Machine Learning Algorithms Illustrated in Python

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Abstract

In order to gain a deeper understanding of *artificial intelligence* algorithms, I will explore a *supervised* learning algorithm, *linear regression*, and an *unsupervised* learning algorithm, *K-means clustering.* After researching these algorithms' mathematical descriptions, I will write implementations both in Python and visualize their outcomes.

1 Introduction

In this paper, I will strictly define a subset of artificial intelligence called *machine learning.* Before diving into the mathematical descriptions and definitions of these algorithms, I will distinguish *supervised learning* from *unsupervised learning.* The *supervised* learning algorithm I will explore is known as a *linear regression* and the *unsupervised* learning algorithm is *K-means clustering.*

Additionally, *supervised learning algorithms* are computationally intensive, so before writing any code it would be most useful to compute the algorithm by hand with a *training set.* Doing this will allow me to understand where inefficiencies in code and computation can occur, or what mathematical concepts and definitions I can apply to my code. Once I have my mathematical descriptions written, I will proceed to write my own code. The popular scientific computing Python library called *NumPy* [2] will be used to handle most of the heavy computational aspects of these algorithms. The Python graphing library called *matplotlib* [1] is used for the visualization of my data and calculations.

2 Machine Learning

Machine learning is one of the many subsets of *artificial intelligence*, known as the study of how to make computers capable of intelligent behavior. Specifically, it deals with the creation of data driven algorithms. These algorithms produce patterns based on given input and use the patterns to predict future cases. The main differentiation of machine learning from another subset of artificial intelligence is that the data drives discovery. For example, say an individual is writing an algorithm that detects what a face looks like. A machine learning algorithm would learn by example, juxtaposed to another type of algorithm that would strictly define what a face looks like in the code the code. Inside of machine learning, there primarily two different types of algorithms: *supervised* and *unsupervised* learning.

3 Supervised Learning Algorithms

3.1 Definition

In *supervised learning* there are two groups of algorithms: classification and regression. Both complete the task of deducing a continuous function from a given *training set*. [4] A *training set* is a vector of discrete values used for the initial discovery of relationships between variables. In order to prevent *overfitting*, deducing conclusions when none exist, a *validation set* is used in case any classification parameter needs to be adjusted. Furthermore, a *test set* is used to gauge the efficiency of a given model. [4] One classic example of a *supervised learning* algorithm is a *linear regression*. Going back to our example of an algorithm classifying a face, a supervised learning algorithm would teach itself through examples what a face looks like in terms of its properties, such as color, structure, and size, so it can classify future inputs based upon these discoveries already made.

3.2 Example: Linear Regression

3.2.1 Definition

A *linear regression* is an approach for modeling the relationship between a scalar dependent variable y and one or more explanatory variables or independent variables) denoted X. Specifically, the case of one explanatory variable is called a *linear regression.* A sample data set for a linear regression would be pairs $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$ where the regression models y_i as a function of x_i

3.2.2 Mathematical Description

The *regression line* can be determined by finding *sum of squares* method. A *fitted linear regression line* can be described as

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 * x \quad [3] \tag{1}$$

$\hat{\beta}_0$ is defined as

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} \tag{2}$$

Given n is the number of data points in the *training set*

$$\bar{y} \equiv \frac{1}{n} \sum y_i \tag{3}$$

$$\bar{x} \equiv \frac{1}{n} \sum x_i \tag{4}$$

$$\hat{\beta}_1 = \left(\frac{n \sum x_i y_i - (\sum x_i)(\sum y_i)}{n \sum x_i^2 - (\sum x_i)^2} \right) \tag{5}$$

An easier way to express $\hat{\beta}_1$ can be defined as

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} \tag{6}$$

Where S_{xy} and S_{xx} are

$$\begin{aligned} S_{xy} &= \sum (x_i - \bar{x})(y_i - \bar{y}) \\ &= \sum x_i y_i - \frac{(\sum x_i)(\sum y_i)}{n} \\ &= \sum x_i y_i - \bar{x} * \bar{y} \end{aligned}$$

$$
\begin{aligned}
S_{xx} &= \sum (x_i - \bar{x})^2 \\
&= \sum (x_i)^2 - \frac{(\sum x_i)^2}{n} \\
&= \sum (x_i)^2 - \bar{x}
\end{aligned}
$$

3.2.3 Example Use Case

You are given a vector of training data, V, such that $V = \{(x_1, y_1), ..., (x_n, y_n)\}$ where x_i is the amount of hours an individual studied for a test and y_i is their score on that test.
Let the pairs of values of V be defined in the table given below.

X: Time Studied (Hours)	Y: Score (Out of 800)
4	390
9	580
10	650
14	730
4	410
7	530
12	600
22	790
1	350
3	400
8	590
11	640
5	450
6	520
10	690
11	690
16	770
13	700
13	730
10	64

3.2.4 Calculations

First, I will calculate $\bar{x}$ and $\bar{y}$, better known as the average values for x and y respectively

$$\begin{aligned}\bar{x} &= \frac{1}{n} * \sum_{i=1}^{20} x_i \\ &= \frac{1}{20} * \sum_{i=1}^{20} x_i \\ &= \frac{1}{20} * 157 \\ &= 8.72\end{aligned}$$

$$\begin{aligned}\bar{y} &= \frac{1}{n} * \sum_{i=1}^{20} y_i \\ &= \frac{1}{20} * \sum_{i=1}^{20} y_i \\ &= \frac{1}{20} * 10420 \\ &= 578.89\end{aligned}$$

Thus, based on our training set defined above $\bar{x} = 8.72$ and $\bar{y} = 578.89$
Next, I will use the previous calculations of $\bar{x}$ and $\bar{y}$ to calculate S_{xy} and S_{xx}

$$\begin{aligned} S_{xx} &= \sum_{i=1}^{20} (x_i)^2 - \bar{x} \\ &= \sum_{i=1}^{i=20} (x_i)^2 - \sum_{i=1}^{i=20} \bar{x} \\ &= 285.31 \\ S_{xy} &= \sum_{i=1}^{20} (x_i)(y_i) - \bar{x}\bar{y} \\ &= \sum_{i=1}^{20} (x_i)(y_i) - \sum_{i=1}^{20} \bar{x}\bar{y} \\ &= 8598.02 \end{aligned}$$

Now, we have all calculations we need to find where β_1

$$\begin{aligned} \beta_1 &= \frac{S_{xy}}{S_{xx}} \\ &= \frac{8598.02}{285.31} \\ &= 30.14 \end{aligned}$$

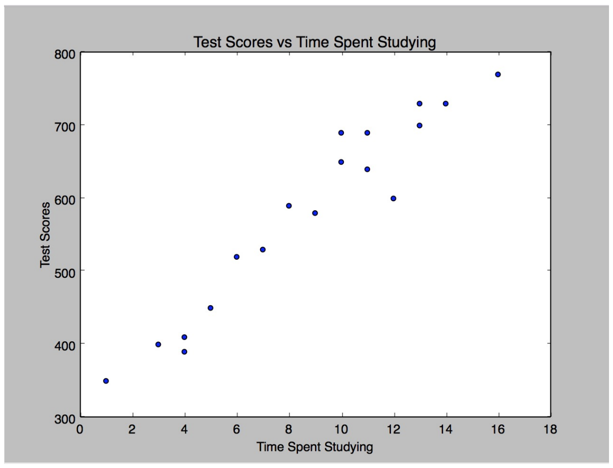
Since we have β_0 we can use it in our final calculation of β_1

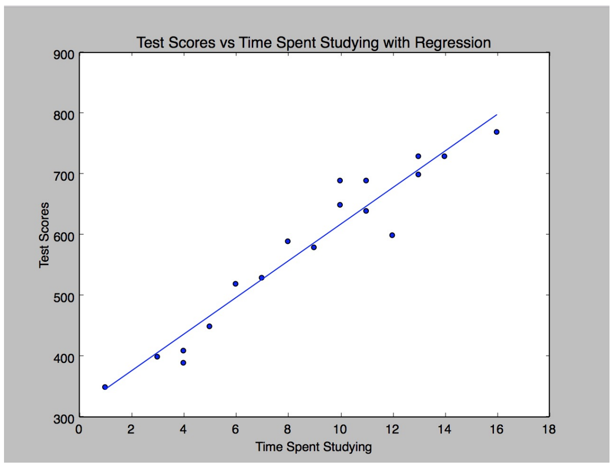
$$\begin{aligned} \beta_0 &= \bar{y} - \beta_1 * \bar{x} \\ &= 578.89 - 8.24 * 9.45 \\ &= 316.82 \end{aligned}$$

Our linear regression line is now

$$y = 316.04 + 30.14x \qquad (7)$$

3.2.5 Geometric Representation





As you can see from the two graphs, our linear regression is a strong approximation of our data set.

3.2.6 Sample Sum of Squares Regression in Python

```
#!/usr/bin/python
import numpy as np # scientific computing library
import matplotlib.pyplot as plt # library to generate
    plots

class SumSquareRegression:
# Creates instance of SumSquareRegression object
class SumSquareRegression:

  def __init__(self, data_set):

    self.data_set = data_set
    self.avg = self.data_avg(self.data_set)
    self.x_bar = self.avg[0]
    self.y_bar = self.avg[1]
    self.sxxy = self.calculate_sxxy(data_set, self.
       x_bar, self.y_bar)
    self.sxx = self.sxxy[0]
    self.sxy = self.sxxy[1]
    self.beta_1 = (self.sxy / self.sxx)
    self.beta_0 = (self.y_bar - self.beta_1 * self.x_bar)

  # O(n) time complexity
  # O(1) space complexity
  # Returns an array containing avg x and avg y values
  def data_avg(self, vector):
    sum_x = 0
    sum_y = 0
    size = len(vector)

    for i in range(0, size ):
      sum_x += vector[i][0]
      sum_y += vector[i][1]

    # type casting to return a decimal
    return [float(sum_x)/size, float(sum_y)/size]

  # O(n) time complexity
  # O(1) space complexity
  # Returns S_xx and S_yy in an array respectively
  def calculate_sxxy(self, vector, x_bar, y_bar):
    sxx_sum = 0
    sxy_sum = 0

    for i in range(0, len(vector) - 1):
      sxx_sum += (vector[i][0] - self.x_bar) ** 2
      sxy_sum += (vector[i][0] - self.x_bar) * (vector[i][1] - self.y_bar)

    return [sxx_sum, sxy_sum]

  # Prints stats related to regression
  def print_regression_stats(self):
    print "x_bar: %.2f" % self.x_bar
    print "y_bar: %.2f" % self.y_bar
    print "s_xx: %.2f" % self.sxx
    print "s_xy: %.2f" % self.sxy
    print "beta_0: %.2f" % self.beta_0
    print "beta_1: %.2f" % self.beta_1
    print "Regression Line: y = %.2fx + %.2f" % (self.beta_1, self.beta_0)

  def plot_data(self, data):
    x_list = [x for [x, y] in data]
    y_list = [y for [x, y] in data]
    plt.scatter(x_list, y_list)
    plt.ylabel('Test Scores')
    plt.xlabel('Time Spent Studying')
    plt.title('Test Scores vs Time Spent Studying')
    plt.show()

  def plot_with_regression(self, data):
    # plot data
    x_list = [x for [x, y] in data]
    y_list = [y for [x, y] in data]
    plt.scatter(x_list, y_list)
    plt.ylabel('Test Scores')
    plt.xlabel('Time Spent Studying')
    # plot regression
    # uses python list comprehension
    y = [self.regression_approximation(x) for [x, y] in data]
    plt.plot(x_list, y)
    # print plot
    plt.title('Test Scores vs Time Spent Studying with Regression')
    plt.show()

  def regression_approximation(self, x):
    return (self.beta_1 * x) + (self.beta_0)

# Test Data
def main():
    sample_data_1 = [[4, 390],[9, 580],[10, 650],[14,
        730],[4, 410],[7, 530],[12, 600],[1, 350],[3,
        400],[8, 590],[11, 640],[5, 450],[6, 520],[10,
        690],[11, 690],[16, 770],[13, 700],[13, 730]]
    regression_1 = SumSquareRegression(sample_data_1)
    regression_1.print_regression_stats()
    regression_1.plot_data(sample_data_1)
    regression_1.plot_with_regression(sample_data_1)

# Runs program automatically
if __name__ == '__main__':
    main()
```

4 Unsupervised Learning Algorithms

4.1 Definition

Our expected outcome from unsupervised learning is to derive some structure from the data where none previously existed. That being said, we are "clustering" the data into groups based on intrinsic relationships found. Hence, this type of algorithm allows user to approach the problem at hand with little to no knowledge of what the result should look like. Back to our example of face classification, an unsupervised algorithm would differentiate faces from cows and dogs, but it would not know or define what each group is.

4.2 Example K-means clustering

4.2.1 Defintion

Grouping a set of objects into similar subsets is a very common task in data analysis and is often referred to as "clustering". This task can be done in a copious amount of ways, however, one of the most prominent algorithms is *K-means clustering*. The *K-means clustering* algorithm aims to partition $n \in \mathbb{N}$ points in a d dimensional space into $k > 0$ distinct clusters. Thus, given a vector of data $X \in \mathbb{R}^d$ with d and n given above, our algorithm seeks to find a set C of k centers. [6]

4.2.2 Mathematical Description

Unfortunately, finding solutions to K-means clustering is *NP Hard*. Computational complexity theory describes *NP Hard* as non-deterministic polynomial time, or it may or may not be able to be solved in polynomial time. *Lloyd's Algorithm* offers an iterative solution to this k-means clustering solution. Let the dataset be a vector X with n points such that $(\forall i \in X)(X_i \in \mathbb{R})$, where $((n > 0) \in \mathbb{N})$ as input, given a parameter $((K > 0) \in \mathbb{N})$ which determines how many clusters to create. Let the output be a set of K cluster centroids, or centers of data clusters, and a labeling of X that assigns each of the points in X to a unique cluster. All points within a cluster are closer in distance to their centroid than they are to any other centroid.
Let C be the set of clusters such that $C_k \subset C$, the set of clusters, C_k be calculated as follows.

$$C_k = \{x_n : ||x_n - \mu_k|| \leq \ \ all \ \ ||x_n - \mu_l||\} \tag{8}$$

μ_k is defined to be the average values clusters

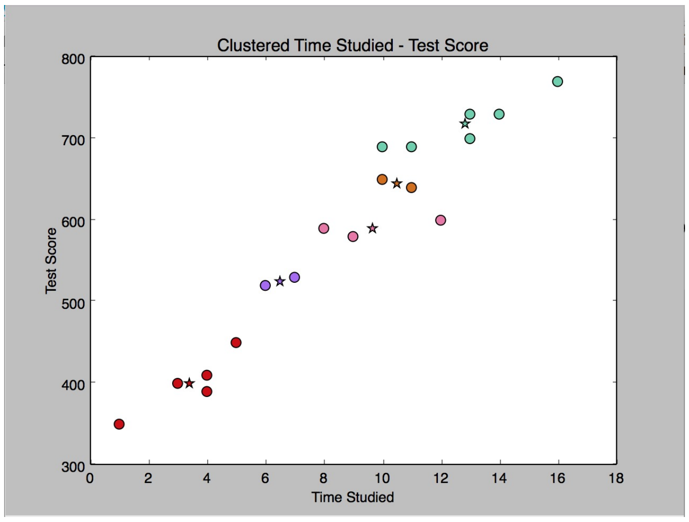
$$\mu_k = \frac{1}{C_k} \sum_{x_n \in C_k} x_n \tag{9}$$

The mathematical condition for the K clusters C_k and the K centroids μ_k can be expressed as:

$$\text{Minimize} \sum_{k=1}^{K} \sum_{x_n \in C_k} (||x_n - \mu_k||)^2 \text{with respect to } C_k, \mu_k \tag{10}$$

[5] The result is a partitioning of data into Voronoi cells. This is why *Lloyd's Algorithm* is also called *Voronoi iteration.*

4.2.3 Geometric Representation



4.2.4 Sample K-means clustering in Python

```
#!/usr/bin/python
import numpy as np # scientific computing library
import matplotlib.pyplot as plt # plotting
import random # used to generate random centroids

class KMeansClustering:

  def __init__(self, data_set, k):
    self.data_set = data_set
    self.k = k

  # for each point in data set,
  # find new subset it belongs too.
  def generate_clusters(self, mu):
    clusters = {}
    for pt in self.data_set:
      # for each pt in our data set
      # find best fitting value
```

```
            best_mu = min([(array[0], np.linalg.norm(pt - mu[array[0]])) \
                        for array in enumerate(mu)], key = lambda t:t[1])[0]
            try:
                clusters[best_mu].append(pt)
            except KeyError:
                clusters[best_mu] = [pt]
        return clusters

    # calcuate new mu values
    def reevaluate_centers(self, mu, clusters):
        new_mu = []
        keys = sorted(clusters.keys())
        for k in keys:
            new_mu.append(np.mean(clusters[k], axis = 0))
        return new_mu

    def has_converged(self, mu, old_mu):
            # we know we have converged if our old and new mu values are the same
        return (set([tuple(a) for a in mu]) == set([tuple(a) for a in old_mu]))

    def k_means(self):
     # at first, randomize centroids
        old_mu = random.sample(self.data_set, self.k)
        mu = random.sample(self.data_set, self.k)

        while not self.has_converged(mu, old_mu):
            old_mu = mu

        # assign pts in data_set to clusters
            clusters = self.generate_clusters(mu)

        # recalculate centers
            mu = self.reevaluate_centers(old_mu, clusters)

        return(mu, clusters)

    def main():
    # Notice this the same as the last dataset
    # Instead of predictive modeling we'll use this data to split into
    # distinct ranges (think A, B, C, D, F) in this case
    sample_data_1 = np.array([[4, 390],[9, 580],[10, 650],[14, 730],[4, 410],[7, 530],[12, 600],[1, 350],[3, 400],[8, 590],[11, 640],[5, 450],[6, 520],[10, 690],[11, 690],[16, 770],[13, 700],[13, 730]])
    k = 5 # how many different clusters do we want?
    clustered = KMeansClustering(sample_data_1, k) # initialize object
    data = clustered.k_means()

    # parse data to plot
    centroids = data[0]
    clusters = data[1]
    i = 0
    for centroid in centroids:
        c = np.random.rand(3,1)
        s = 70,
        plt.scatter(centroid[0],centroid[1], s, c, marker = '*')
        data = clusters[i]
        for pt in data:
            plt.scatter(pt[0],pt[1], s ,c)
        i += 1
    plt.xlabel('Time Studied')
    plt.ylabel('Test Score')
    plt.title('Clustered Time Studied - Test Score')
    plt.show()

    if __name__ == '__main__':
    main()
```

References

[1] http://matplotlib.org/

[2] http://www.numpy.org/

[3] http://www2.isye.gatech.edu/s̃man/courses/6739SimpleLinearRegression.pdf

[4] http://cs229.stanford.edu/notes/cs229-notes1.pdf

[5] https://datasciencelab.wordpress.com/2013/12/12/clustering-with-k-means-in-python/

[6] Mackay, David J. C. (2002) *Information Theory, Inference & Learning Algorithms* Cambridge University Press

[7] https://github.com/skamdart

Acknowledgement

Source code for this .tex file and my algorithms can be found at my GitHub [7]