Week 7 Lab (KNN)

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About The Data

In this lab you will learn how to use sklearn to build a machine learning model using k-Nearest Neighbors algorithm to predict whether the patients in the "Pima Indians Diabetes Dataset" have diabetes or not.

The dataset that we'll be using for this task comes from kaggle.com and contains the following attributes:

- Pregnancies: Number of times pregnant
- Glucose: Plasma glucose concentration a 2 hours in an oral glucose tolerance test
- BloodPressure: Diastolic blood pressure (mm Hg)
- SkinThickness: Triceps skin fold thickness (mm)
- Insulin: 2-Hour serum insulin (mu U/ml)
- BMI: Body mass index (weight in kg/(height in m)^2)
- DiabetesPedigreeFunction: Diabetes pedigree function
- Age (in years)
- Outcome: Class variable (0 or 1)

Exploratory Data Analysis

Let's begin by importing some necessary libraries that we'll be using to explore the data.

In [1]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
```

In [2]:
```
from matplotlib import rcParams
rcParams['figure.figsize'] = 15, 5
sns.set_style('darkgrid')
```

Our first step is to load the data into a pandas DataFrame

In [3]:
```
diabetes_df = pd.read_csv('diabetes.csv')
diabetes_df.head()
```

Out[3]:

	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	BMI	DiabetesPedigreeFunction	Age	Outcome
0	6	148	72	35	0	33.6	0.627	50	1
1	1	85	66	29	0	26.6	0.351	31	0
2	8	183	64	0	0	23.3	0.672	32	1
3	1	89	66	23	94	28.1	0.167	21	0
4	0	137	40	35	168	43.1	2.288	33	1

From here, it's always a good step to use ***describe()*** and ***info()*** to get a better sense of the data and see if we have any missing values.

In [4]:
```
diabetes_df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 768 entries, 0 to 767
Data columns (total 9 columns):
 #   Column                    Non-Null Count  Dtype
---  ------                    --------------  -----
 0   Pregnancies               768 non-null    int64
 1   Glucose                   768 non-null    int64
 2   BloodPressure             768 non-null    int64
 3   SkinThickness             768 non-null    int64
 4   Insulin                   768 non-null    int64
 5   BMI                       768 non-null    float64
 6   DiabetesPedigreeFunction  768 non-null    float64
 7   Age                       768 non-null    int64
 8   Outcome                   768 non-null    int64
dtypes: float64(2), int64(7)
memory usage: 54.1 KB
```

Looking at the info summary, we can see that there are 768 entries in the DataFrame, and 768 non-null entries in each feature/colum. Thus, there are no missing values, but there is something strange when we look at the describe summary below.

For certain columns below, does a value of zero make sense? For example, if an individual had a glucose or blood pressure level of 0, they'd probably be dead, so it's likely that the true values were excluded from the data for some reason.

Therefore, we'll consider the following columns to have missing values where there's an invalid zero value:

- Glucose
- BloodPressure
- SkinThickness
- Insulin
- BMI

In [5]:
```
diabetes_df.describe()
```

Out[5]:

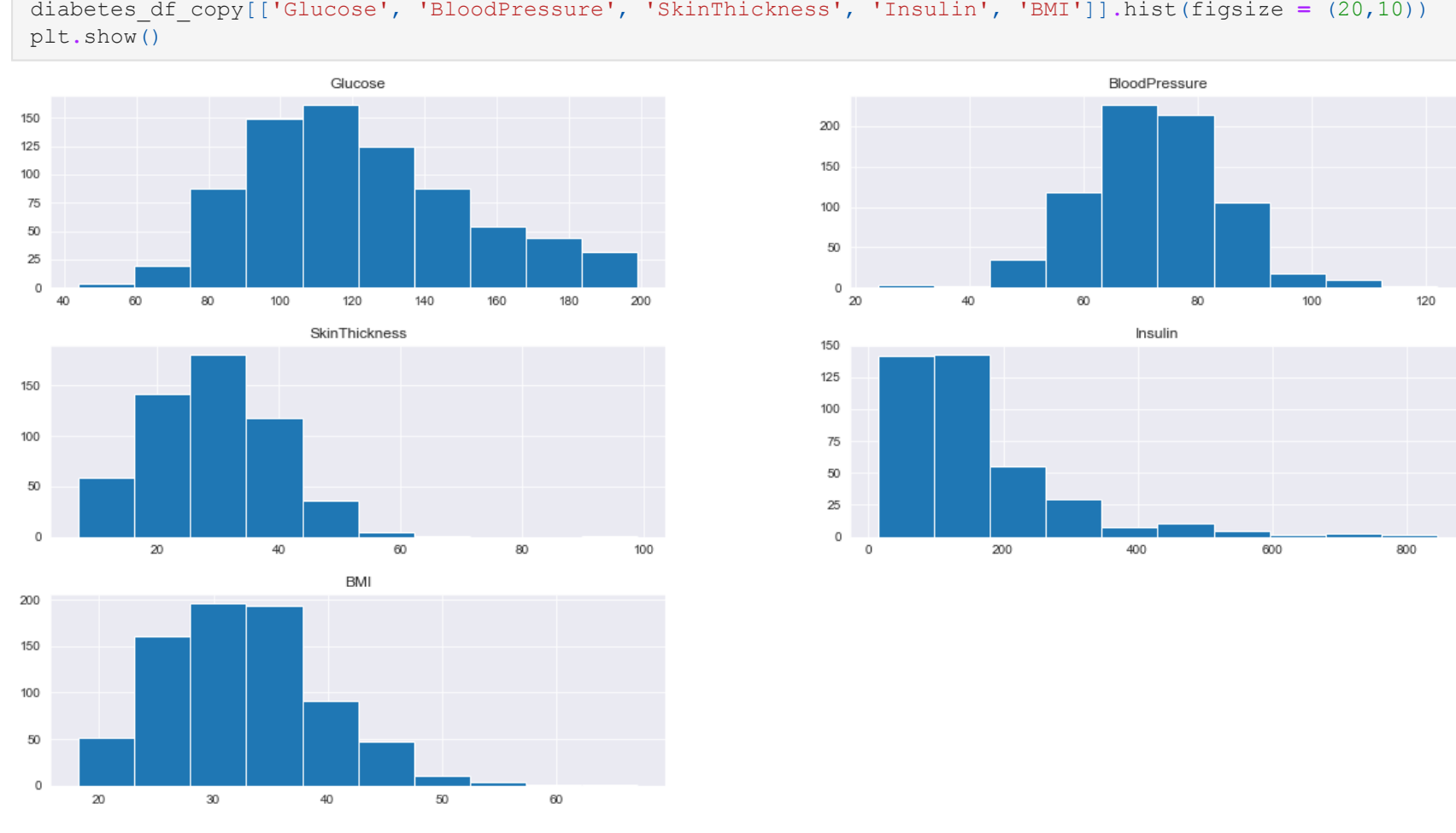
	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	BMI	DiabetesPedigreeFunction	Age
count	768.000000	768.000000	768.000000	768.000000	768.000000	768.000000	768.000000	768.000000
mean	3.845052	120.894531	69.105469	20.536458	79.799479	31.992578	0.471876	33.240885
std	3.369578	31.972618	19.355807	15.952218	115.244002	7.884160	0.331329	11.760232
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.078000	21.000000
25%	1.000000	99.000000	62.000000	0.000000	0.000000	27.300000	0.243750	24.000000
50%	3.000000	117.000000	72.000000	23.000000	30.500000	32.000000	0.372500	29.000000
75%	6.000000	140.250000	80.000000	32.000000	127.250000	36.600000	0.626250	41.000000
max	17.000000	199.000000	122.000000	99.000000	846.000000	67.100000	2.420000	81.000000

Let's go ahead and replace out invalid zero values with nan, since they technically missing values. We'll go ahead and make a copy of our diabetes_df and modify the zeros in the copy just incase we need to refer back to the original. We can make copies of DataFrames using ***.copy(deep=True)***. There's also a very convenient function we can call ***.replace(x, y)*** that will replace all x values with the y value specified.

In [6]:
```
diabetes_df_copy = diabetes_df.copy(deep=True)
diabetes_df_copy['Glucose'] = diabetes_df_copy['Glucose'].replace(0,np.NaN)
diabetes_df_copy['BloodPressure'] = diabetes_df_copy['BloodPressure'].replace(0,np.NaN)
diabetes_df_copy['SkinThickness'] = diabetes_df_copy['SkinThickness'].replace(0,np.NaN)
diabetes_df_copy['Insulin'] = diabetes_df_copy['Insulin'].replace(0,np.NaN)
diabetes_df_copy['BMI'] = diabetes_df_copy['BMI'].replace(0,np.NaN)
```

Before choosing how to impute these missing values, let's take a look at their distributions.

In [7]:
```
diabetes_df_copy[['Glucose', 'BloodPressure', 'SkinThickness', 'Insulin', 'BMI']].hist(figsize = (20,10))
plt.show()
```

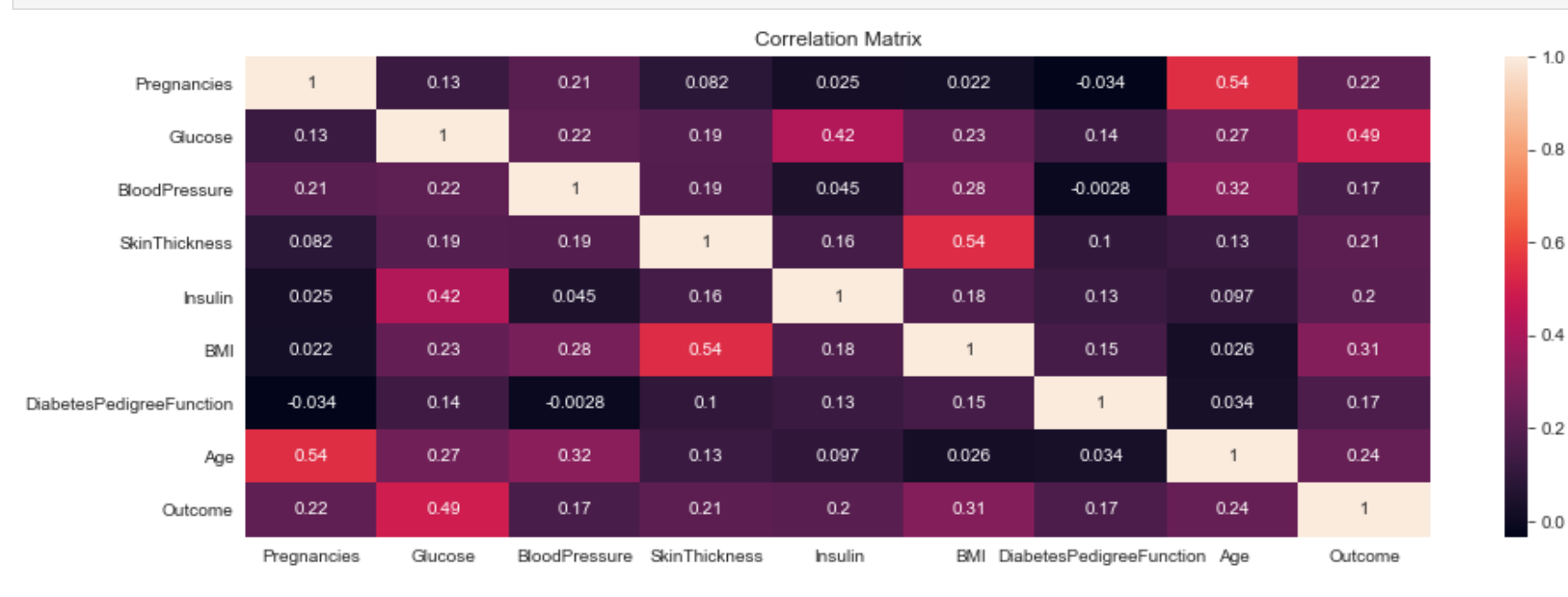


Since SkinThickness, Insulin, and BMI look skewed, we'll go ahead and replace their missing values with median instead of mean. Glucose and BloodPressure should be ok if we stick with mean for imputing. Recall that mean can be effected by outliers.

In [8]:
```
diabetes_df_copy['Glucose'].fillna(diabetes_df_copy['Glucose'].mean(), inplace = True)
diabetes_df_copy['BloodPressure'].fillna(diabetes_df_copy['BloodPressure'].mean(), inplace = True)
diabetes_df_copy['SkinThickness'].fillna(diabetes_df_copy['SkinThickness'].median(), inplace = True)
diabetes_df_copy['Insulin'].fillna(diabetes_df_copy['Insulin'].median(), inplace = True)
diabetes_df_copy['BMI'].fillna(diabetes_df_copy['BMI'].median(), inplace = True)
```

Let's first create a heatmap and see if there are any correlations in our dataset.

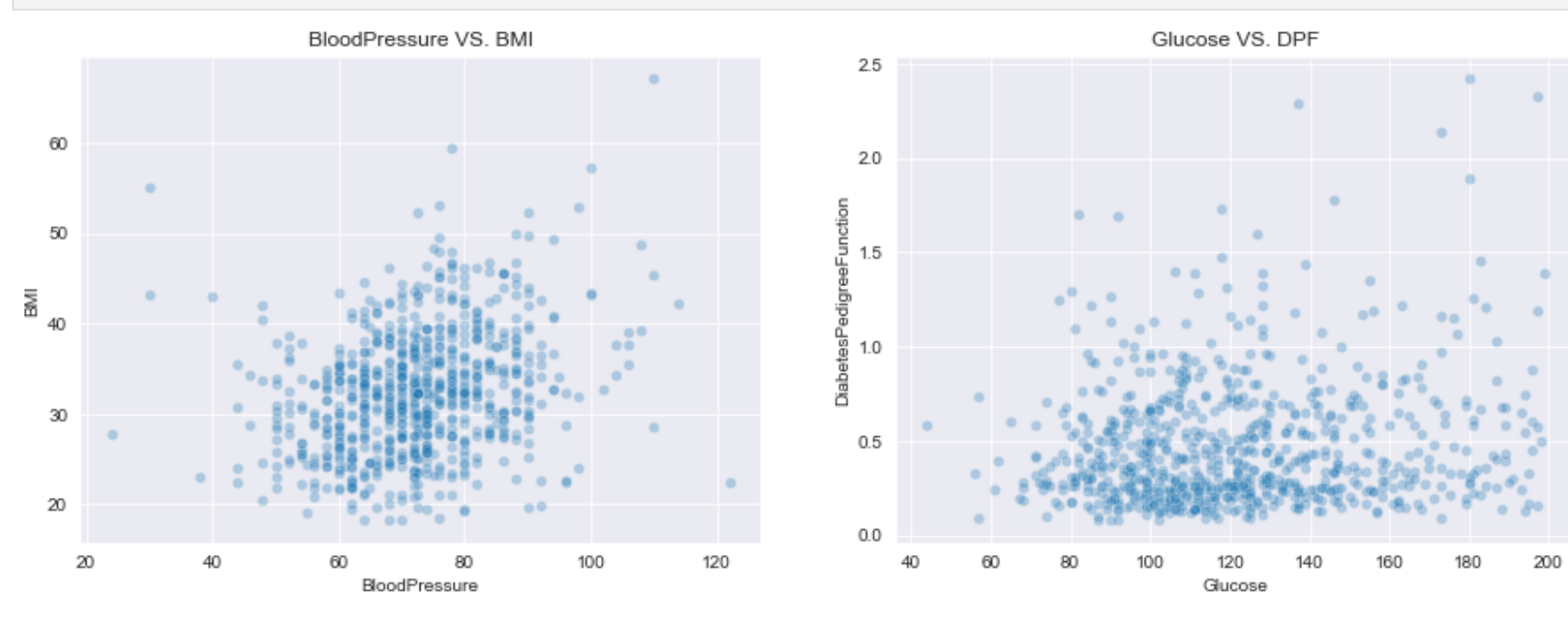
In [9]:
```
sns.heatmap(diabetes_df_copy.corr(), annot=True)
plt.title('Correlation Matrix')
plt.show()
```



Interpretation: No significant case of multi collinearity is observed.

Let's also check out a few scatterplots of our data.

In [10]:
```
fig, axes = plt.subplots(nrows=1, ncols=2, figsize=(15, 5))

# alpha parameter adjusts the point transparency. points with much more overlap will appear darker.
sns.scatterplot(x='BloodPressure', y='BMI', data=diabetes_df_copy, alpha=0.3, ax=axes[0])
axes[0].set_title('BloodPressure VS. BMI')

sns.scatterplot(x='Glucose', y='DiabetesPedigreeFunction', data=diabetes_df_copy, alpha=0.3, ax=axes[1])
axes[1].set_title('Glucose VS. DPF')

plt.show()
```

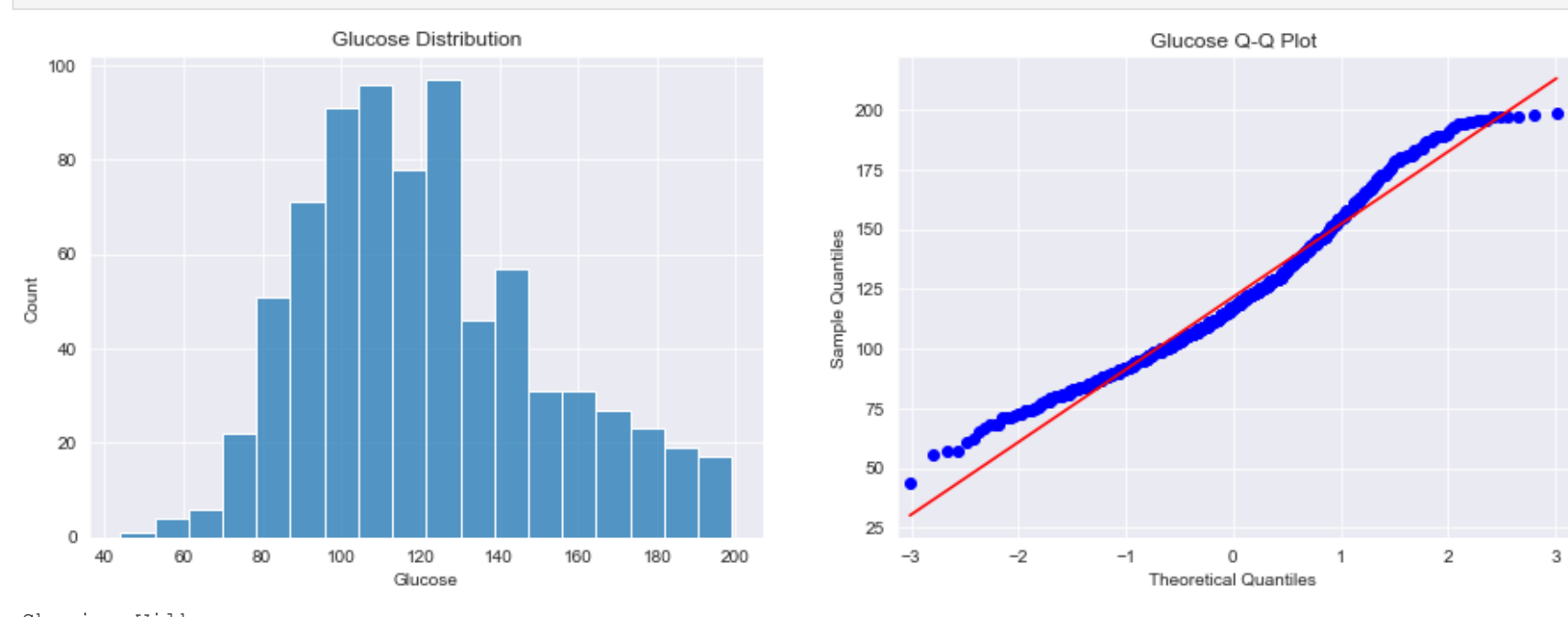


Interpretation:

- BMI seems to have a slight increase as blood pressure increases. However, majority of the data seems to be centered and cluster at around a blood pressure of 50-95 and BMI of 20-45. We've also got some outliars scattered around the main cluster.
- There's a very subtle increase in diabetes pedigree function as glucose increases. Majority of the data tends to fall between a 75 and 175 glucose level. We also have some outliars with very high diabetes pedigree function and again the zeros outliars which were removed in the no_zeros_df

Note: Don't worry if you can't replicate the plot to the right. You should have learned about QQ plots in math 3339. In case anyone needs these type of plots or a certain statistical test with p-values for their project, statsmodels is a great place to find these.

In [11]:
```
import statsmodels.api as sm
import scipy
import pylab

fig, axes = plt.subplots(nrows=1, ncols=2, figsize=(15, 5))

sns.histplot(diabetes_df_copy['Glucose'], ax=axes[0])
axes[0].set_title('Glucose Distribution')

sm.qqplot(diabetes_df_copy['Glucose'], line='s', ax=axes[1])
axes[1].set_title('Glucose Q-Q Plot')

pylab.show()

w, p_val = scipy.stats.shapiro(diabetes_df_copy['Glucose'])
print('Shapiro-Wilk: \nw:{}, p-value:{}\n'.format(w,p_val))

d, p_val = scipy.stats.kstest(diabetes_df_copy['Glucose'], 'norm')
print('Kolmogorov-Smirnov: \nd:{}, p-value:{}\n'.format(w,p_val))

print('Skewness of the data: \n{}\n'.format(scipy.stats.skew(diabetes_df_copy['Glucose'])))
```



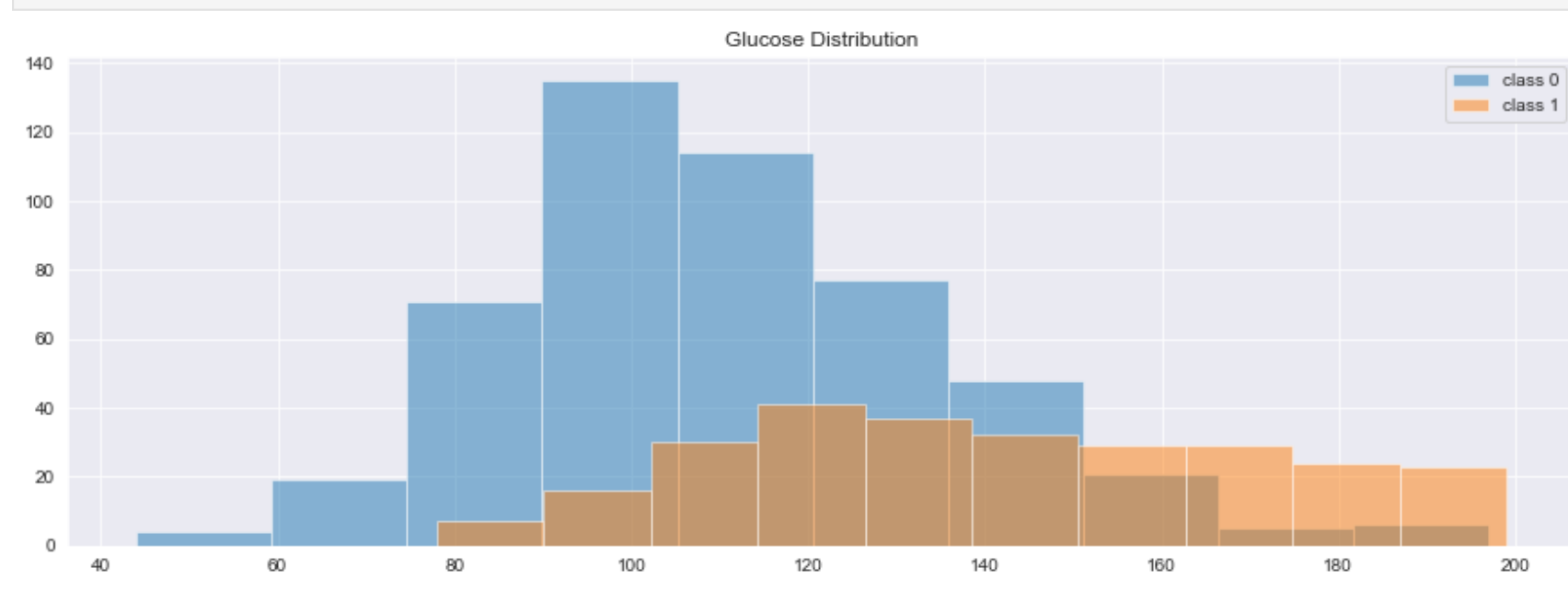

```
Shapiro-Wilk:
w:0.969902515411377, p-value:1.7774986343921384e-11

Kolmogorov-Smirnov:
d:0.969902515411377, p-value:0.0

Skewness of the data:
0.531677628850459
```

Interpretation:

- The distribution of glucose is unimodal, and appears to be roughly bell shaped, but it's certainly not a near perfect normal distribution. The provided Q-Q plot, Shapiro-Wilk, and Kolmogorov-Smirnov tests seem to reject the null hypothesis of the data being a normal distribution at the .05 significance level. We can also see both by the graph and provided skewness score (should be about zero for normally distributed data) below that the data has a slight right skew. The distribution peaks at around 120 with most of the data between 100 and 140.

How does the glucose distribution of people with diabetes vary from those without?

In [12]:
```
class_zero = diabetes_df_copy[(diabetes_df_copy['Outcome'] == 0)]
class_one = diabetes_df_copy[(diabetes_df_copy['Outcome'] == 1)]

plt.hist(x=class_zero['Glucose'], label='class 0', alpha=0.5)
plt.hist(x=class_one['Glucose'], label='class 1', alpha=0.5)
plt.legend()
plt.title('Glucose Distribution')

plt.show()
```



Interpretation:

- Majority of people in class 0 lie between 93 and 125, where as majority of people in class 1 lie between 119 and 167. With that said, this attribute could serve as a good indicator to determine whether somone is diabetic or not since those in class 1 tend to be in the higher end compared to class 0.

I encourage you to go ahead and explore the dataset some more to see if you can find some more interesting points, but I'll jump to the pre-processing now since the main goal of this lab is KNN.

Pre-Processing

The most important step here is to standardize our data. Because the KNN classifier predicts the class of a given test observation by identifying the observations that are nearest to it, the scale of the variables matters. If this is not taken into account, any variables that are on a large scale will have a much larger effect on the distance between the observations, and hence on the KNN classifier, than variables that are on a small scale.

If you recall from math 3339, data Z is rescaled such that and , and is done through this formula:

But lucky for us sklearn can do all of this for us. 🙂

In [13]:
```
from sklearn.preprocessing import StandardScaler

# all columns except 'Outcome'
X = diabetes_df_copy.drop('Outcome', axis=1)
y = diabetes_df_copy['Outcome']

# create our scaler object
scaler = StandardScaler()
# use our scaler object to transform/scale our data and save it into X_scaled
X_scaled = scaler.fit_transform(X)
# reassign X to a new DataFrame using the X_scaled values.
X = pd.DataFrame(data=X_scaled, columns=X.columns)
```

Taking a look at the data again, we see that it is now scaled.

In [14]:
```
X.head()
```

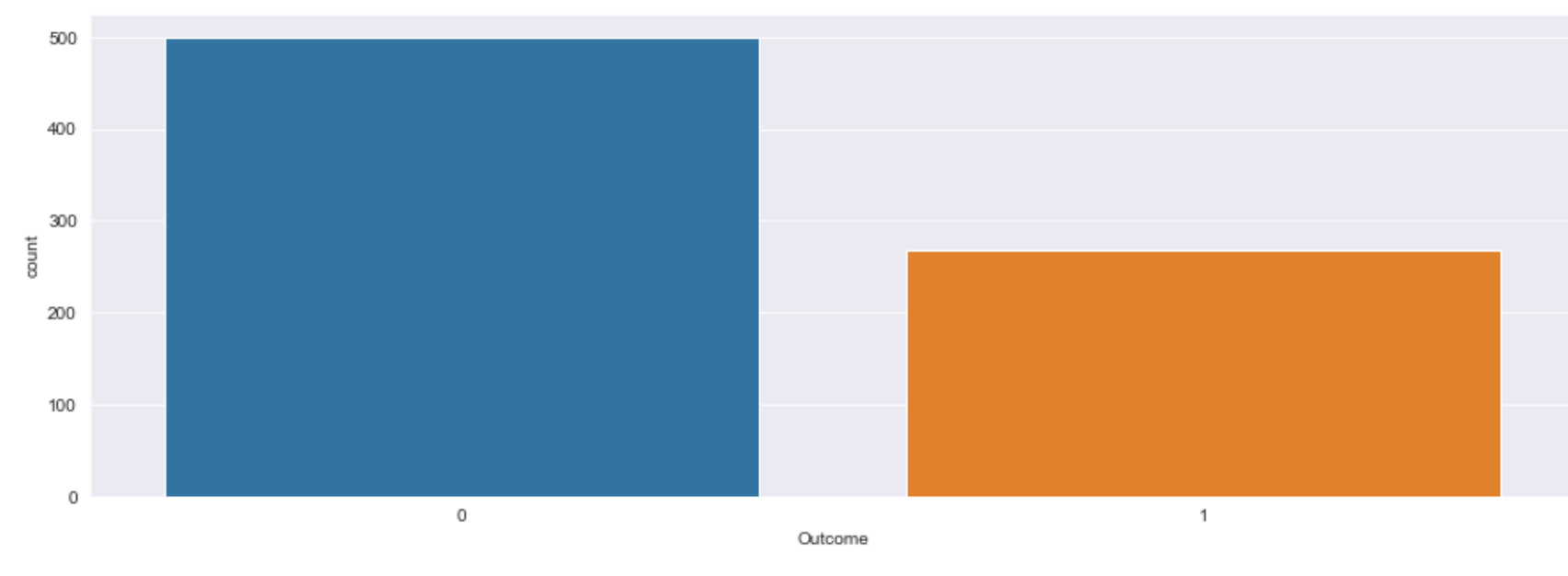
Out[14]:

	Pregnancies	Glucose	BloodPressure	SkinThickness	Insulin	BMI	DiabetesPedigreeFunction	Age
0	0.639947	0.865108	-0.033518	0.670643	-0.181541	0.166619	0.468492	1.425995
1	-0.844885	-1.206162	-0.529859	-0.012301	-0.181541	-0.852200	-0.365061	-0.190672
2	1.233880	2.015813	-0.695306	-0.012301	-0.181541	-1.332500	0.604397	-0.105584
3	-0.844885	-1.074652	-0.529859	-0.695245	-0.540642	-0.633881	-0.920763	-1.041549
4	-1.141852	0.503458	-2.680669	0.670643	0.316566	1.549303	5.484909	-0.020496

Creating our Model

We're now ready to begin creating and training our model. We first need to split our data into training and testing sets. This can be done using sklearn's ***train_test_split(X, y, test_size)*** function. This function takes in your features (X), the target variable (y), and the test_size you'd like (Generally a test size of around 0.3 is good enough). It will then return a tuple of X_train, X_test, y_train, y_test sets for us. We will train our model on the training set and then use the test set to evaluate the model.

In [15]:
```
sns.countplot(x=diabetes_df_copy['Outcome'])
plt.show()
```



The above graph shows that the data is biased towards datapoints having outcome value as 0 (diabetes was not present actually). The number of non-diabetics is almost twice the number of diabetic patients. This is where an additional parameter ***stratify*** can come in handy. Stratified sampling aims at splitting a data set so that each split is similar with respect to something. In a classification setting, it is often chosen to ensure that the train and test sets have approximately the same percentage of samples of each target class as the complete set.

In [16]:
```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, stratify=y, random_state=42)
```

Recall from lecture, KNN requires us to find some optimal k value. How we'll do this is by plotting different k values on the x axis, and the model score for that k value on the y-axis.

Note: You can also plot the error on the y-axis, which is quite common as well.

In [17]:
```
from sklearn.neighbors import KNeighborsClassifier

# will append scores here for plotting later
test_scores = []
train_scores = []

# testing k values from 1-14
for i in range(1,15):
    # create a model with k=i
    knn = KNeighborsClassifier(i)
    # train the model
    knn.fit(X_train,y_train)

    # append scores.
    train_scores.append(knn.score(X_train,y_train))
    test_scores.append(knn.score(X_test,y_test))
```

In [20]:
```
sns.lineplot(x=range(1,15), y=train_scores, marker='*', label='Train Score')
sns.lineplot(x=range(1,15), y=test_scores, marker='o', label='Test Score')
plt.title('K vs. Score')
plt.xlabel('K')
plt.ylabel('Score')
plt.show()
```

The best result seems to be captured at k = 11 thus 11 will be used for the final model. At this value our train and test scores don't vary significantly.

In [21]:
```
knn = KNeighborsClassifier(11)

knn.fit(X_train,y_train)
knn.score(X_test,y_test)
```

Out[21]: 0.7532467532467533

Note: You should also take into account cross validation when considering different models. A separate exercise however will be created covering different cross validation techniques.

Not bad, but could be better. See if you can mess with the data and imporve on this score.

Lastly, let's just print out a confusion matrix and classification report of our results.

In [22]:
```
from sklearn.metrics import confusion_matrix
from sklearn.metrics import classification_report

y_pred = knn.predict(X_test)
print(classification_report(y_test,y_pred))
print(confusion_matrix(y_test,y_pred))
```

```
              precision    recall  f1-score   support

           0       0.79      0.85      0.82       150
           1       0.67      0.58      0.62        81

    accuracy                           0.75       231
   macro avg       0.73      0.71      0.72       231
weighted avg       0.75      0.75      0.75       231

[[127  23]
 [ 34  47]]
```

Great job! You now know how to use KNeighborsClassifier in sklearn. Try using this on your own dataset and refer back to this lecture if you get stuck.