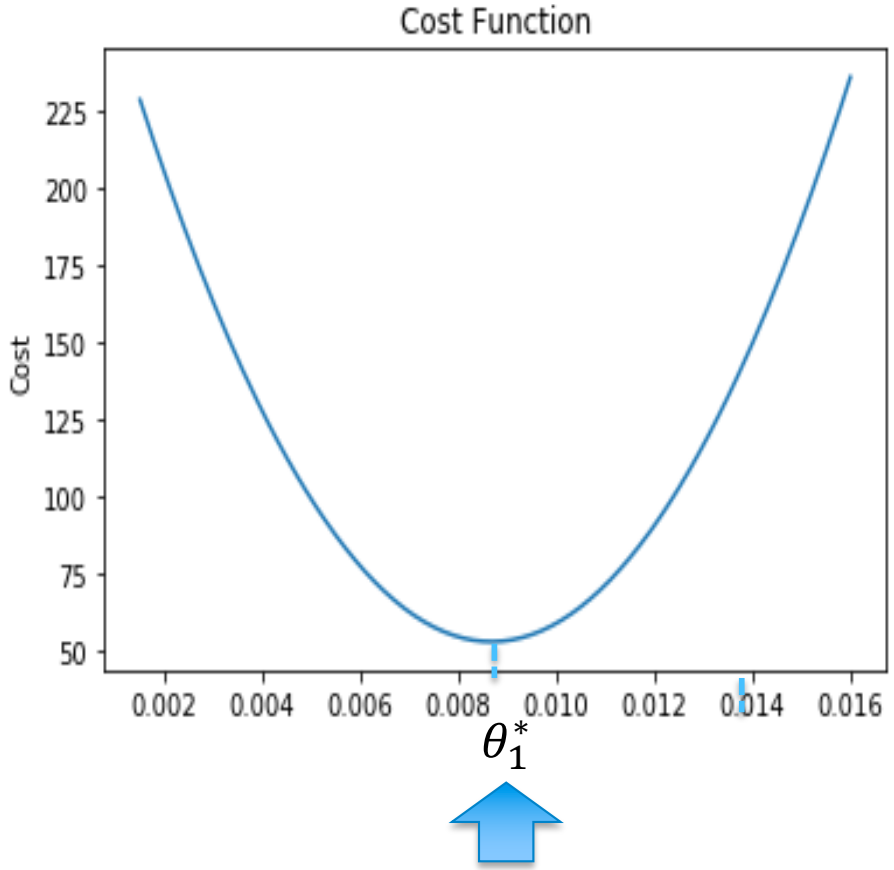
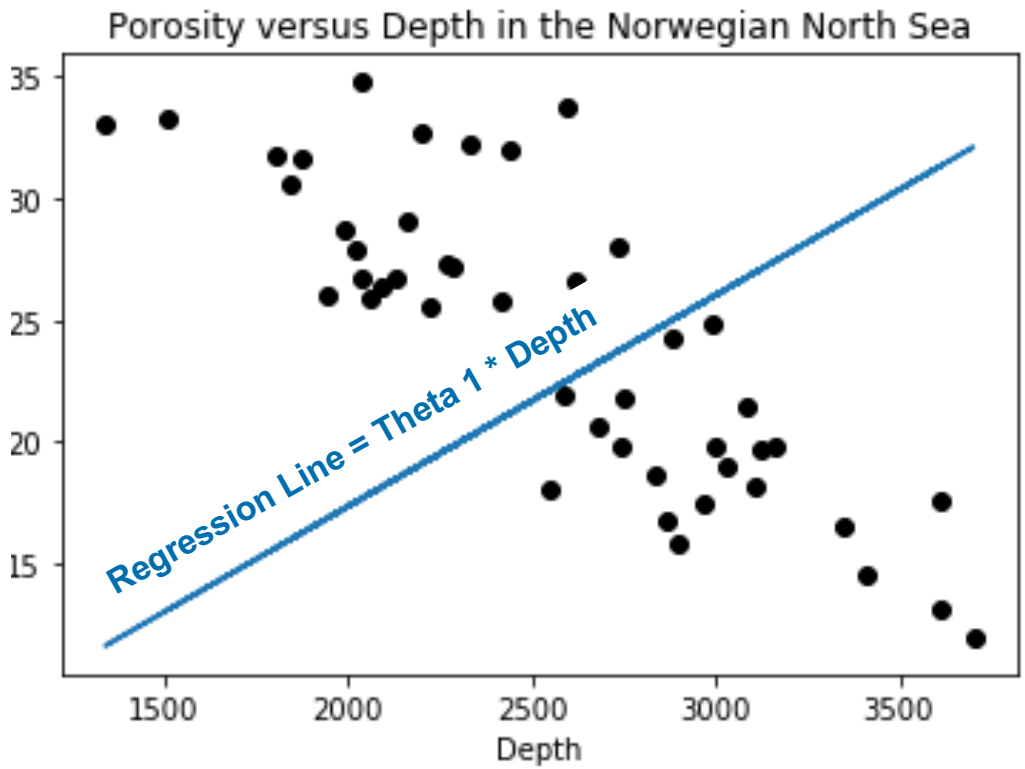
Cost Function is Convex for Regression





Cost Function Minimum at θ_1^* = 0.00876

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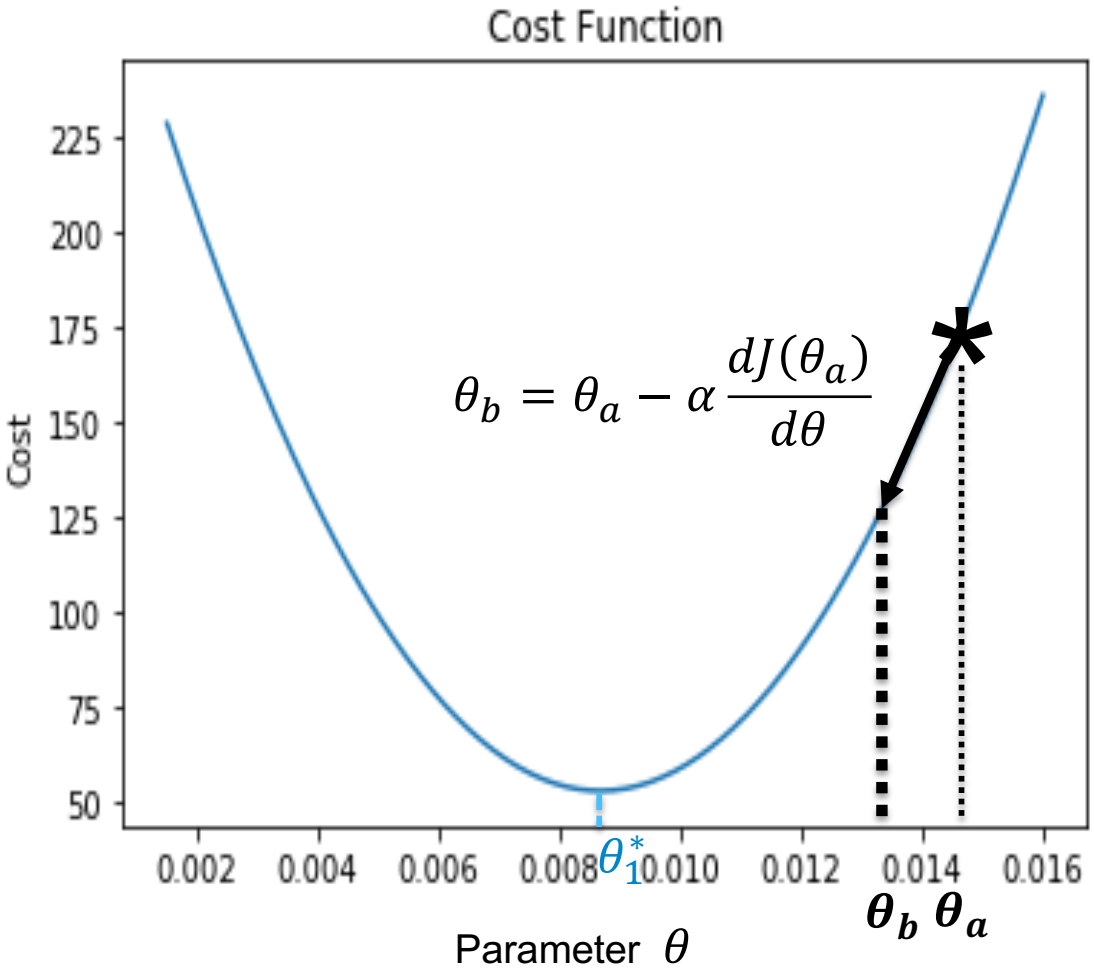
Gradient Descent on a Convex Function

α *is the* ***learning rate****, fixed by the user.*



If α is too small , convergence can be too slow, if α is too large it may miss the minimum.

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Result with a Bias Term in the Linear Regression

The cost function $J(\theta_0,\theta_1)$ can be easily developed

$$\boldsymbol{J(\theta_0,\theta_1)} = \frac{1}{2m}\sum_{i=1}^{m}\left(y^{(i)} - \theta_0 - \theta_1 x^{(i)}\right)^2 = \frac{1}{2m}\sum_{i=1}^{m} y^{(i)2} + \frac{\boldsymbol{\theta_0^2}}{2} + \boldsymbol{\theta_1^2}\left(\frac{1}{2m}\sum_{i=1}^{m} x^{(i)2}\right)$$
$$-2\boldsymbol{\theta_0}\left(\frac{1}{2m}\sum_{i=1}^{m} y_i\right) + 2\boldsymbol{\theta_0\theta_1}\left(\frac{1}{2m}\sum_{i=1}^{m} x_i\right) - 2\boldsymbol{\theta_1}\left(\frac{1}{2m}\sum_{i=1}^{m} x^{(i)}y^{(i)}\right)$$

The cost function is simply a second degree polynomial in θ_0 and θ_1. It reaches its minimum for the values of $\theta_0$and θ_1 given by the so-called normal equations

$$\theta_0^* = \frac{\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)2}\right)\left(\frac{1}{m}\sum_{i=1}^{m} y^{(i)}\right) - \left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right)\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}y^{(i)}\right)}{\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)2}\right) - \left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right)^2} \quad \theta_1^* = \frac{\frac{1}{m}\sum_{i=1}^{m} x^{(i)}y^{(i)} - \left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right)\left(\frac{1}{m}\sum_{i=1}^{m} y^{(i)}\right)}{\left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)2}\right) - \left(\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right)^2}$$

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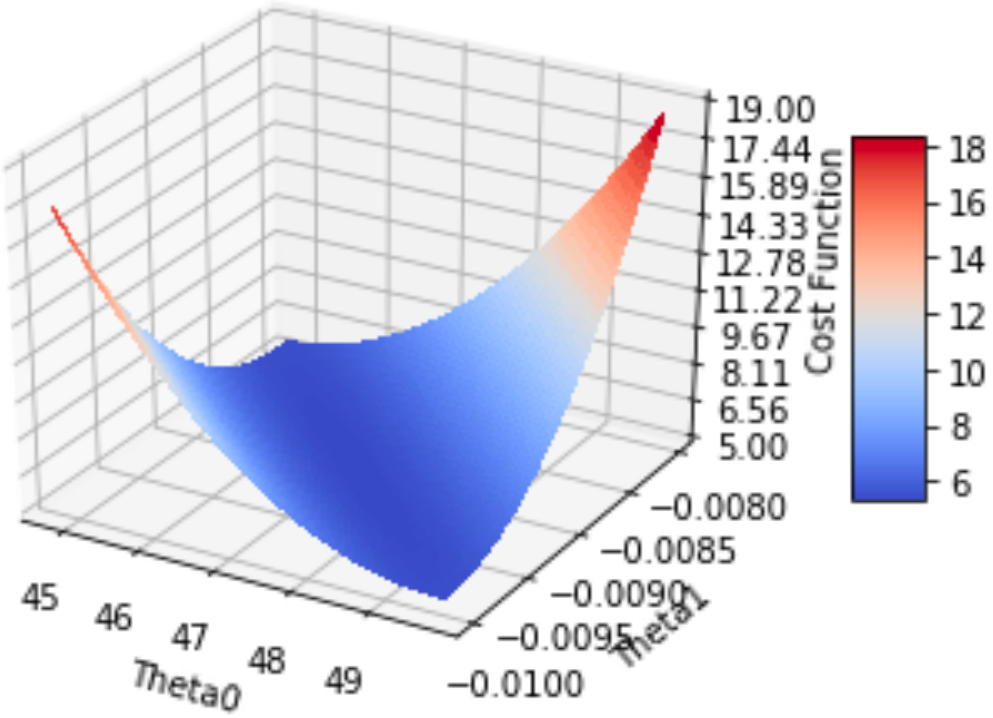
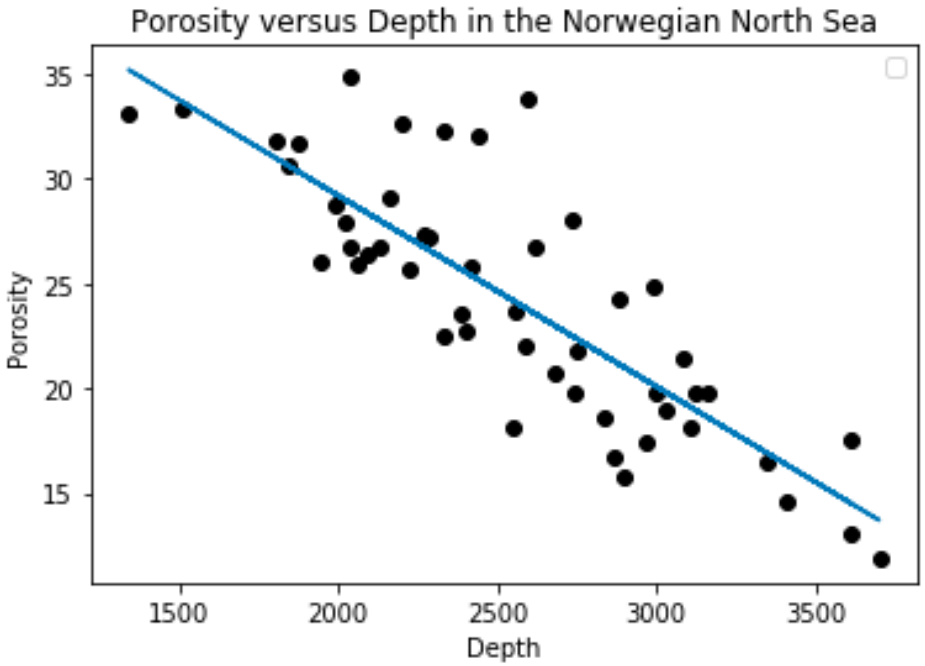
Cost Function for θ_0 and θ_1





A nice property of a convex cost function is that it has no local minima. If you cannot decrease the objective function anymore, it means you have reached the global minimum.

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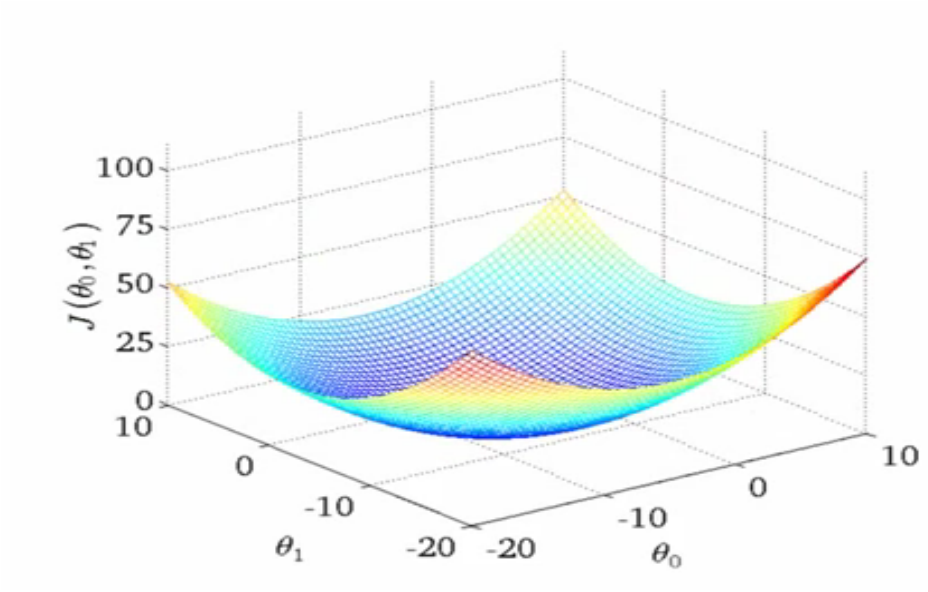
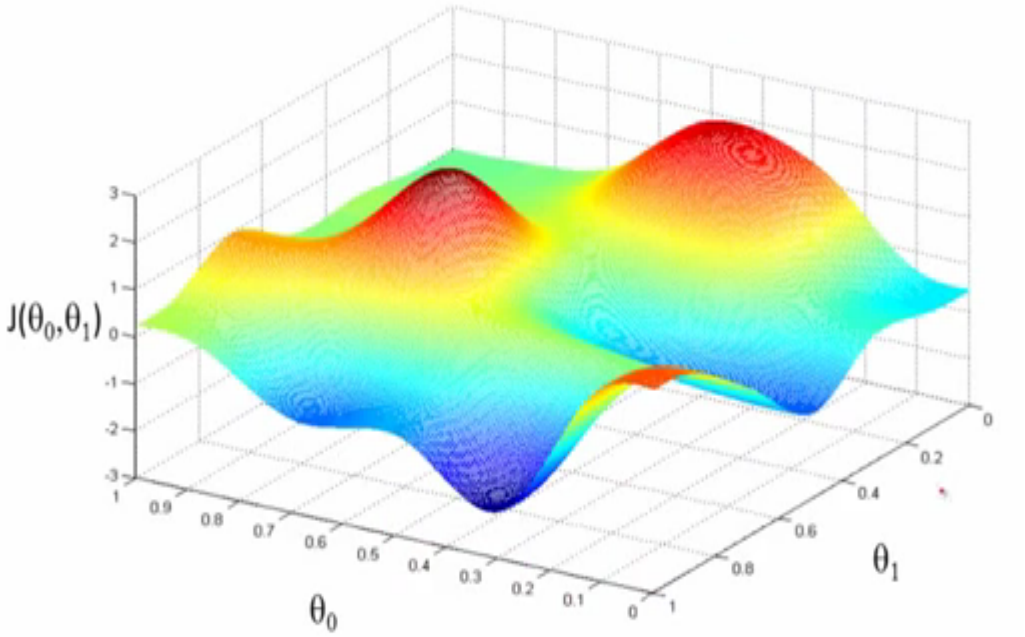
Convex vs Non-Convex Objective Function

Convex



Non-Convex



Unfortunately, many cost functions in non-linear problems are non-convex

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Multiple Linear Regression

From: $h_\theta(x) = \theta_0 + \theta_1 x$

To: $h_\theta(x_1, x_2, \ldots, x_n) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$

$y^{(i)}$ is the value of the target in the example i of the training set

$x_j^{(i)}$ is the value of the feature j in the example i of the training set

m is the number of examples in the training set

n is the number of features in each example of the training set

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Examples of Multiple Linear Regression

Predict House Price from its squared footage, number of bedrooms, number of bathrooms, …

Predict child height from both parents' sizes, nutrition, environment factor….

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Vector Notation for Multiple Linear Regression

The hypothesis function is, if we have n input features x_i:

$$y = h_\theta(x_1, x_2, \ldots, x_n) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$

With the vector notation $x = \begin{pmatrix} 1 \\ x_1 \\ \ldots \\ x_n \end{pmatrix}$ $\theta = \begin{pmatrix} \theta_0 \\ \theta_1 \\ \ldots \\ \theta_n \end{pmatrix}$ We have $h_\theta(x) = \theta^T x$

We write the m data vectors as: $(x^{(i)}, y^{(i)})$ $x^{(i)} = \begin{pmatrix} x_1^{(i)} \\ \ldots \\ x_n^{(i)} \end{pmatrix}$ and $y^{(i)}$ real for $i = 1 \ldots m$

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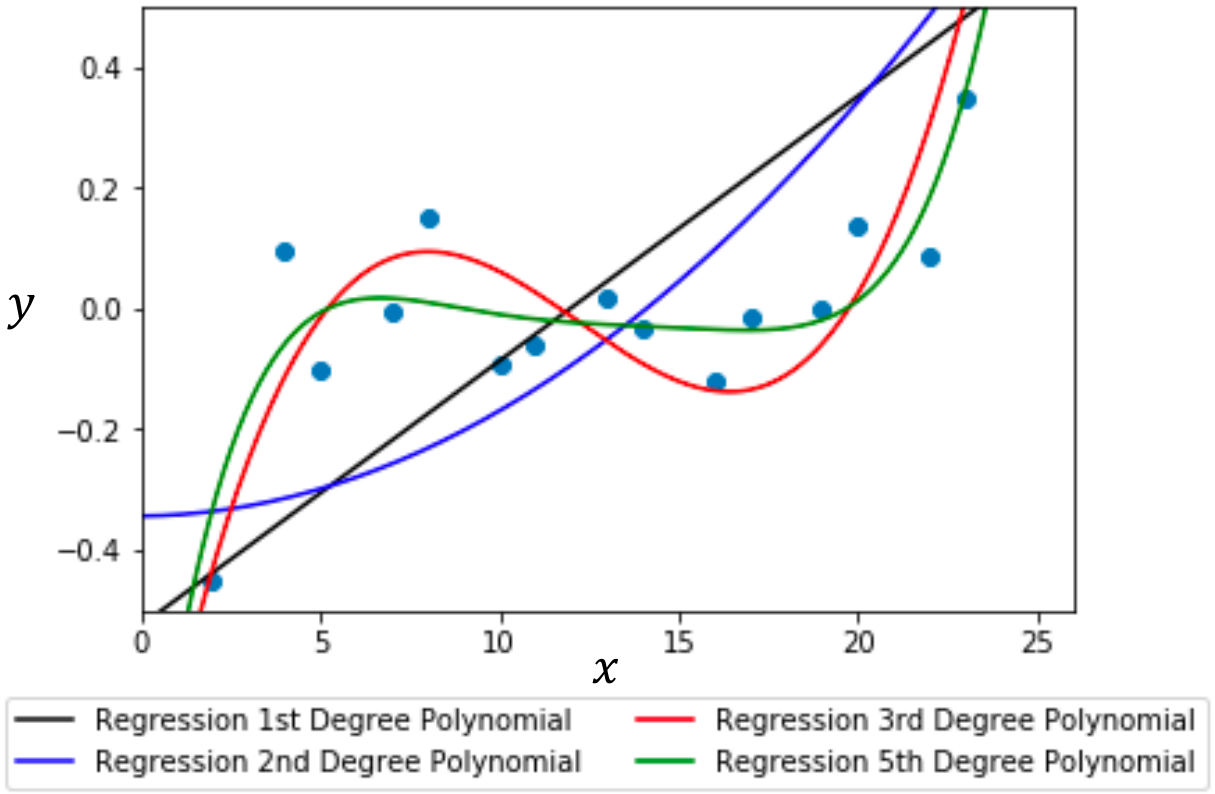
Example of Non-Linear Regression

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_n x^n$$



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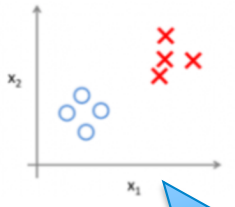
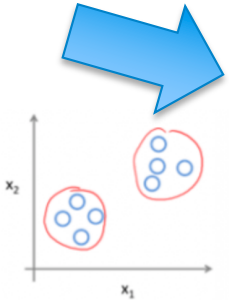
Reminder: Supervised vs Unsupervised Learning

MACHINE LEARNING

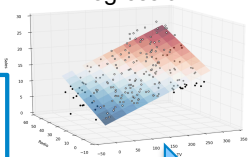


SUPERVISED LEARNING
Training Set:
Data x with labels y

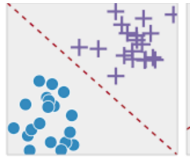


UNSUPERVISED LEARNING
Training Set:
Just Data x

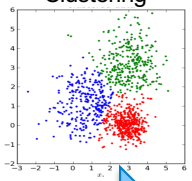
Regression



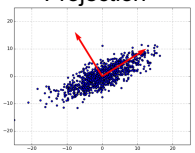
Classification



Clustering



Projection



Regression
(y is real number/vector)

Classification
(y is class or integer number/vector)

Clustering
(group x's in clusters)

Dimensionality Reduction
(compress x's)

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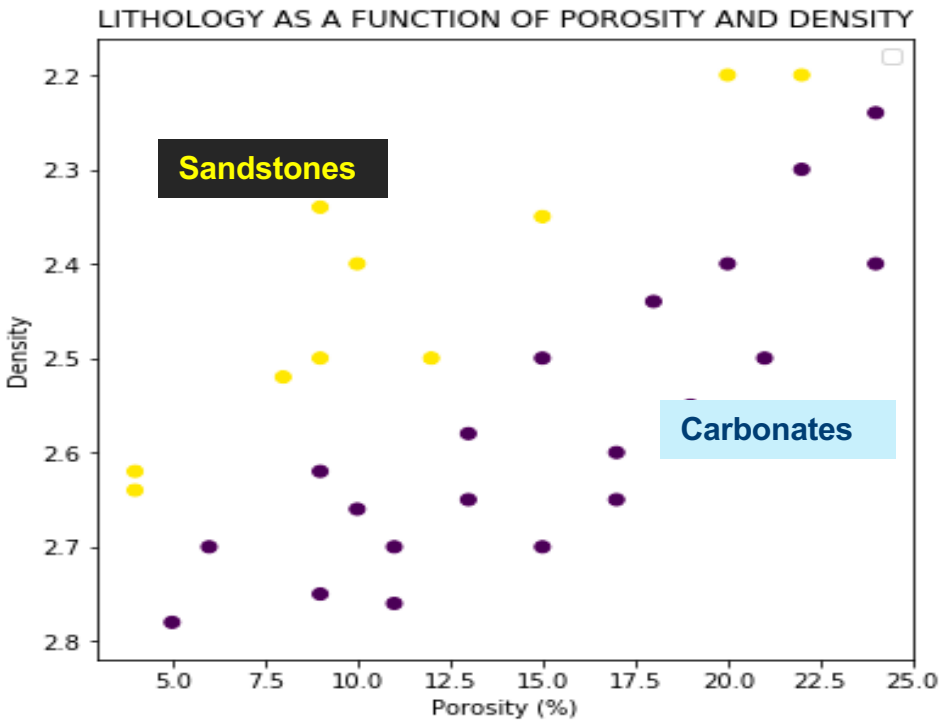
Logistic Regression Problem



30 rock samples with Porosity, Density and Lithology as a label.

We wish to predict Lithology from Density and Porosity: this is a Supervised Classification problem .

Cannot use Linear Regression : need a transform from the domain of real values to the 0 or 1 indicator

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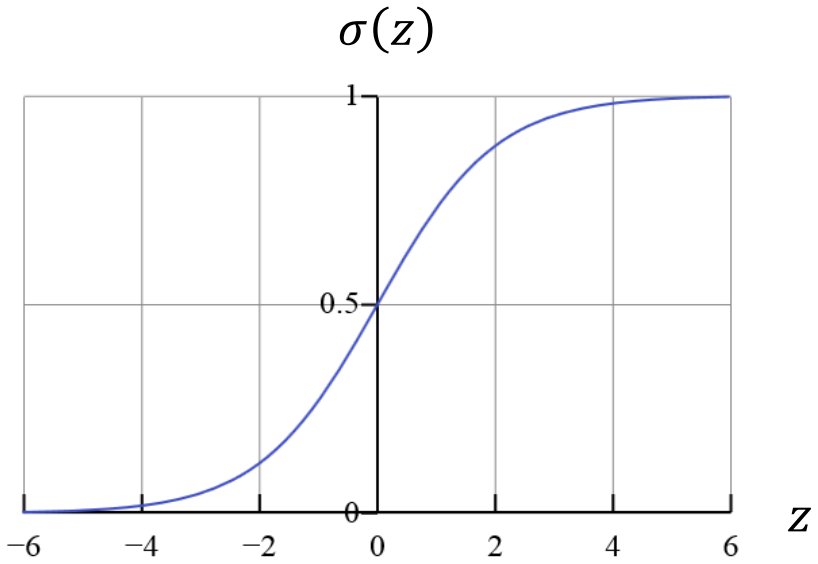
Sigmoid Function for transformation to [0,1] domain.

- It is also called the **Logistic** Function
- It takes any real value z and transforms it into a value between 0 and 1



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

It is easy to prove that

$$\sigma'(z) = \big(1 - \sigma(z)\big)\sigma(z)$$

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Interpreting the output of the Logistic function

- Say that y is the outcome of a regression equation for an input x

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_n x_n$$

- In vector form:

$$y = \theta^T x$$

- y is a real number which can take any positive or negative value.

- If we apply the sigmoid (or logistic) function $\sigma(y)$ we obtain a value between 0 and 1, which **we interpret as the probability for the class to be 1**

$$h_\theta(x) = P(y = 1|\theta, x) = \sigma(\theta^T x) = \frac{1}{1 + e^{-\theta^T x}}$$

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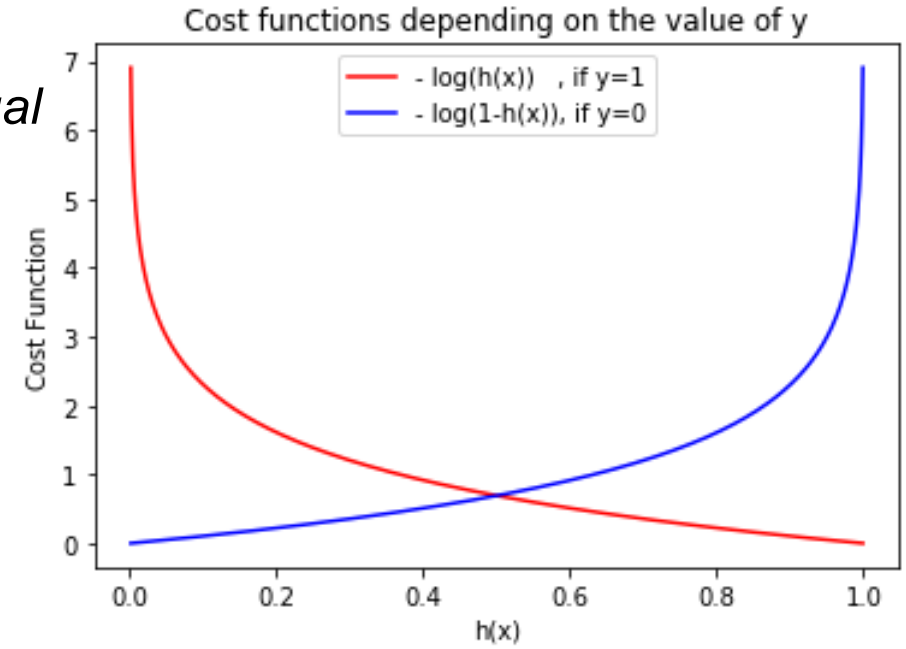
Cost Function for Logistic Regression (one data point)

For one data point , how to measure the discrepancy between the actual data value y (equal to 0 or 1) and the estimated probability $h_\theta(x)$?

$$Cost(h_\theta(x), y) = -\log\big(h_\theta(x)\big) \qquad if\ y = 1$$

$$Cost(h_\theta(x), y) = -\log\big(1 - h_\theta(x)\big) \quad if\ y = 0$$



Combining the two possibilities above into one single equation:

$$Cost(h_\theta(x), y) = -\mathrm{y}\log\big(h_\theta(x)\big) - (1 - y)\log\big(1 - h_\theta(x)\big)$$

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Cost function for a Training whole Set: $\left(\left(x^{(i)}\right),\left(y^{(i)}\right)\right)\ i = 1 \ldots \mathrm{m}$

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} Cost\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)$$

$$= -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log\left(h_\theta\left(x^{(i)}\right)\right) + \left(1-y^{(i)}\right)\log\left(1-h_\theta\left(x^{(i)}\right)\right)\right] = \underline{\textbf{Cross-Entropy}}$$

To minimize, just calculate the derivatives $\frac{\partial J(\theta)}{\partial \theta_j}$ for $\mathrm{j} = 1 \ldots . \mathrm{n}$ and apply Gradient Descent

$$\frac{\partial J(\theta)}{\partial \theta_j} = \frac{1}{m}\sum_{i=1}^{m}\left[h_\theta\left(x^{(i)}\right) - y^{(i)}\right]x_j^{(i)}$$

Exercise: prove this relationship!

In spite of its name, Logistic Regression is for <u>C</u>lassification rather than Regression!

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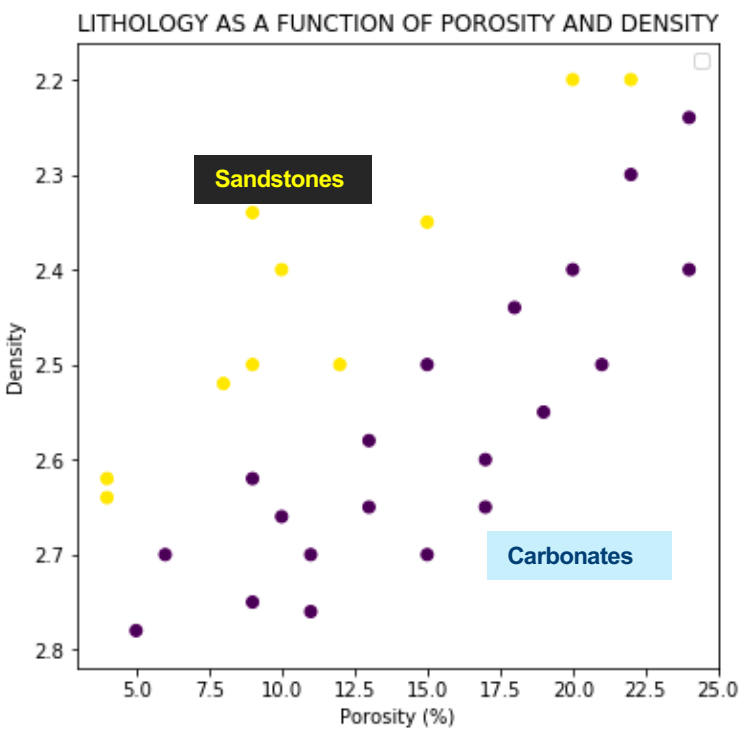
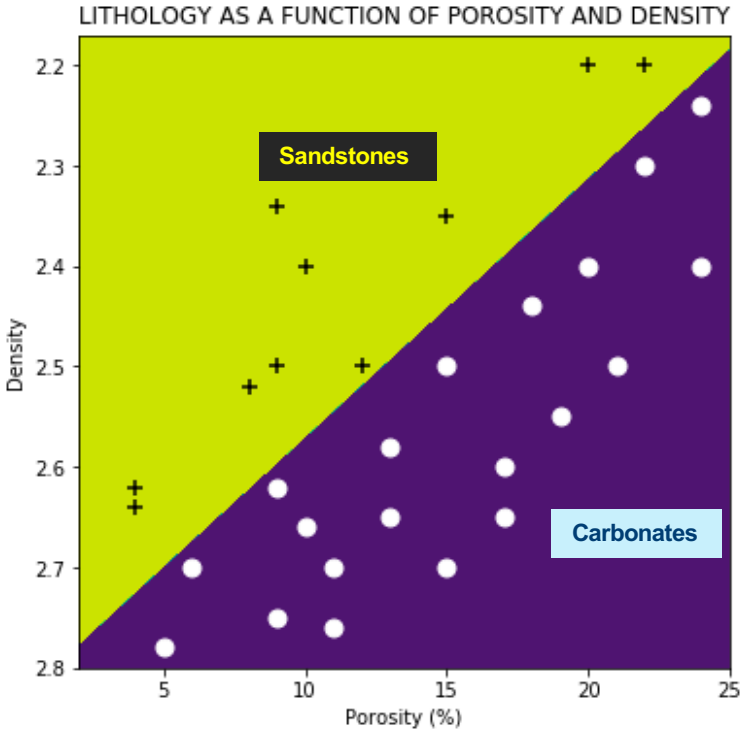
Example of Binary Logistic Regression Result





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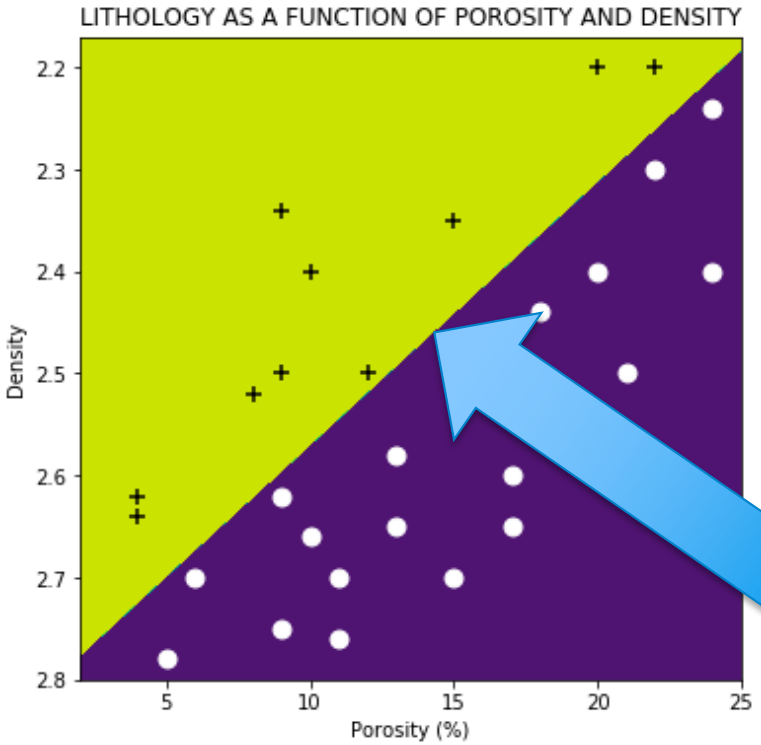
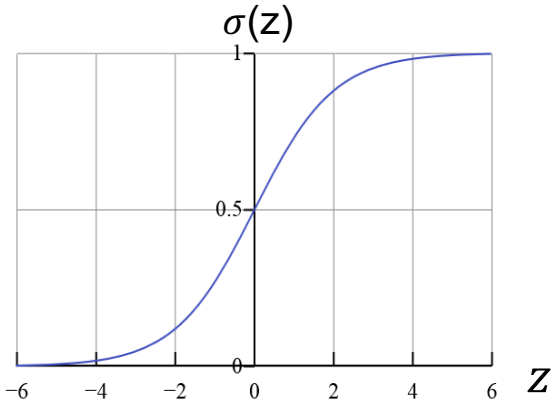
Definition of the Decision Boundary



$$P(y = 1|\theta, x) = \sigma(\theta^T x)$$



Sigmoid function $\sigma(z)$ is >0.5 if $\theta^T x$>0

Hence the Decision Boundary in 2D is the line of equation $\theta^T x$=0

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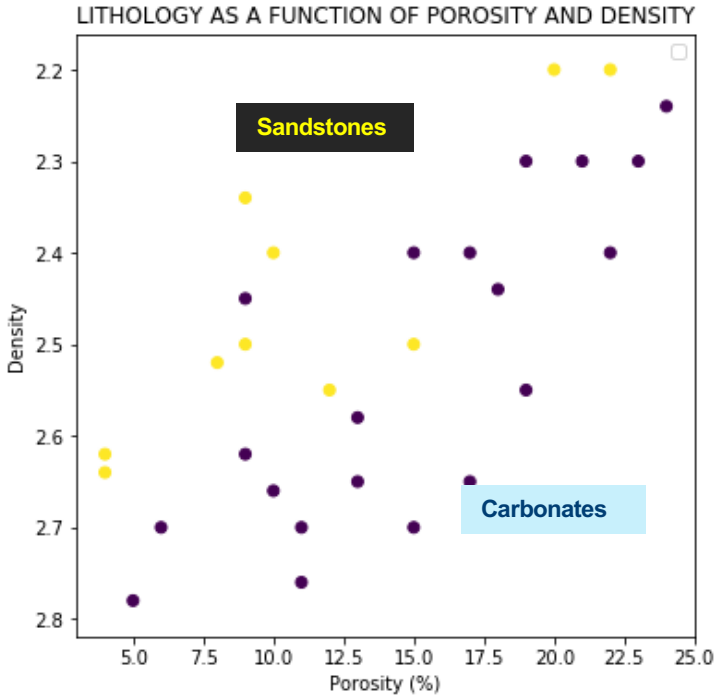
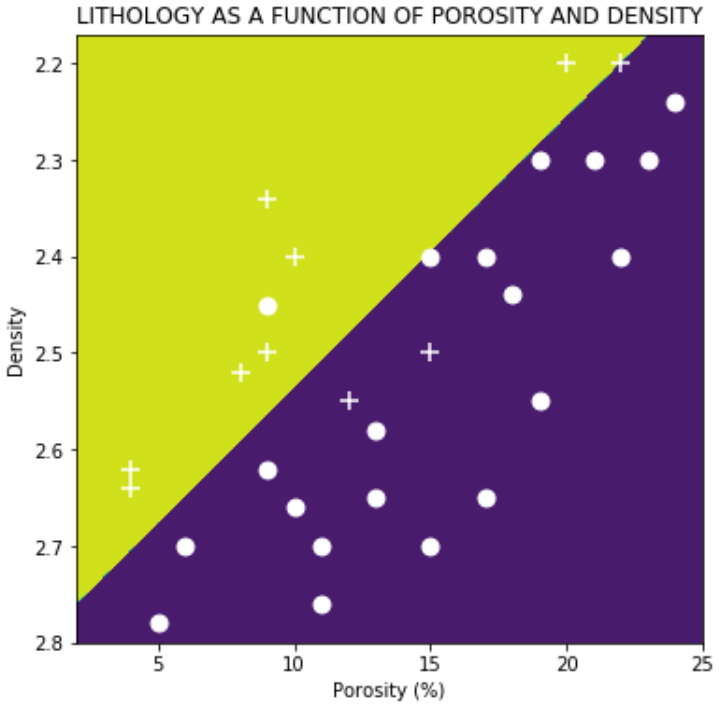
Example where the Data are not Linearly Separated





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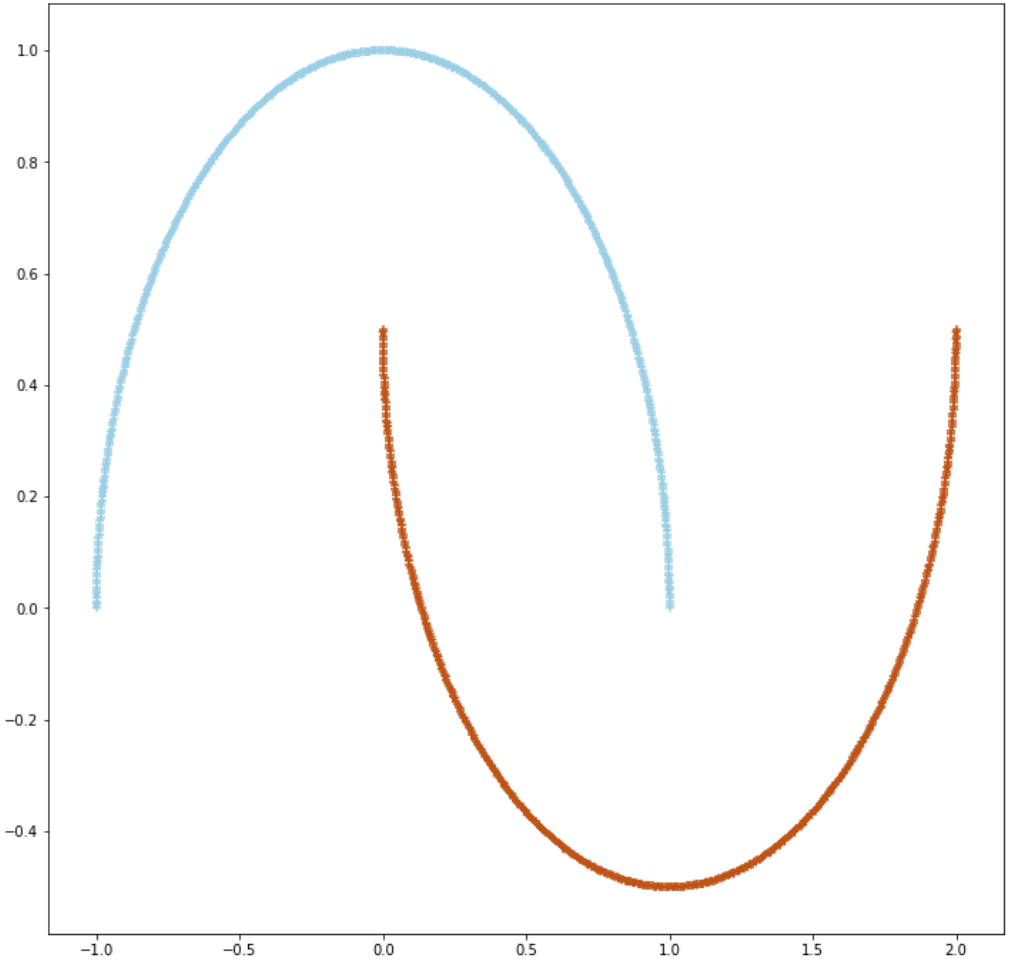
Simple Example of Non-Linear Logistic Regression(1)



The m =1000 data points $\left(x_1^i, x_2^i\right)_{i=1,1000}$ are in the plane.

A group of data are one color, the other group another color.

Question: predict the color at each location of the plane.

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Simple Example of Non-Linear Logistic Regression (2)

Model used for Logistic Regression:

$$h_\theta(x_1, x_2) = \sigma\big(\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_1^2 + \theta_4 x_2^2 + \theta_5 x_1 x_2 + \ldots\ldots + \theta_{16} x_1^5 + \theta_{17} x_2^5 + \theta_{18} x_1^4 x_2 + \theta_{19} x_1 x_2^4 + \theta_{20} x_1^3 x_2^2 + \theta_{21} x_1^2 x_2^3\big)$$

Decision Boundary will be be a polynomial of degree 5.

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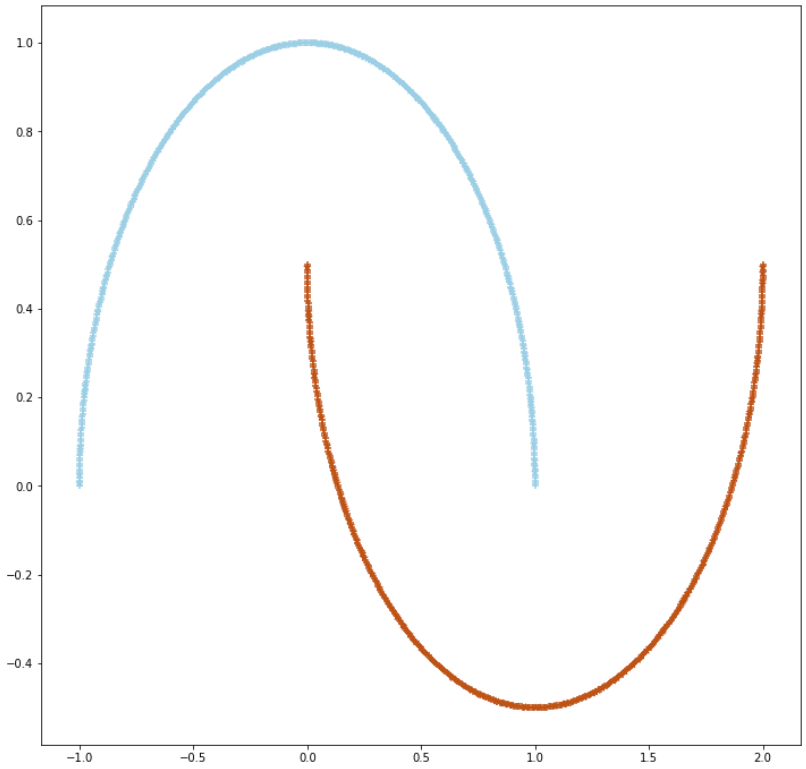
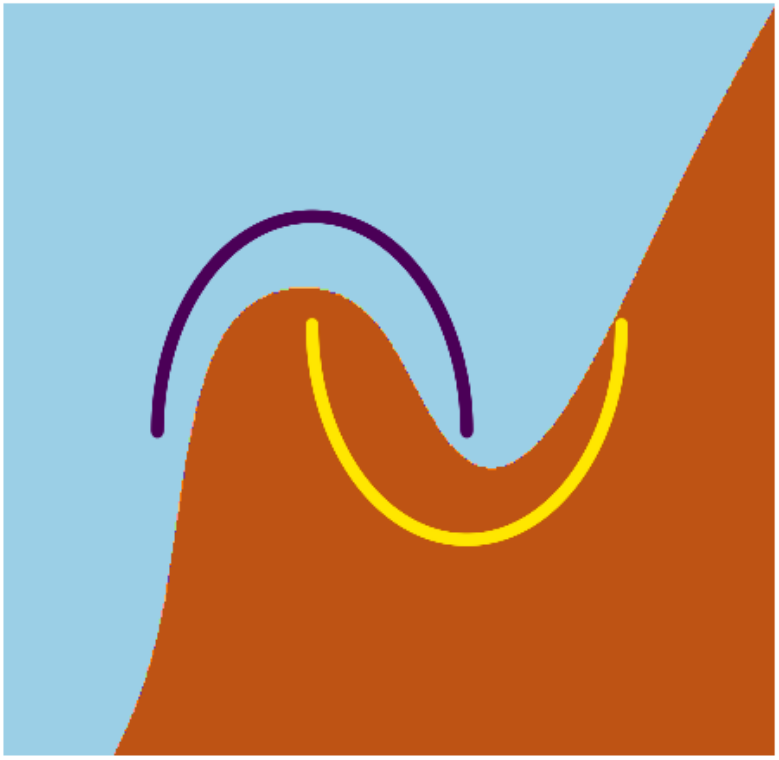
Simple Example of Non-Linear Logistic Regression (3)



Input: 1000 Points of coordinates (x_1, x_2) taking two different colours



Output: Decision Boundary if a degree 5 polynomial in (x_1, x_2) is used

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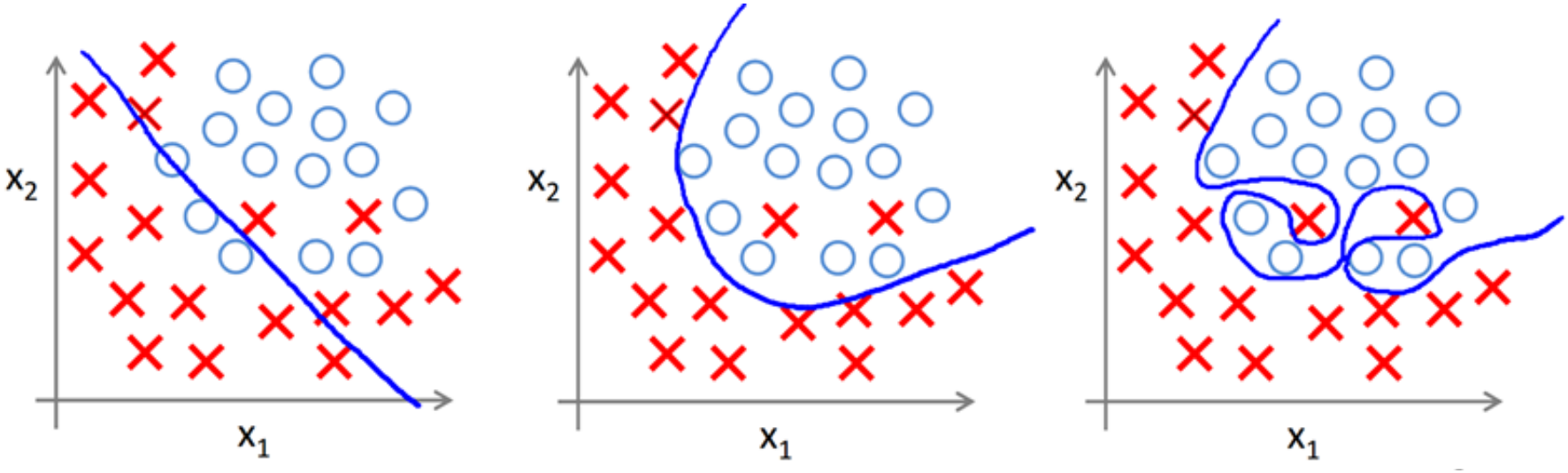
Configurations for Non-Linear Logistic Regression



First Degree Polynomial

Second Degree Polynomial

nth Degree Polynomial

Will have to decide which polynomial degree is statistically reasonable and which one is too high and causes "overfitting" (as seen with the third example).

Source: Machne Learning Course, Andrew Ng

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Applying Logistic Regression to MNIST

Extract from the MNIST Dataset

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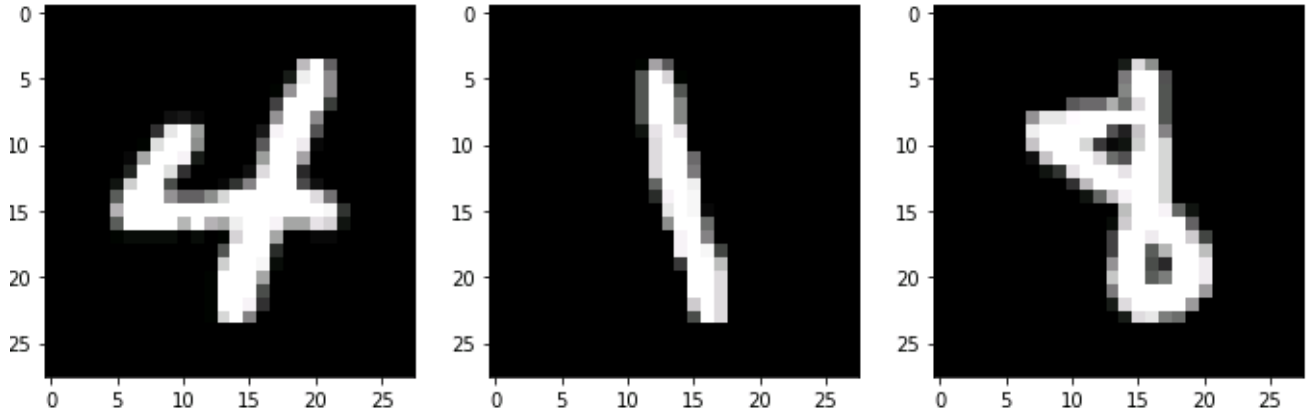
Input to Logistic Regression on MNIST

Each label is the digit (between 0 and 9) associated with the image

Label = 4 Label = 1 Label = 8



(60000 Training Examples)

Each Image is coded as a 28x28 array of grey level pixels. Each pixel value varies between 0 and 255

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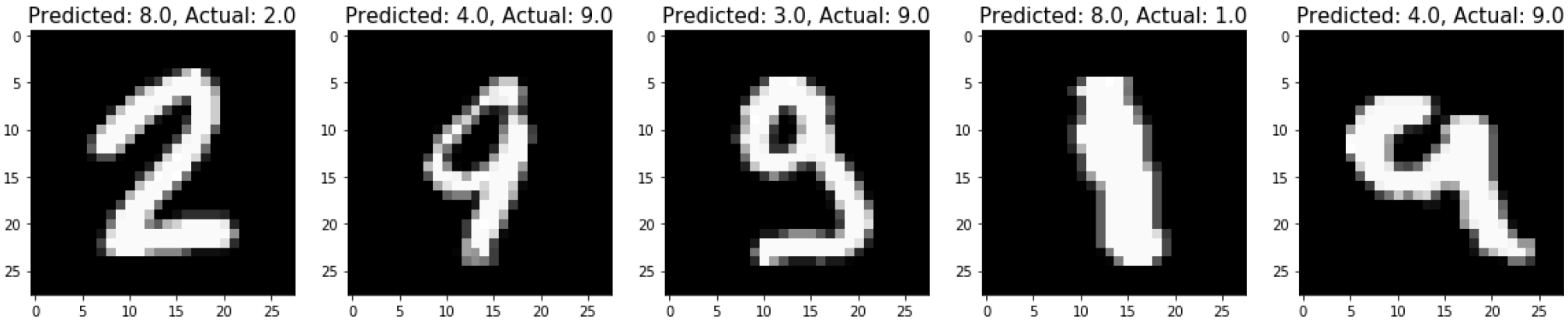
Results of Softmax Regression on MNIST Dataset

(Softmax, a generalization of Logistic Regression >2 classes, to be discussed in next session)

Examples of Misclassified Images



https://www.kdnuggets.com/2016/07/softmax-regression-related-logistic-regression.html

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Softmax Regression on MNIST

The Results:

On the 60000 Training Images	On the 10000 Test Images
Mean Accuracy: 0.94	Mean Accuracy: 0.92
Misclassified Images: 3893 (6.5%)	Misclassified Images: 817 (8.2%)

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Introduction to Machine Learning

1. What is Machine Learning
2. Unsupervised vs Supervised Learning
3. Linear Regression
4. Logistic Regression
5. K-Means and PCA

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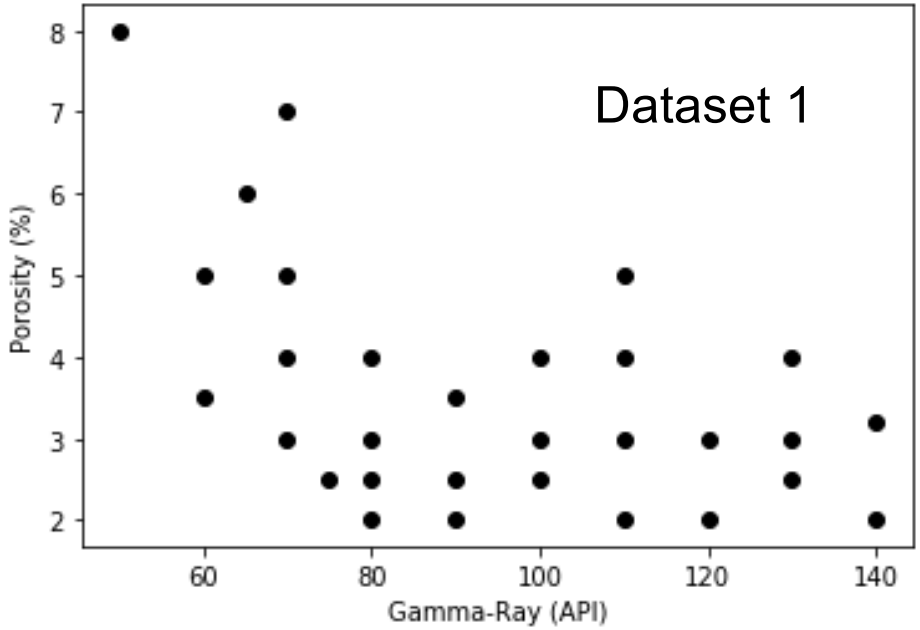
Clustering is an Unsupervised Learning Approach



The Training set has no labels $y^{(i)}$, it only has two features $x^{(i)}$
Clustering automatically groups the input training examples into a small number of clusters of « similar » examples.

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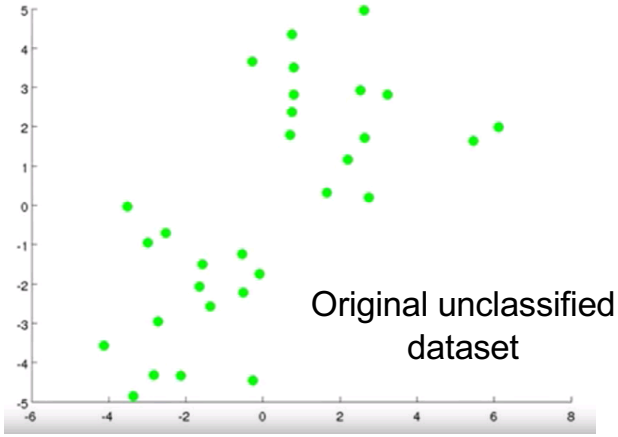
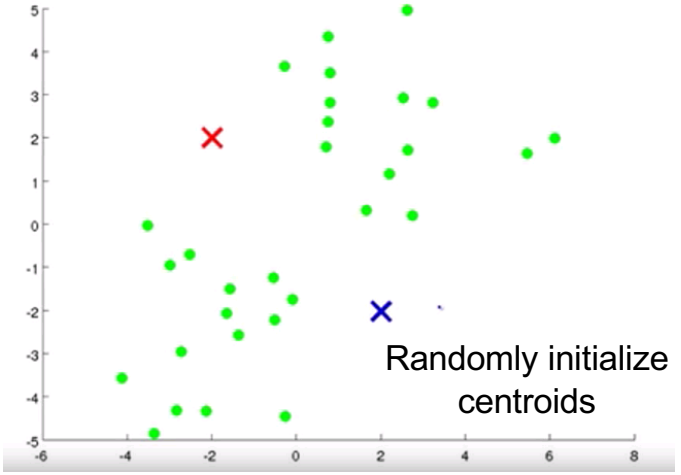
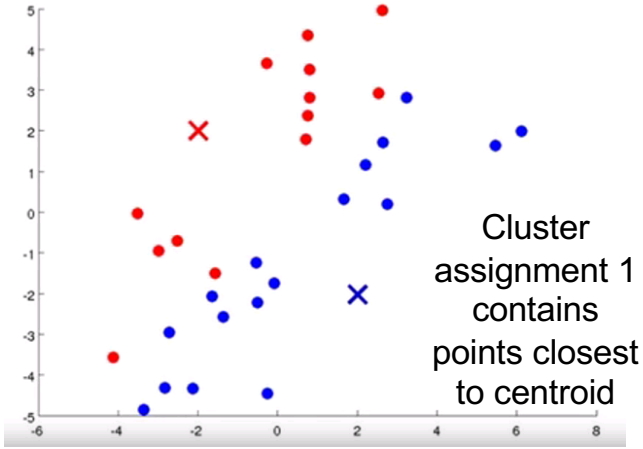
K-Means: The Algorithm (1)



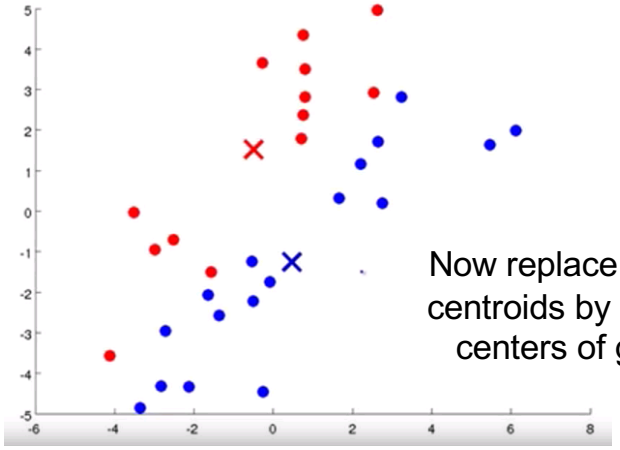
Original unclassified dataset



Randomly initialize centroids



Cluster assignment 1 contains points closest to centroid



Now replace random centroids by clusters' centers of gravity

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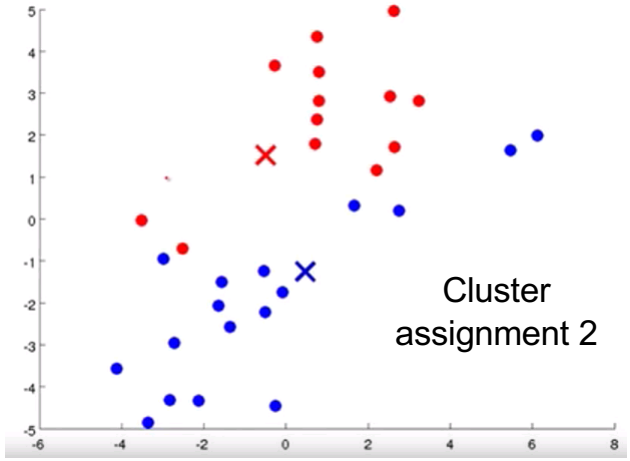
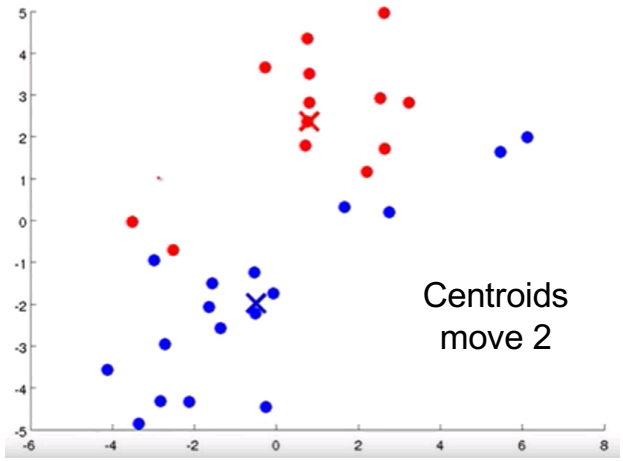
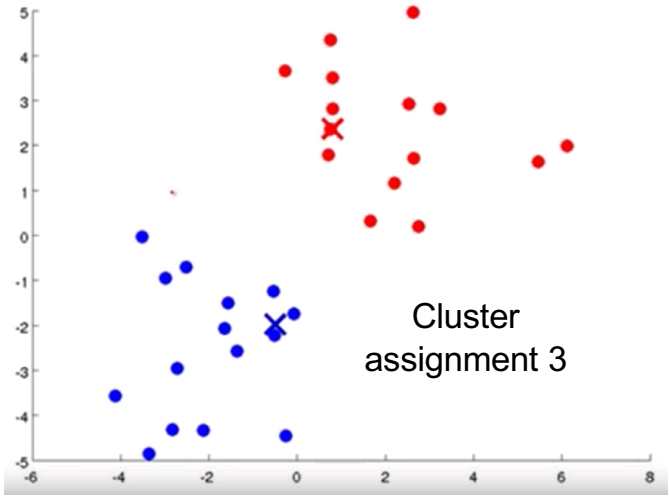
K-Means: The Algorithm (2)







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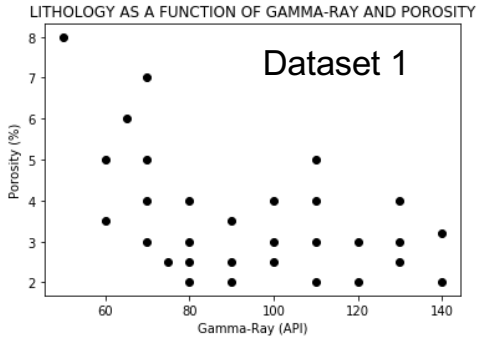
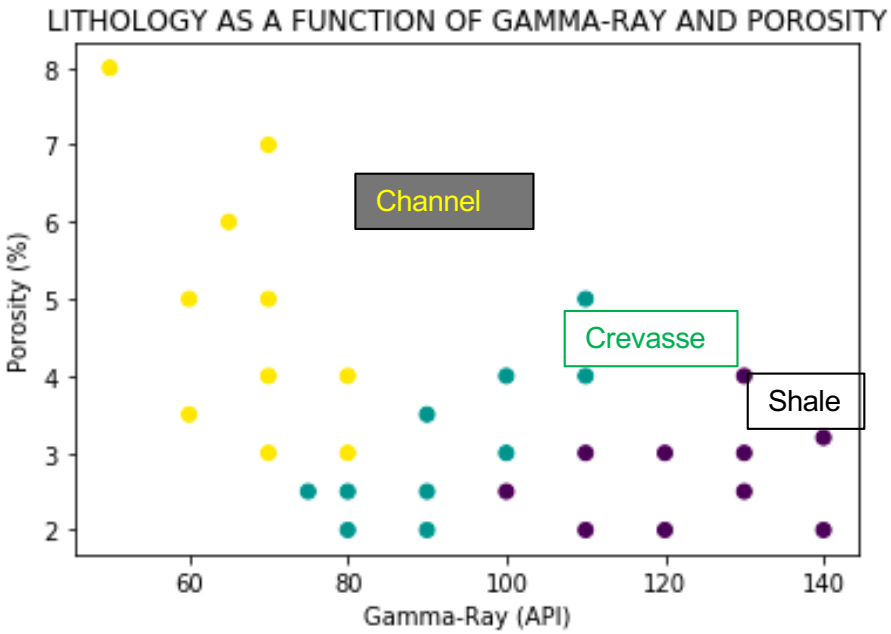
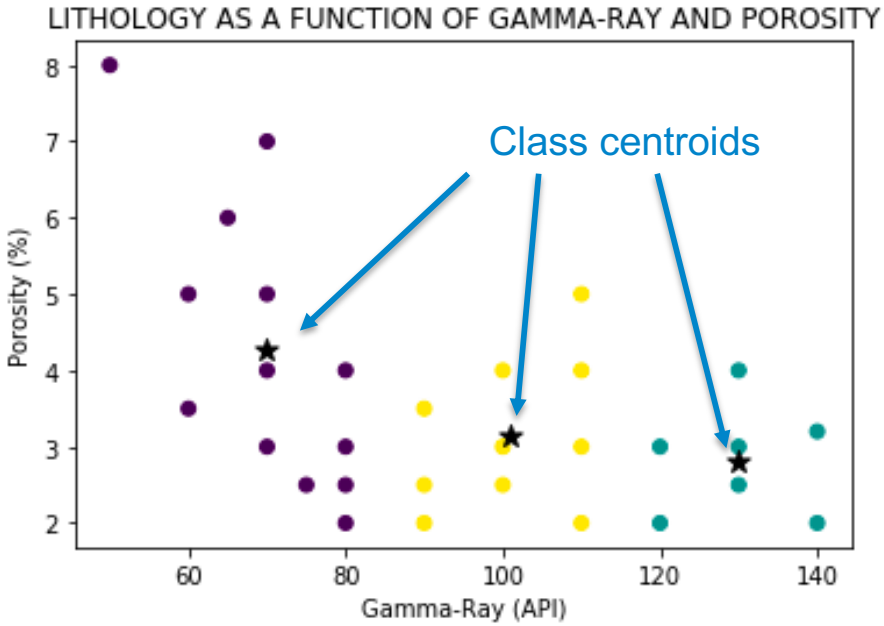


K-Means on Lithology Dataset 1

ACTUAL CLASSES



CLASSES FROM K-MEANS



Good!

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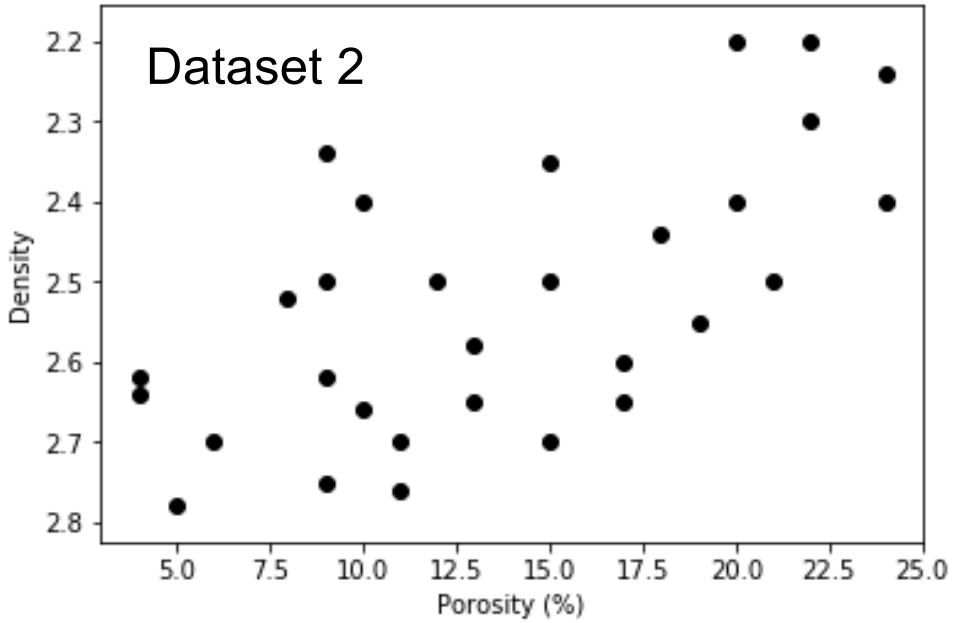
Clustering is an Unsupervised Learning Approach



The Training set has no labels $y^{(i)}$, it only has features $x^{(i)}$
Clustering automatically groups the input training examples into a small number of clusters of « similar » examples.

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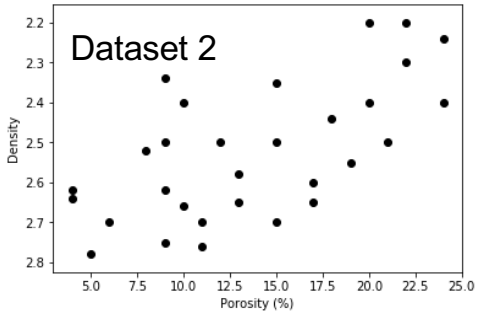
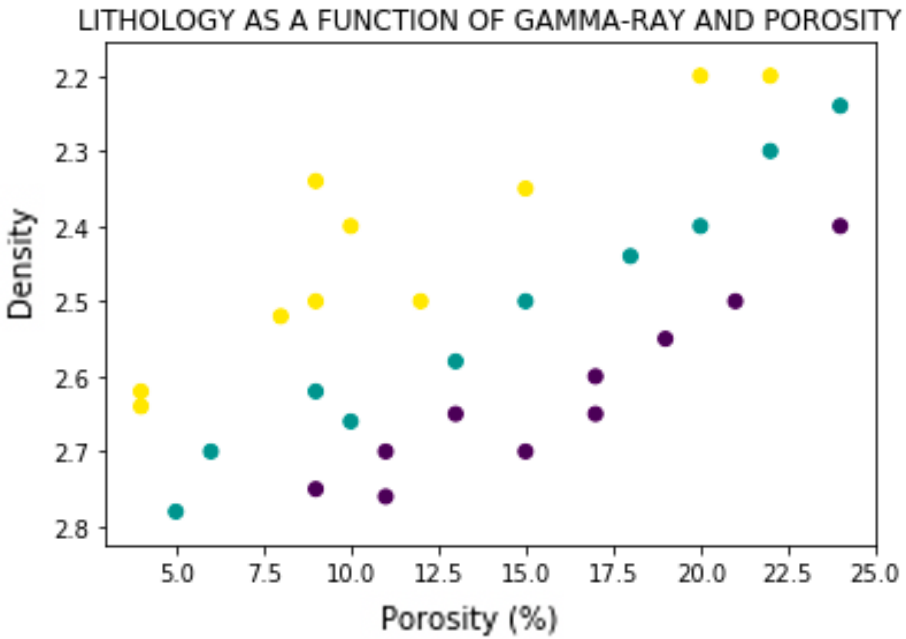
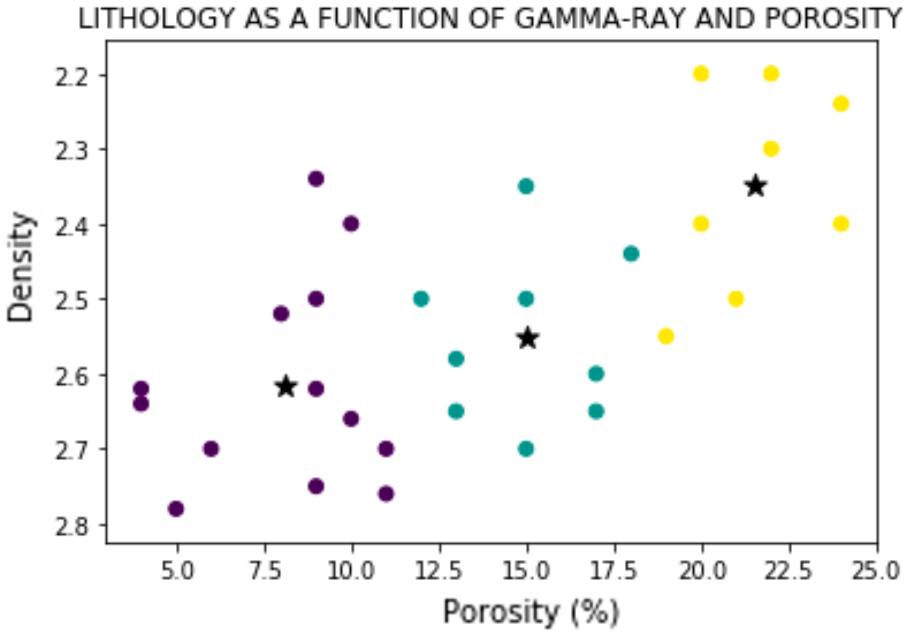


K-Means on Lithology Dataset 2

ACTUAL CLASSES



CLASSES FROM K-MEANS



Poor!

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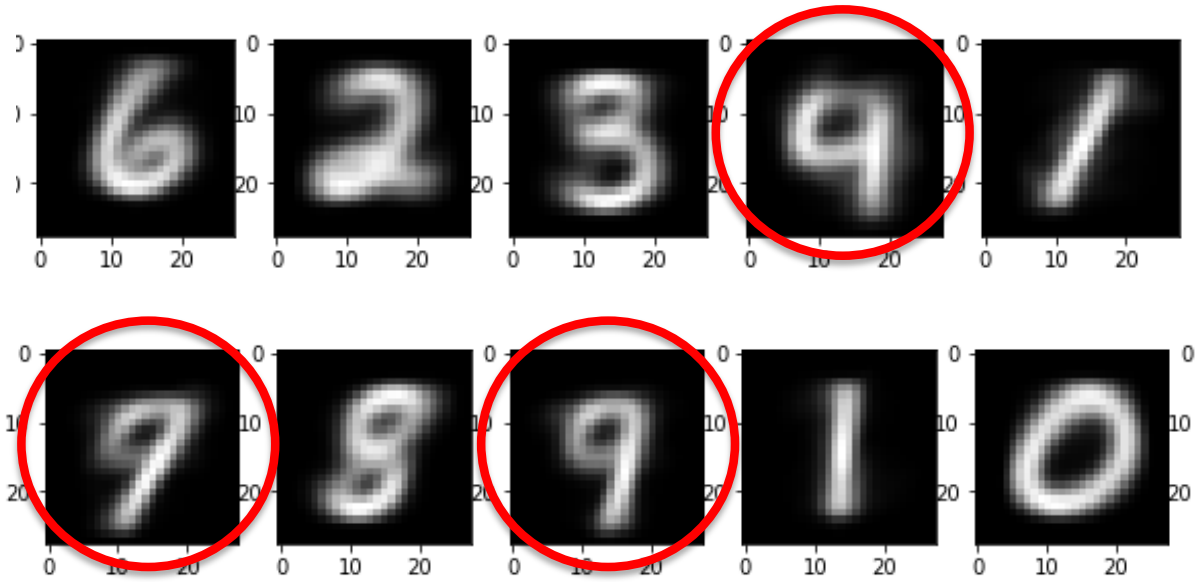
Applying K-Means to the MNIST Example

Number of classes:
k=10

Each square is a
class centroid
(or class mean)



Digits 4, 5, 7 are not represented as individual classes.
There are three classes that look like a mixture of 4, 7 and 9

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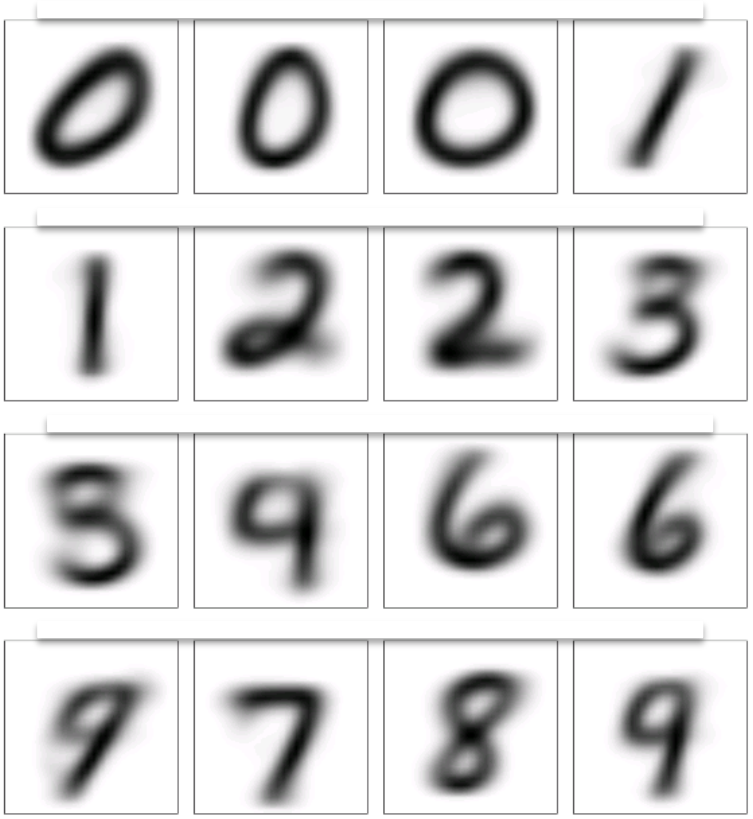
Applying K-Means with 16 Classes to MNIST

Number of classes:
k=16

Each square is a
class centroid
(or class mean)



Source: http://johnloeber.com/docs/kmeans.html

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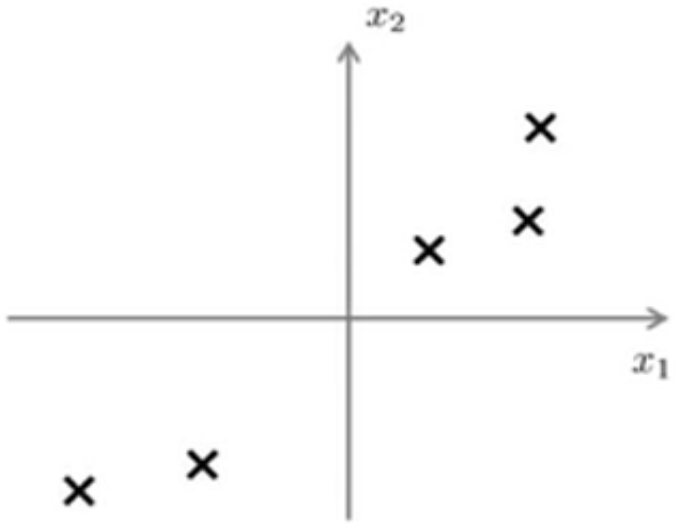
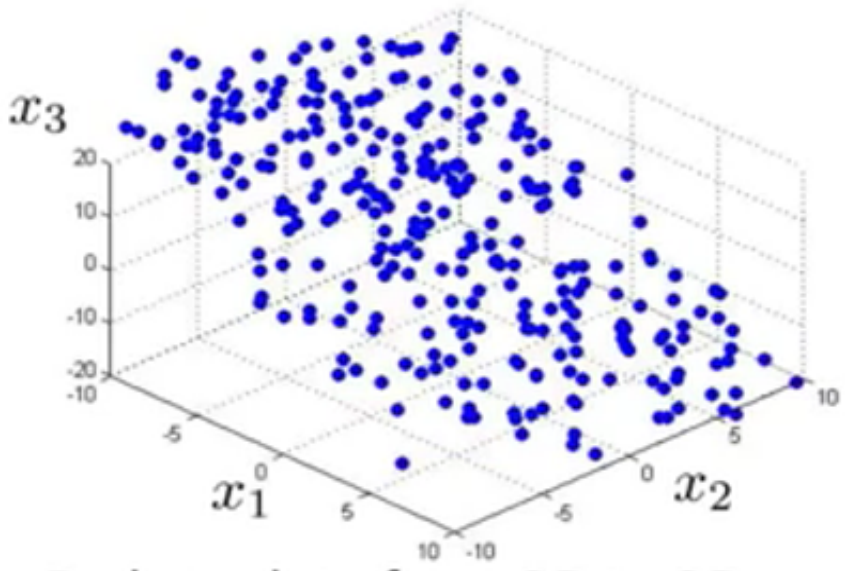
Dimensionality Reduction: the PCA approach



Opportunity to Project 2-D Data into 1-D Space



Opportunity to Project 3-D Data into 2-D Space

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The PCA Approach: Preliminary Data Normalization

Training Set vectors: $x^{(1)}, x^{(2)}, \ldots \ldots, x^{(m)}$. (no label)

Calculate mean of coordinates of the training vectors: $\mu_j = \frac{1}{m}\sum_{i=1}^{m} x_j^{(i)}$

Calculate standard deviation s_j of coordinates of the training vectors: $s_j^2 = \frac{1}{m}\sum_{i=1}^{m} x_j^{(i)2} - \mu_j^2$

Replace each input feature by normalized value: $\boldsymbol{x_j^{(i)} := \frac{x_j^{(i)} - \mu_j}{s_j}}$

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Dimensionality Reduction: the PCA algorithm

Training Set vectors: $x^{(1)}, x^{(2)}, \ldots \ldots, x^{(m)}$ (no label).

To project data from n-dimensional to k-dimensional space, calculate covariance matrix:

$$\Sigma = \frac{1}{m}\sum_{i=1}^{m}\left(x^{(i)}\right)\left(x^{(i)}\right)^{T}$$

Then compute eigenvalues $(\lambda_i)_{i=1\ldots m}$ of matrix Σ

Keep the p largest eigenvalues $(\lambda_i)_{i=1\ldots p}$ and project on the space of dimension p defined by the associated p eigenvectors, also called principal components.

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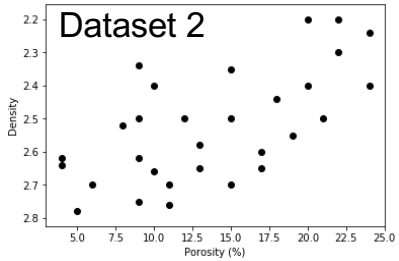
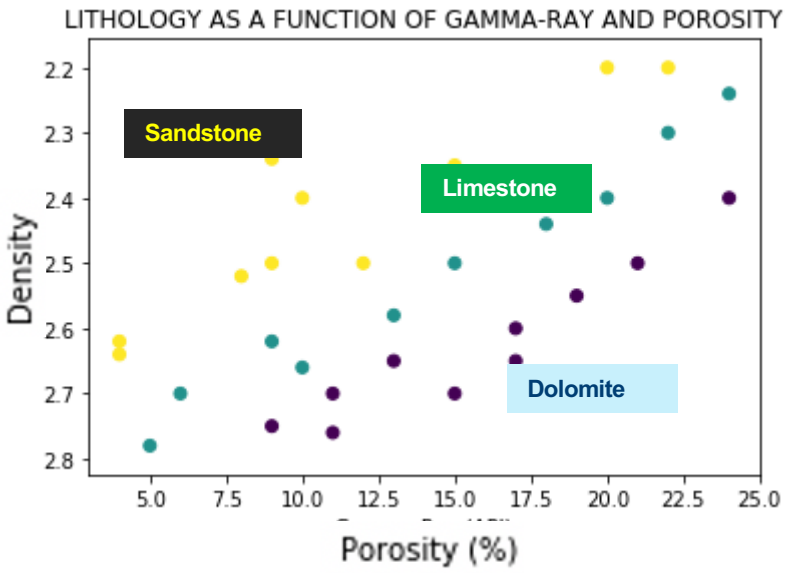


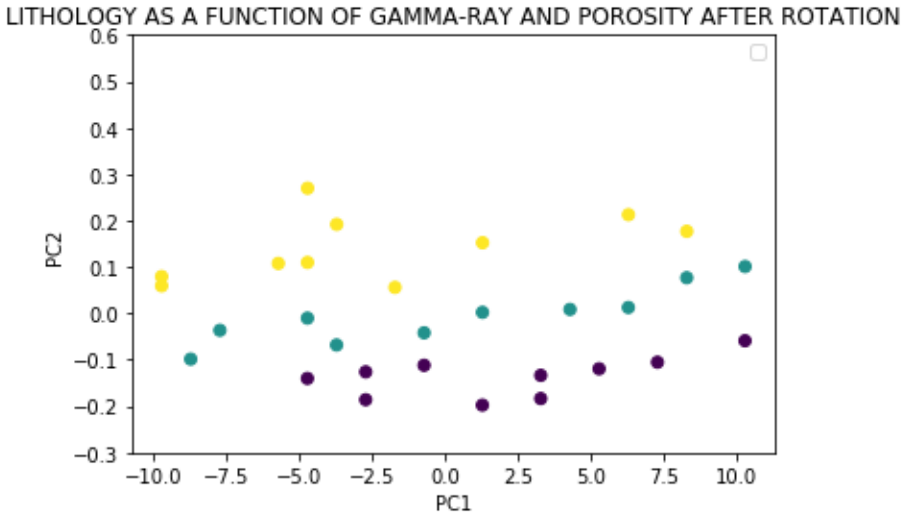
Dimensionality Reduction: PCA on Dataset 2

Original Data Space



PCA

Principal Components Space



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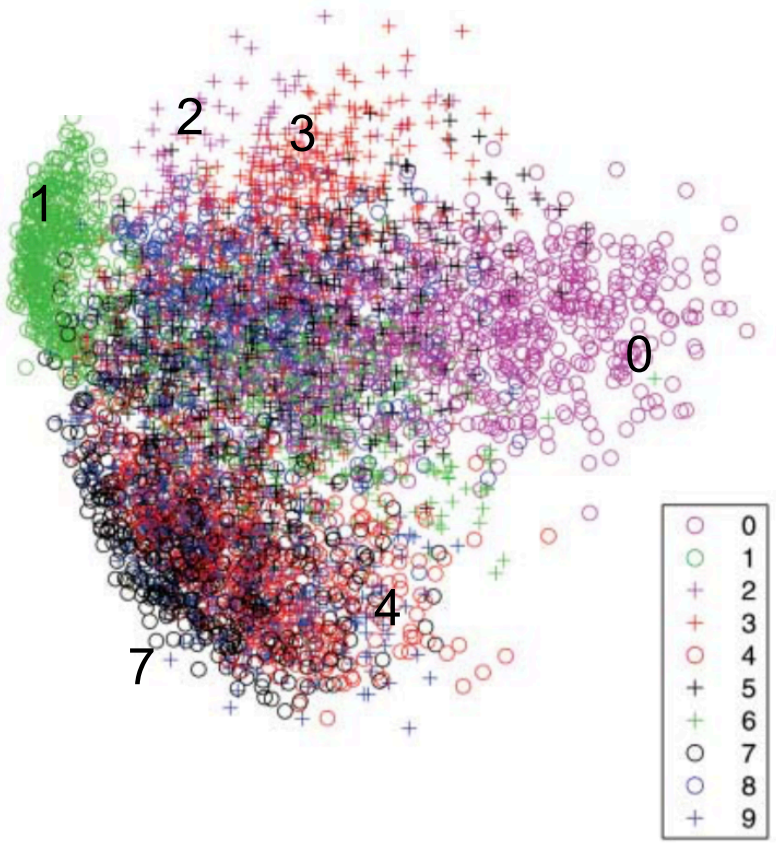
MNIST Results with PCA



The two first principal components for 500 digits of each class produced by taking the first two principal components of all 60,000 training images. The labels were not used for PCA, they are just posted on the PCA results.

From Hinton and Salakhutdinov, Science, Science, July 2006

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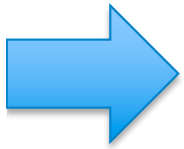
First Session Conclusion

- **Supervised vs Unsupervised Learning**
- **Regression: The Elementary Machine Learning Approach**
- **Logistic Regression: The Elementary Supervised Classification Approach**
- **K-Means and PCA: The Elementary Unsupervised Classification Approaches**
- **Mathematical Notations are Important.**



Neural Nets and Deep Learning are going to be a generalization of the above to more complex (non-linear) approaches applied to huge datasets.