Hello Clustering

Recall from lecture that K-means has two main steps: the points assignment step, and the mean update step. After the initialization of the centroids, we assign each data point to a centroid. Then, each centroids are updated by re-estimating the means.

Concretely, if we are given N data points, x1, x2, ..., xN , and we would like to form K clusters. We do the following;

1. **Initialization**: Pick K random data points as K centroid locations c1, c2, ..., cK .
2. **Assign**: For each data point k, find the closest centroid. Assign that data point to the centroid. The distance used is typically Euclidean distance.
3. **Update**: For each centroid, calculate the mean from the data points assigned to it.
4. **Repeat**: repeat step 2 and 3 until the centroids stop changing (conver-gence).

   Given the following data points in x-y coordinates (2 dimensional)

x	y
1	2
3	3
2	2
8	8
6	6
7	7
-3	-3
-2	-4
-7	-7

In [693…

```
# Install all modules
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import copy
```

In [694…

```
# Initialize dataframe
x = np.array([1, 3, 2, 8, 6, 7, -3, -2, -7])
y = np.array([2, 3, 2, 8, 6, 7, -3, -4, -7])
dataframe_points = pd.DataFrame({'x': x, 'y': y})
```

In [695…

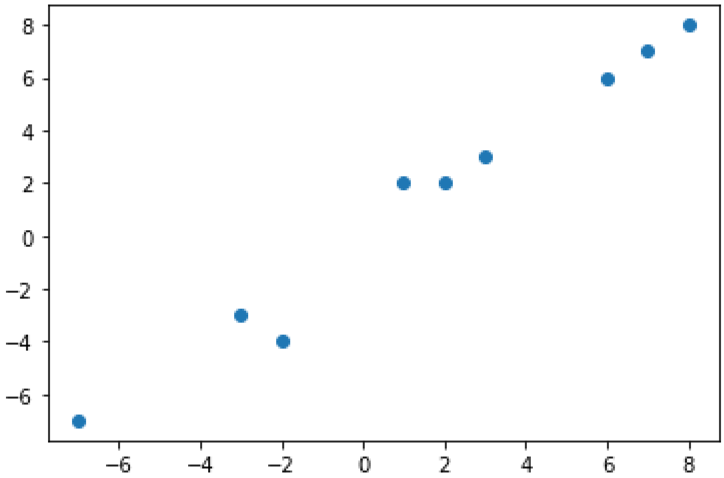
```
# Print dataframe
dataframe_points
```

Out[695]:

	x	y
0	1	2
1	3	3
2	2	2
3	8	8
4	6	6
5	7	7
6	-3	-3
7	-2	-4
8	-7	-7

In [696…

```
# Plot dataframe
plt.scatter(dataframe_points['x'], dataframe_points['y'])
plt.show()
```



In [697…

```
# Create KMeans class
class KMeans:
  def __init__(self, points, starting_centriods):
    self.points = points
    self.centriods = starting_centriods
    self.clusters = self.__find_clusters()
    self.iterations = 0

  # Find clusters
  def __find_clusters(self):
    # Copy data
    centriods = self.centriods.copy()
    points = self.points.copy()
    # Initialize clusters
    clusters = [[] for _ in range(len(centriods))]
    # Find clusters
    for point in points.to_numpy():
      distances = []
      for centroid in centriods.to_numpy():
        # Calculate distance from each point to each centroid using Euclide
        distance = np.linalg.norm(point - centroid)
        distances.append(distance)
      # Assign point to cluster
      clusters[np.argmin(distances)].append(point)
```

```
    # Update clusters
    self.clusters = clusters
    # Return clusters
    return clusters

  # Update centriods
  def __update_centriods(self):
    # Copy data
    centriods = self.centriods.copy()
    clusters = self.clusters.copy()
    # Update centriods
    for i in range(len(clusters)):
      clustered_points = clusters[i]
      centriods.iloc[i] = np.mean(clustered_points, axis=0)
    # Return updated centriods
    return centriods

  def run(self):
    self.centriods = self.__update_centriods()
    self.clusters = self.__find_clusters()
    self.iterations += 1

  def plot(self):
    colors = ['violet', 'limegreen', 'skyblue']
    darken_colors = ['indigo', 'green', 'blue']
    for i in range(len(self.clusters)):
      clustered_points = np.array(self.clusters[i])
      plt.scatter(clustered_points[:, 0], clustered_points[:, 1], label=i, 
      plt.scatter(self.centriods['x'][i], self.centriods['y'][i], marker='*
    plt.legend()
    plt.show()
```

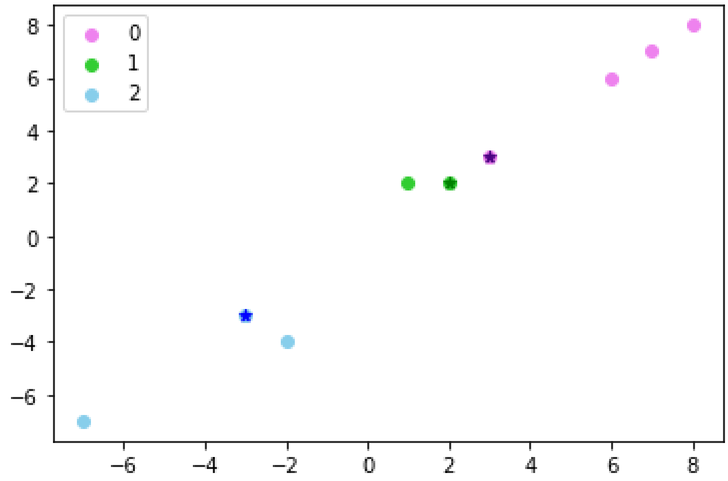
T1

If the starting points are (3,3), (2,2), and (-3,-3). Describe each assign and update step. What are the points assigned? What are the updated centroids? You may do this calculation by hand or write a program to do it.

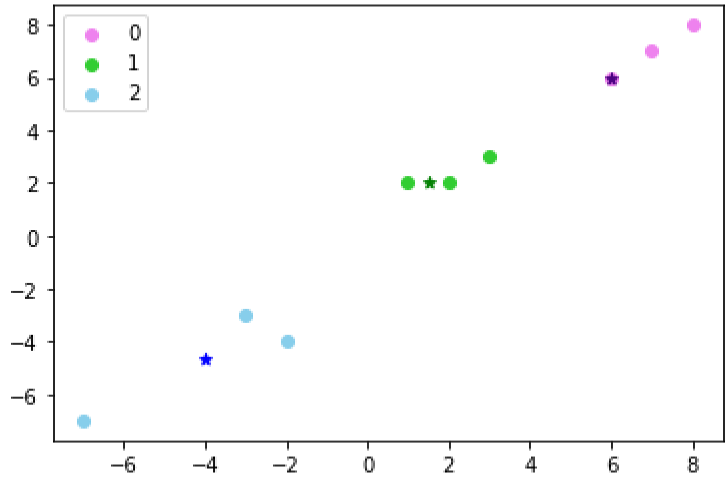
In [698…

```
# Initialize centroids
starting_centriods = pd.DataFrame({
  'x': [3, 2, -3],
  'y': [3, 2, -3]
})
kMeans = KMeans(dataframe_points, starting_centriods)
print(kMeans.centriods)
kMeans.plot()
kMeans.run()
print(kMeans.centriods)
kMeans.plot()
```

```
   x  y
0  3  3
1  2  2
2 -3 -3
```




```
     x         y
0   6.0   6.000000
1   1.5   2.000000
2  -4.0  -4.666667
```



Answer

updated centroids คือ

1. (6, 6)
2. (1.5, 2)
3. (-4, -4.67) ตามลำดับ

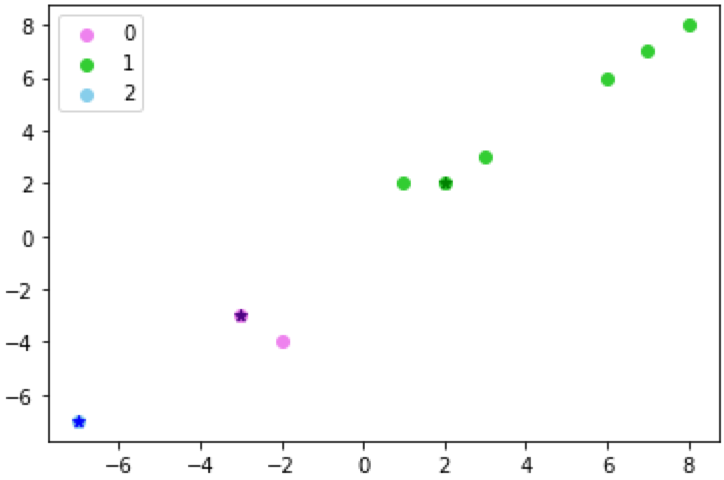
T2

If the starting points are (-3,-3), (2,2), and (-7,-7), what happens?

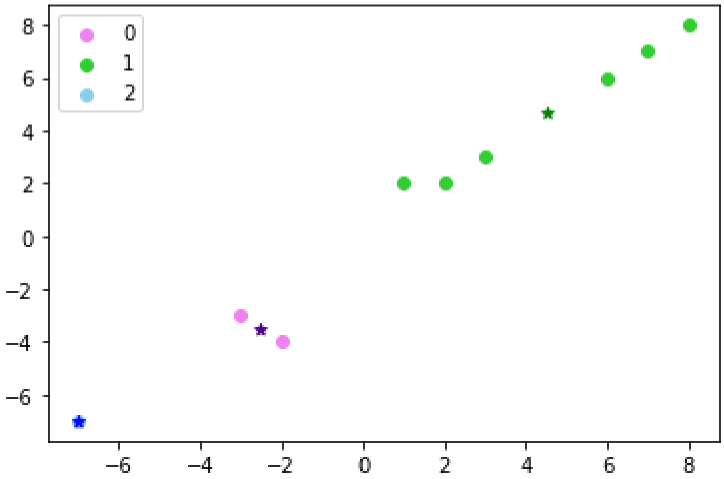
In [699…

```
# Initialize centroids
starting_centriods = pd.DataFrame({
   'x': [-3, 2, -7],
   'y': [-3, 2, -7]
})
kMeans = KMeans(dataframe_points, starting_centriods)
print(kMeans.centriods)
kMeans.plot()
kMeans.run()
print(kMeans.centriods)
kMeans.plot()
```

```
   x  y
0 -3 -3
1  2  2
2 -7 -7
```




```
     x         y
0 -2.5 -3.500000
1  4.5  4.666667
2 -7.0 -7.000000
```



Answer

updated centroids คือ

1. (-2.5, -3.5)
2. (4.5, 4.67)
3. (-7, -7) ตามลำดับ

T3

Between the two starting set of points in the previous two questions, which one do you think is better? How would you measure the 'goodness' quality of a set of starting points?

In general, it is important to try different sets of starting points when doing k-means.

Answer

แบบแรกจะดีกว่า เพราะสังเกตว่า แบบที่สองกลุ่มที่อยู่บนขวา กับกลุ่มที่อยู่แถวกลาง ๆ ถูกจัดให้อยู่ใน cluster เดียวกัน ซึ่งจริง ๆ แล้ว 2 กลุ่มนี้แยกออกจากกันชัดเจน เมื่อมองด้วยตา

โดยทั่วไปแล้ว การเลือกจุดเริ่มต้นของ centriods ค่อนข้างสำคัญ เพราะถ้าเราเลือก centroid ได้ไม่ดี เช่น centriod ไปกระจุกตัวอยู่แถว ๆ เดียวกัน จะทำให้ Algorithm ในการแบ่งกลุ่มทำงานได้ไม่ดีพอที่เราจะเอามาใช้ตีความต่อ

OT1

What would be the best K for this question? Describe your reason- ing.

Answer

สำหรับโจทย์ข้อนี้น่าจะเป็น K = 4 เพราะเมื่อมองด้วยตาเปล่าเราจะเห็นว่ามี 4 กลุ่มแบ่งออกจากกันชัดเจน ไล่จากล่างซ้าย ขึ้นไปยัง บนขวา

My heart will go on

In this part of the exercise we will work on the Titanic dataset provided by Kaggle. The Titanic dataset contains information of the passengers boarding the Titanic on its final voyage. We will work on predicting whether a given passenger will survive the trip.

Let's launch Jupyter and start coding! We start by importing the data using Pandas

```
train_url =
"http://s3.amazonaws.com/assets.datacamp.com/course/Kaggle/train.csv'

train = pd.read_csv(train_url) #training set

test_url =
"http://s3.amazonaws.com/assets.datacamp.com/course/Kaggle/test.csv"

test = pd.read_csv(test_url) #test set
```

Both train and test are dataframes. Use the function train.head() and train.tail() to explore the data. What do you see? Use the function describe() to get a better understanding of the data. You can read the meaning of the data fields at https://www.kaggle.com/c/titanic/data

Looking at the data, you will notice a lot of missing values. For example, some age is NaN. This is normal for real world data to have some missing values. There are several ways to handle missing values. The simplest is to throw away any rows that have missing values. However, this usually reduce the amount of training data you have. Another method is to guess what the missing value should be. The simplest guess is to use the Median or Mode of the data. For this exercise we will proceed with this.

In [700…

```
# Install traning set and test set

train_url = "http://s3.amazonaws.com/assets.datacamp.com/course/Kaggle/trai
```

```
train = pd.read_csv(train_url) #training set

test_url = "http://s3.amazonaws.com/assets.datacamp.com/course/Kaggle/test.
test = pd.read_csv(test_url) #test set

# Define dataset
dataset = [train, test]
```

In [701…

```
dataset[0].head(10)
```

Out[701]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fa
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.25(
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.28:
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.92!
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.10(
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.05(
5	6	0	3	Moran, Mr. James	male	NaN	0	0	330877	8.45!
6	7	0	1	McCarthy, Mr. Timothy J	male	54.0	0	0	17463	51.86:
7	8	0	3	Palsson, Master. Gosta Leonard	male	2.0	3	1	349909	21.07!
8	9	1	3	Johnson, Mrs. Oscar W (Elisabeth Vilhelmina Berg)	female	27.0	0	2	347742	11.13:
9	10	1	2	Nasser, Mrs. Nicholas (Adele Achem)	female	14.0	1	0	237736	30.07(

In [702…

```
dataset[1].head(10)
```

Out[702]:

	PassengerId	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	E
0	892	3	Kelly, Mr. James	male	34.5	0	0	330911	7.8292	NaN	
1	893	3	Wilkes, Mrs. James (Ellen Needs)	female	47.0	1	0	363272	7.0000	NaN	
2	894	2	Myles, Mr. Thomas Francis	male	62.0	0	0	240276	9.6875	NaN	
3	895	3	Wirz, Mr. Albert	male	27.0	0	0	315154	8.6625	NaN	
4	896	3	Hirvonen, Mrs. Alexander (Helga E Lindqvist)	female	22.0	1	1	3101298	12.2875	NaN	
5	897	3	Svensson, Mr. Johan Cervin	male	14.0	0	0	7538	9.2250	NaN	
6	898	3	Connolly, Miss. Kate	female	30.0	0	0	330972	7.6292	NaN	
7	899	2	Caldwell, Mr. Albert Francis	male	26.0	1	1	248738	29.0000	NaN	
8	900	3	Abrahim, Mrs. Joseph (Sophie Halaut Easu)	female	18.0	0	0	2657	7.2292	NaN	
9	901	3	Davies, Mr. John Samuel	male	21.0	2	0	A/4 48871	24.1500	NaN	

In [703…

```
for data in dataset:
  print(data.describe())
```

```
       PassengerId    Survived      Pclass         Age       SibSp  \
count   891.000000  891.000000  891.000000  714.000000  891.000000
mean    446.000000    0.383838    2.308642   29.699118    0.523008
std     257.353842    0.486592    0.836071   14.526497    1.102743
min       1.000000    0.000000    1.000000    0.420000    0.000000
25%     223.500000    0.000000    2.000000   20.125000    0.000000
50%     446.000000    0.000000    3.000000   28.000000    0.000000
75%     668.500000    1.000000    3.000000   38.000000    1.000000
max     891.000000    1.000000    3.000000   80.000000    8.000000

            Parch        Fare
count  891.000000  891.000000
mean     0.381594   32.204208
std      0.806057   49.693429
min      0.000000    0.000000
25%      0.000000    7.910400
50%      0.000000   14.454200
75%      0.000000   31.000000
max      6.000000  512.329200
       PassengerId      Pclass         Age       SibSp       Parch        Fa
re
count   418.000000  418.000000  332.000000  418.000000  418.000000  417.0000
00
mean   1100.500000    2.265550   30.272590    0.447368    0.392344   35.6271
88
std     120.810458    0.841838   14.181209    0.896760    0.981429   55.9075
76
min     892.000000    1.000000    0.170000    0.000000    0.000000    0.0000
00
25%     996.250000    1.000000   21.000000    0.000000    0.000000    7.8958
00
50%    1100.500000    3.000000   27.000000    0.000000    0.000000   14.4542
00
75%    1204.750000    3.000000   39.000000    1.000000    0.000000   31.5000
00
max    1309.000000    3.000000   76.000000    8.000000    9.000000  512.3292
00
```

T4

What is the median age of the training set? You can easily modify the age in the dataframe by

In [704…

```python
for data in dataset:
  data["Age"] = data["Age"].fillna(data["Age"].median())
```

In [705…

```python
# Normailize age
for data in dataset:
  data["Age"] = (data["Age"] - data["Age"].min()) / (data["Age"].max() - da
```

T5

Some fields like ‘Embarked’ are categorical. They need to be converted to numbers first. We will represent S with 0, C with 1, and Q with 2. What is the mode of Embarked? Fill the missing values with the mode. You can set the value of Embarked easily with the following command

Do the same for Sex.

In [706…

```
# S = 0
# C = 1
# Q = 2
for data in dataset:
  data["Age"] = data["Age"].fillna(data["Age"].median())
  data.loc[data["Embarked"] == "S", "Embarked"] = 0
  data.loc[data["Embarked"] == "C", "Embarked"] = 1
  data.loc[data["Embarked"] == "Q", "Embarked"] = 2
  data["Embarked"] = data["Embarked"].fillna(data["Embarked"].median())
```

In [707…

```
# male = 0
# female = 1
for data in dataset:
  data.loc[data["Sex"] == "male", "Sex"] = 0
  data.loc[data["Sex"] == "female", "Sex"] = 1
```

T6

Write a logistic regression classifier using gradient descent as learned in class. Use PClass, Sex, Age, and Embarked as input features. You can extract the features from Pandas to Numpy by

In [708…

```
# Define cleaned data

train_df = copy.deepcopy(dataset)[0]
test_df  = copy.deepcopy(dataset)[1]

train_data = np.array(train_df[["Pclass","Sex","Age","Embarked"]].values, d
test_data = np.array(test_df[["Pclass","Sex","Age","Embarked"]].values, dty

train_y = np.array(train_df[["Survived"]].values, dtype = float)
train_y = train_y.reshape(train_y.size)
```

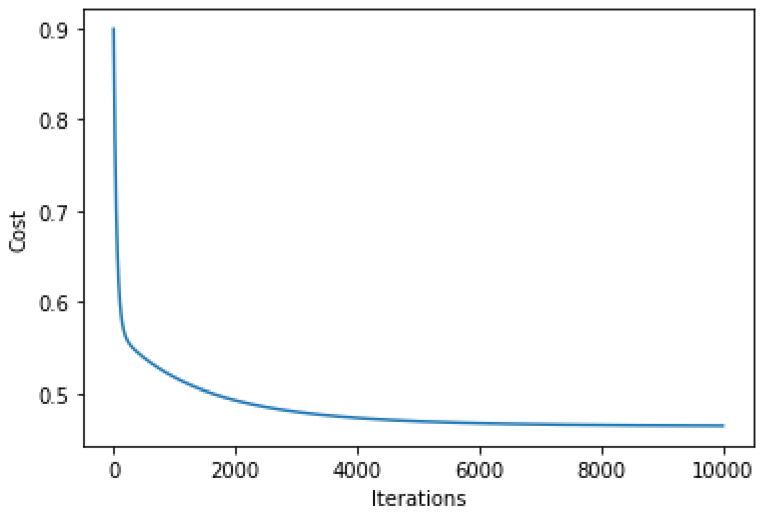
In [709…

```
# Define sigmoid function
def sigmoid(x):
  return np.array(1/(1+np.exp(-x)))
# Define cost function
def cost(theta, data, y):
  m = data.shape[0]
  predictions = np.array(sigmoid(np.dot(data, theta)))
  cost = -(1/m)*(np.dot(y, np.log(predictions.T+1e-5)) + np.dot((1-y), np.l
  return cost
# Define gradient function
def gradient(theta, data, y):
  m = data.shape[0]
  predictions = sigmoid(np.dot(data, theta))
  error = predictions - y
  gradient = (1/m)*np.dot(data.T, error)
  return gradient
# Define gradient descent function
def gradient_descent(theta, data, y, alpha, iteration=10000):
  cost_history = []
  for _ in range(iteration):
    cost_history.append(cost(theta, data, y))
```

```
    theta = theta - alpha*gradient(theta, data, y)
  return theta, cost_history
def predict(data, theta, raw):
  predictions = np.array(sigmoid(np.dot(data, theta)))
  predictions = np.where(predictions >  0.5, 1, predictions)
  predictions = np.where(predictions <= 0.5, 0, predictions)
  predictions = np.array(predictions, dtype = int)
  print("Survived", np.count_nonzero(predictions))
  result = pd.DataFrame({
    "PassengerId": raw["PassengerId"],
    "Survived": predictions
  })
  return result
def compare_prediction(actual, prediction):
  df = pd.DataFrame({
    "Actual": actual,
    "Prediction": prediction,
    "Compare": actual == prediction
  })
  return df["Compare"].sum()/len(actual)
```

In [710…

```
# Initialize features number
features = train_data.shape[1]
# Random pick theta
theta = np.random.random(features)
# Initialize learning rate
alpha = 0.007
# Run gradient descent
theta, cost_history = gradient_descent(theta, train_data, train_y, alpha)
# Plot cost history
plt.plot(cost_history)
plt.ylabel('Cost')
plt.xlabel('Iterations')
plt.show()

print(theta)
```




```
[-0.71967932  2.50169202 -0.09922443  0.34264704]
```

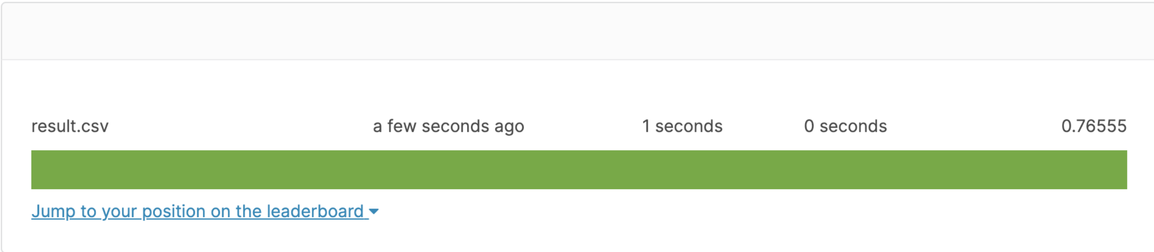
In [711…

```
print("Train Survived", np.count_nonzero(train["Survived"]))
result = predict(train_data, theta, train_df)
print("Accuracy", compare_prediction(train_y, result["Survived"]))
result = predict(test_data, theta, test_df)
result.to_csv("./result.csv", index = False)
```

```
Train Survived 342
Survived 314
Accuracy 0.7867564534231201
Survived 152
```

T7

My predictions score



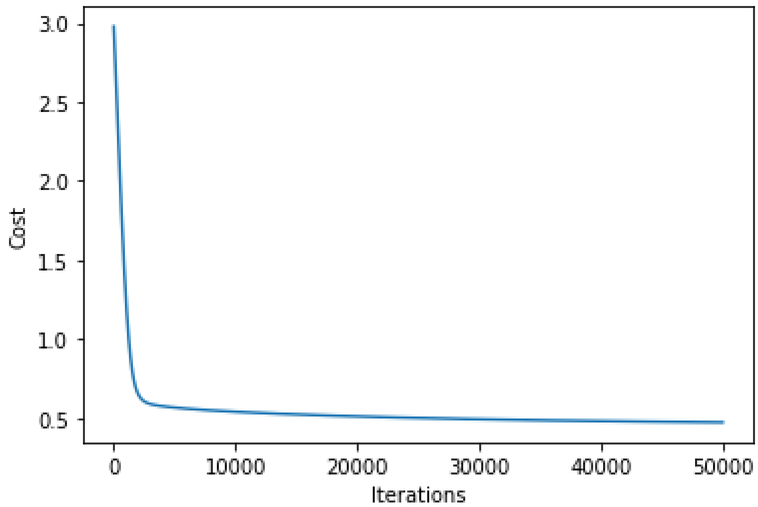
T8

Try adding some higher order features to your training (x21, x1x2,...). Does this model has better accuracy on the training set? How does it perform on the test set?

In [719…

```
# Copy dataset
dataset_1 = copy.deepcopy(dataset)
data_1 = []

# Add new features
for i in range(len(dataset_1)):
  d = dataset_1[i]
  d.replace('', np.nan, inplace=True)
  d["Age*Class"] = d["Age"]*d["Pclass"]
  d["SibSp"] = d["SibSp"].fillna(0)
  d["Parch"] = d["Parch"].fillna(0)
  d["Family_Size"] = d["SibSp"]+d["Parch"]+1
  d["Fare"] = d["Fare"].fillna(d["Fare"].median())
  d["Fare_Per_Person"] = d["Fare"]/d["Family_Size"]
  d["Fare_Per_Person"] = (d["Fare_Per_Person"] - d["Fare_Per_Person"].min()
  data_1.append(np.array(d[["Pclass","Age","Sex","Embarked","Age*Class","Fa

# Extract dataset
train_data_1 = data_1[0]
test_data_1  = data_1[1]

# Initialize features number
features_1 = train_data_1.shape[1]
# Random pick theta
theta_1 = np.random.random(features_1)

train_y_1 = np.array(train[["Survived"]].values, dtype = float)
train_y_1 = train_y_1.reshape(train_y_1.size)

# Initialize learning rate
alpha = 0.0005
iteration = 50000

# Run gradient descent
theta_1, cost_history = gradient_descent(theta_1, train_data_1, train_y_1,
# Plot cost history
```

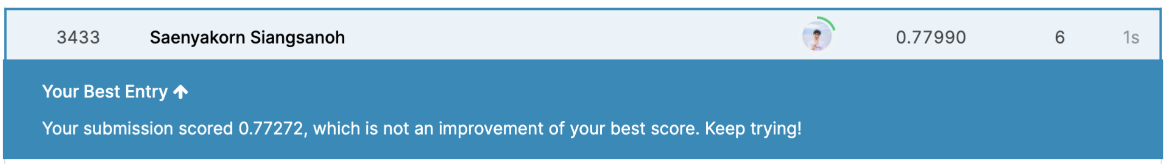
```
plt.plot(cost_history)
plt.ylabel('Cost')
plt.xlabel('Iterations')
plt.show()

# Print theta
print(theta_1)

# Predict test set
print(dataset_1[0]["Survived"].value_counts())
result = predict(train_data_1, theta_1, dataset_1[0])
print("Accuracy", compare_prediction(train_y_1, result["Survived"]))
result = predict(test_data_1, theta_1, dataset_1[1])
result.to_csv("./result_1.csv", index = False)
```




```
[-5.54555750e-01  7.22923702e-02  1.81313447e+00  4.10982154e-01
 -2.65926154e-01 -4.22421403e-04  5.43272178e-01]
0    549
1    342
Name: Survived, dtype: int64
Survived 249
Accuracy 0.8035914702581369
Survived 121
```

Answer

การทำนายที่ได้ fit กับ train data มากขึ้น แต่เมื่อลองส่งไปแล้วพบว่าคะแนนความถูกต้องลดลง (Overfitting) แต่เมื่อลองเอา Fare per person ออกพบว่าการทำนายได้คะแนนเพิ่มขึ้นดังรูป



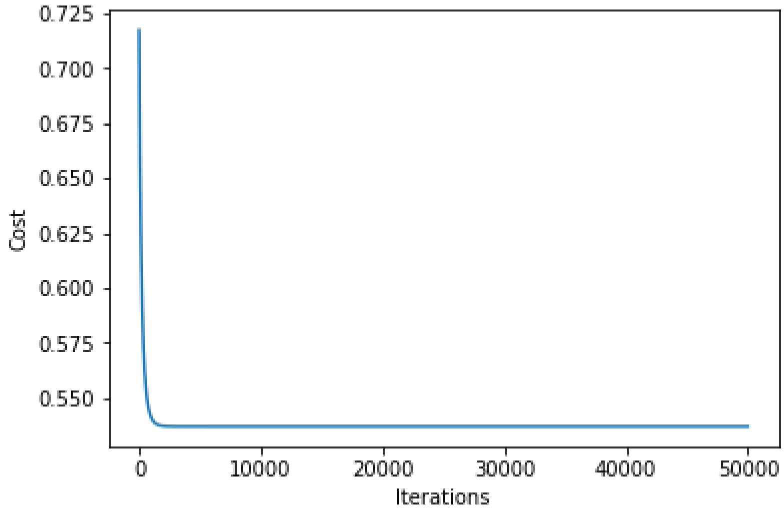
T9

What happens if you reduce the amount of features to just Sex and Age?

In [713…

```
# Copy dataset
dataset_2 = copy.deepcopy(dataset)
data_2 = []

# Add new features
```

```
for i in range(len(dataset_2)):
  d = dataset_2[i]
  data_2.append(np.array(d[["Age","Sex"]].values, dtype = float))

# Extract dataset
train_data_2 = data_2[0]
test_data_2  = data_2[1]

# Initialize features number
features_2 = train_data_2.shape[1]
# Random pick theta
theta_2 = np.random.random(features_2)

train_y_2 = np.array(train[["Survived"]].values, dtype = float)
train_y_2 = train_y_1.reshape(train_y_2.size)

# Initialize learning rate
alpha = 0.1
iteration = 50000

# Run gradient descent
theta_2, cost_history = gradient_descent(theta_2, train_data_2, train_y_2,
# Plot cost history
plt.plot(cost_history)
plt.ylabel('Cost')
plt.xlabel('Iterations')
plt.show()

# Print theta
print(theta_2)

# Predict test set
print(dataset_2[0]["Survived"].value_counts())
result = predict(train_data_2, theta_2, dataset_2[0])
print("Accuracy", compare_prediction(train_y_2, result["Survived"]))
result = predict(test_data_2, theta_2, dataset_2[1])
```




```
[-3.23752429  2.23751753]
0    549
1    342
Name: Survived, dtype: int64
Survived 305
Accuracy 0.7789001122334456
Survived 138
```

Answer

Model ทำนายผู้โดยสารได้แย่ลง เพราะขาดข้อมูลอื่นในการประกอบการตัดสินใจ

Fun with matrix algebra

Prove the following statements. All of them can be solved by first expanding out the matrix notation as a combination of their elements, and then use the definitions of trace and matrix derivatives to help finish the proof. For example, the (i, j) element of $Y = AB$ is $Y_{i,j} = \Sigma_m A_{i,m} B_{m,j}$.

OT4

1. $\nabla_A trAB = B^T$

   Let $Y = AB$

   Then, $Y_{i,j} = \Sigma_m A_{i,m} B_{m,j}$

   So, $tr(Y) = tr(AB) = \Sigma_m A_{i,m} B_{m,i}$

   Since,

$$\nabla_A f(A) = \begin{bmatrix} \frac{\delta f}{\delta A_{1,1}} & \dots & \frac{\delta f}{\delta A_{1,n}} \\ \dots & \dots & \dots \\ \frac{\delta f}{\delta A_{n,1}} & \dots & \frac{\delta f}{\delta A_{n,n}} \end{bmatrix}$$

```
So,
```

$$\nabla_A(tr(AB)) = \nabla_A(\Sigma_m A_{i,m} B_{m,i}) = \begin{bmatrix} \frac{\delta \Sigma_m A_{i,m} B_{m,i}}{\delta A_{1,1}} & \dots & \frac{\delta \Sigma_m A_{i,m} B_{m,i}}{\delta A_{1,n}} \\ \dots & \dots & \dots \\ \frac{\delta \Sigma_m A_{i,m} B_{m,i}}{\delta A_{n,1}} & \dots & \frac{\delta \Sigma_m A_{i,m} B_{m,i}}{\delta A_{n,n}} \end{bmatrix}$$

```
Fianlly,
```

$$\nabla_A(\Sigma_m A_{i,m} B_{m,i}) = \begin{bmatrix} B_{1,1} & \dots & B_{n,1} \\ \dots & \dots & \dots \\ B_{1,n} & \dots & B_{n,n} \end{bmatrix} = B^T$$

```
Q.E.D
```

OT5

1. $\nabla_{A^T} f(A) = (\nabla_A f(A))^T$

   Since,

$$\nabla_A f(A) = \begin{bmatrix} \frac{\delta f}{\delta A_{1,1}} & \dots & \frac{\delta f}{\delta A_{1,n}} \\ \dots & \dots & \dots \\ \frac{\delta f}{\delta A_{n,1}} & \dots & \frac{\delta f}{\delta A_{n,n}} \end{bmatrix}$$

Then,

$$\nabla_{A^T} f(A) = \begin{bmatrix} \frac{\delta f}{\delta A_{1,1}} & \dots & \frac{\delta f}{\delta A_{n,1}} \\ \dots & \dots & \dots \\ \frac{\delta f}{\delta A_{1,n}} & \dots & \frac{\delta f}{\delta A_{n,n}} \end{bmatrix} = \begin{bmatrix} \frac{\delta f}{\delta A_{1,1}} & \dots & \frac{\delta f}{\delta A_{1,n}} \\ \dots & \dots & \dots \\ \frac{\delta f}{\delta A_{n,1}} & \dots & \frac{\delta f}{\delta A_{n,n}} \end{bmatrix}^T = (\nabla_A f(A))^T$$