AML_Homework_3_CS4090

April 1, 2022

1 Homework 3

1.1 Part 1: Imbalanced Dataset

This part of homework helps you practice to classify a highly imbalanced dataset in which the number of examples in one class greatly outnumbers the examples in another. You will work with the Credit Card Fraud Detection dataset hosted on Kaggle. The aim is to detect a mere 492 fraudulent transactions from 284,807 transactions in total.

1.1.1 Instructions

Please push the .ipynb, .py, and .pdf to Github Classroom prior to the deadline. Please include your UNI as well.

Due Date : 2nd April 2022

1.1.2 Name: Chandan Suri

1.1.3 UNI: CS4090

1.2 0 Setup

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

import sklearn
from sklearn.metrics import confusion_matrix
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from imblearn.pipeline import make_pipeline as imb_make_pipeline
from imblearn.under_sampling import RandomUnderSampler
from imblearn.over_sampling import RandomOverSampler
from imblearn.over_sampling import SMOTE
```

1.3 1 Data processing and exploration

Download the Kaggle Credit Card Fraud data set. Features V1, V2, … V28 are the principal components obtained with PCA, the only features which have not been transformed with PCA are

'Time' and 'Amount'. Feature 'Time' contains the seconds elapsed between each transaction and the first transaction in the dataset. The feature 'Amount' is the transaction Amount, this feature can be used for example-dependant cost-sensitive learning. Feature 'Class' is the response variable and it takes value 1 in case of fraud and 0 otherwise.

[2]:
```
raw_df = pd.read_csv('https://storage.googleapis.com/download.tensorflow.org/
↪data/creditcard.csv')
raw_df.head()
```

[2]:

	Time	V1	V2	V3	V4	V5	V6	V7	\
0	0.0	-1.359807	-0.072781	2.536347	1.378155	-0.338321	0.462388	0.239599	
1	0.0	1.191857	0.266151	0.166480	0.448154	0.060018	-0.082361	-0.078803	
2	1.0	-1.358354	-1.340163	1.773209	0.379780	-0.503198	1.800499	0.791461	
3	1.0	-0.966272	-0.185226	1.792993	-0.863291	-0.010309	1.247203	0.237609	
4	2.0	-1.158233	0.877737	1.548718	0.403034	-0.407193	0.095921	0.592941	

	V8	V9	…	V21	V22	V23	V24	V25	\
0	0.098698	0.363787	…	-0.018307	0.277838	-0.110474	0.066928	0.128539	
1	0.085102	-0.255425	…	-0.225775	-0.638672	0.101288	-0.339846	0.167170	
2	0.247676	-1.514654	…	0.247998	0.771679	0.909412	-0.689281	-0.327642	
3	0.377436	-1.387024	…	-0.108300	0.005274	-0.190321	-1.175575	0.647376	
4	-0.270533	0.817739	…	-0.009431	0.798278	-0.137458	0.141267	-0.206010	

	V26	V27	V28	Amount	Class
0	-0.189115	0.133558	-0.021053	149.62	0
1	0.125895	-0.008983	0.014724	2.69	0
2	-0.139097	-0.055353	-0.059752	378.66	0
3	-0.221929	0.062723	0.061458	123.50	0
4	0.502292	0.219422	0.215153	69.99	0

[5 rows x 31 columns]

1.3.1 1.1 Examine the class label imbalance

Let's look at the dataset imbalance:

Q1. How many observations are there in this dataset? How many of them have positive label (labeled as 1)?

[3]:
```
target_feature_name = "Class"
credit_card_data_num_rows = len(raw_df)

# This will add up all the 1's in the class which is the label for the dataset.
# Summing all the 1's essentially gives us the number of positive labels in the␣
↪dataset.
positive_labels_num = raw_df[target_feature_name].sum()

print(f"The number of observatons in the dataset: {credit_card_data_num_rows}")
```

```
print(f"The number of rows marked with Class 1 (positive label):␣
 ↪{positive_labels_num}")
```

```
The number of observatons in the dataset: 284807
The number of rows marked with Class 1 (positive label): 492
```

As shown above, the total number of observations in our dataset is 284807 and the number of positive labels in the dataset are 492 that corresponds to rows in the dataset with class label as 1.

1.3.2 1.2 Clean, split and normalize the data

The raw data has a few issues. First the `Time` and `Amount` columns are too variable to use directly. Drop the `Time` column (since it's not clear what it means) and take the log of the `Amount` column to reduce its range.

[4]:
```
cleaned_df = raw_df.copy()

# You don't want the `Time` column.
cleaned_df.pop('Time')

# The `Amount` column covers a huge range. Convert to log-space.
eps = 0.001 # 0 => 0.1¢
cleaned_df['Log Ammount'] = np.log(cleaned_df.pop('Amount')+eps)
```

Q2. Split the dataset into development and test sets. Please set test size as 0.2 and random state as 42.

[5]:
```
# Extract the label as separate variable and get the features as separate␣
 ↪variable.
credit_card_cleaned_data_labels = cleaned_df[target_feature_name]
credit_card_cleaned_data_features = cleaned_df.drop(target_feature_name, axis =␣
 ↪1)

X_dev, X_test, y_dev, y_test =␣
 ↪train_test_split(credit_card_cleaned_data_features,
                                                    credit_card_cleaned_data_labels,
                                                    stratify =␣
 ↪credit_card_cleaned_data_labels,
                                                    test_size = 0.2,
                                                    random_state = 42)

print(f"The shape of the Development Set Features: {X_dev.shape}")
print(f"The shape of the Testing Set Features: {X_test.shape}")
print(f"The shape of the Development Set Labels: {y_dev.shape}")
print(f"The shape of the Testing Set Labels: {y_test.shape}")
```

```
The shape of the Development Set Features: (227845, 29)
The shape of the Testing Set Features: (56962, 29)
The shape of the Development Set Labels: (227845,)
```

```
The shape of the Testing Set Labels: (56962,)
```

Q3. Normalize the input features using the sklearn StandardScaler. Print the shape of your development features and test features.

[6]:
```
std_scaler = StandardScaler()

X_dev_scaled = pd.DataFrame(std_scaler.fit_transform(X_dev), columns = X_dev.
 ↪columns)
X_test_scaled = pd.DataFrame(std_scaler.transform(X_test), columns = X_test.
 ↪columns)

print(f"The shape of the Scaled Development Set Features: {X_dev_scaled.shape}")
print(f"The shape of the Scaled Testing Set Features: {X_test_scaled.shape}")
```

```
The shape of the Scaled Development Set Features: (227845, 29)
The shape of the Scaled Testing Set Features: (56962, 29)
```

1.3.3 1.3 Define the model and metrics

Q4. First, fit a default logistic regression model. Print the AUC and average precision of 5-fold cross validation.

[7]:
```
# Additional Imports
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import cross_validate
```

[8]:
```
lr_default_model = LogisticRegression()
scores = cross_validate(lr_default_model, X_dev_scaled, y_dev,
                        cv = 5, scoring = ['roc_auc', 'average_precision'])

print(f"The AUC values are as follows: {scores['test_roc_auc']}")
print(f"The AUC of the default Logistic Regression model is:␣
 ↪{scores['test_roc_auc'].mean()}")
print(f"The Average Precision of the default Logistic Regression model is: " + \
      f"{scores['test_average_precision'].mean()}")
```

```
The AUC values are as follows: [0.96867681 0.98255313 0.96207234 0.97842981
0.99011106]
The AUC of the default Logistic Regression model is: 0.9763686302709351
The Average Precision of the default Logistic Regression model is:
0.7620017185050845
```

[9]:
```
# Get the fitted model
lr_default_model = LogisticRegression()
lr_default_model = lr_default_model.fit(X_dev_scaled, y_dev)
```

Q5.1. Perform random under sampling on the development set. What is the shape of your development features? How many positive and negative labels are there in

your development set? (Please set random state as 42 when performing random under sampling)

[10]:
```
ru_sampler = RandomUnderSampler(replacement = False, random_state = 42)
X_dev_undersampled, y_dev_undersampled = ru_sampler.fit_resample(X_dev_scaled,␣
 ↪y_dev)

print(f"The shape of the Development Features is: {X_dev_scaled.shape} ")
print(f"The shape of the Development Features after Under Sampling is:␣
 ↪{X_dev_undersampled.shape}")
print(f"The positive and negative labels are as follows: \n {y_dev_undersampled.
 ↪value_counts()}")
```

```
The shape of the Development Features is: (227845, 29)
The shape of the Development Features after Under Sampling is: (788, 29)
The positive and negative labels are as follows:
 0    394
1    394
Name: Class, dtype: int64
```

There are 788 rows with 29 columns/features in the development dataset having all the features after random under sampling has been performed. Also, the number of positive and negative labels in the development set are the same and equal to 394. This makes sense as in random under sampling, the minority class is the one with class label 1 (positive label) and has only 394 rows in the development dataset so, the majority class will be down sampled to have the same number of rows as in the majority class here which is equal to 394.

Q5.2. Fit a default logistic regression model using under sampling. Print the AUC and average precision of 5-fold cross validation. (Please set random state as 42 when performing random under sampling)

[11]:
```
ru_sampler = RandomUnderSampler(replacement = False, random_state = 42)
lr_under_sampled_pipeline = imb_make_pipeline(ru_sampler, LogisticRegression())

scores = cross_validate(lr_under_sampled_pipeline, X_dev_scaled, y_dev,
                        cv = 5, scoring = ['roc_auc', 'average_precision'])

print(f"The AUC values are as follows: {scores['test_roc_auc']}")
print(f"The AUC of the default Logistic Regression model (& Under Sampling) is:␣
 ↪" + \
      f"{scores['test_roc_auc'].mean()}")
print(f"The Average Precision of the default Logistic Regression model (& Under␣
 ↪Sampling) is: " + \
      f"{scores['test_average_precision'].mean()}")
```

```
The AUC values are as follows: [0.96614574 0.9753319  0.98044194 0.97379755
0.99099009]
The AUC of the default Logistic Regression model (& Under Sampling) is:
0.9773414443783114
```

```
The Average Precision of the default Logistic Regression model (& Under
Sampling) is: 0.5687868062162817
```

[12]:
```
# Get the Under sampled fitted model from the pipeline
ru_sampler = RandomUnderSampler(replacement = False, random_state = 42)
lr_under_sampled_pipeline = imb_make_pipeline(ru_sampler, LogisticRegression())
lr_under_sampled_model = lr_under_sampled_pipeline.fit(X_dev_scaled, y_dev)
```

Q6.1. Perform random over sampling on the development set. What is the shape of your development features? How many positive and negative labels are there in your development set? (Please set random state as 42 when performing random over sampling)

[13]:
```
ro_sampler = RandomOverSampler(random_state = 42)
X_dev_oversampled, y_dev_oversampled = ro_sampler.fit_resample(X_dev_scaled,␣
 ↪y_dev)

print(f"The shape of the Development Features is: {X_dev_scaled.shape} ")
print(f"The shape of the Development Features after Over Sampling is:␣
 ↪{X_dev_oversampled.shape}")
print(f"The positive and negative labels are as follows: \n {y_dev_oversampled.
 ↪value_counts()}")
```

```
The shape of the Development Features is: (227845, 29)
The shape of the Development Features after Over Sampling is: (454902, 29)
The positive and negative labels are as follows:
 0    227451
1    227451
Name: Class, dtype: int64
```

There are 454902 rows with 29 columns in the development feature set after random over sampling has been performed. Also, the number of negative labels (class label 0) in the development set is equal to 227451 which is the same as the number of the positive labels (class label 1). This makes sense as in random over sampling, the number of rows in the minority class (class label 1) are randomly sampled to create number of rows equal to that of the majority class (class label 0).

Q6.2. Fit a default logistic regression model using over sampling. Print the AUC and average precision of 5-fold cross validation. (Please set random state as 42 when performing random over sampling)

[14]:
```
ro_sampler = RandomOverSampler(random_state = 42)
lr_over_sampled_pipeline = imb_make_pipeline(ro_sampler, LogisticRegression())

scores = cross_validate(lr_over_sampled_pipeline, X_dev_scaled, y_dev,
                        cv = 5, scoring = ['roc_auc', 'average_precision'])

print(f"The AUC values are as follows: {scores['test_roc_auc']}")
print(f"The AUC of the default Logistic Regression model (& Over Sampling) is:␣
 ↪" + \
```

```
      f"{scores['test_roc_auc'].mean()}")
print(f"The Average Precision of the default Logistic Regression model (& Over␣
 ↪Sampling) is: " + \
      f"{scores['test_average_precision'].mean()}")
```

```
The AUC values are as follows: [0.95932134 0.98132348 0.98764035 0.98166547
0.99338205]
The AUC of the default Logistic Regression model (& Over Sampling) is:
0.9806665368543067
The Average Precision of the default Logistic Regression model (& Over Sampling)
is: 0.7522653129344974
```

[15]:
```
# Get the Over sampled fitted model from the pipeline
ro_sampler = RandomOverSampler(random_state = 42)
lr_over_sampled_pipeline = imb_make_pipeline(ro_sampler, LogisticRegression())
lr_over_sampled_model = lr_over_sampled_pipeline.fit(X_dev_scaled, y_dev)
```

Q7.1. Perform Synthetic Minority Oversampling Technique (SMOTE) on the development set. What is the shape of your development features? How many positive and negative labels are there in your development set? (Please set random state as 42 when performing SMOTE)

[16]:
```
smote_sampler = SMOTE(random_state = 42)
X_dev_smote_sampled, y_dev_smote_sampled = smote_sampler.
 ↪fit_resample(X_dev_scaled, y_dev)

print(f"The shape of the Development Features is: {X_dev_scaled.shape} ")
print(f"The shape of the Development Features after SMOTE Sampling is:␣
 ↪{X_dev_smote_sampled.shape}")
print(f"The positive and negative labels are as follows: \n␣
 ↪{y_dev_smote_sampled.value_counts()}")
```

```
The shape of the Development Features is: (227845, 29)
The shape of the Development Features after SMOTE Sampling is: (454902, 29)
The positive and negative labels are as follows:
 0    227451
1    227451
Name: Class, dtype: int64
```

There are 454902 rows with 29 columns in the development feature set after SMOTE has been performed. Also, the number of negative labels (class label 0) in the development set is equal to 227451 which is the same as the number of the positive labels (class label 1). This makes sense as in SMOTE, the number of rows in the minority class (class label 1) are used to morph and create new data/rows such that the number of rows in the minority class are equal to that of the number of rows in the majority class (class label 0).

Q7.2. Fit a default logistic regression model using SMOTE. Print the AUC and average precision of 5-fold cross validation. (Please set random state as 42 when performing SMOTE)

[17]:
```
smote_sampler = SMOTE(random_state = 42)
lr_smote_pipeline = imb_make_pipeline(smote_sampler, LogisticRegression())

scores = cross_validate(lr_smote_pipeline, X_dev_scaled, y_dev,
                        cv = 5, scoring = ['roc_auc', 'average_precision'])

print(f"The AUC values are as follows: {scores['test_roc_auc']}")
print(f"The AUC of the default Logistic Regression model (& SMOTE) is: " + \
      f"{scores['test_roc_auc'].mean()}")
print(f"The Average Precision of the default Logistic Regression model (&␣
 ↪SMOTE) is: " + \
      f"{scores['test_average_precision'].mean()}")
```

```
The AUC values are as follows: [0.95776313 0.97980138 0.98119548 0.97971317
0.99339012]
The AUC of the default Logistic Regression model (& SMOTE) is:
0.9783726532901543
The Average Precision of the default Logistic Regression model (& SMOTE) is:
0.7509401146877034
```

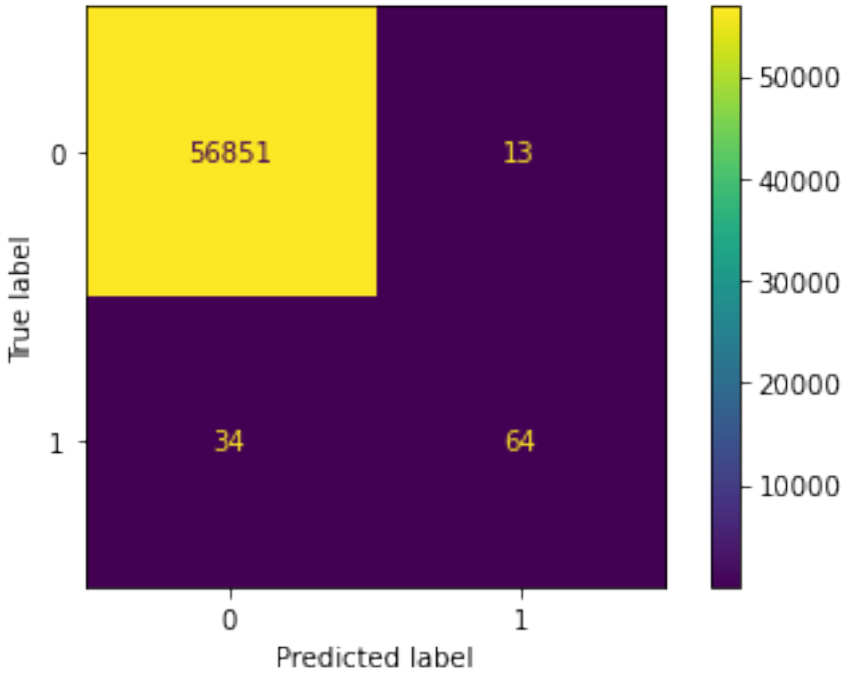
[18]:
```
# Get the fitted model after applying SMOTE from the pipeline
smote_sampler = SMOTE(random_state = 42)
lr_smote_pipeline = imb_make_pipeline(smote_sampler, LogisticRegression())
lr_smote_model = lr_smote_pipeline.fit(X_dev_scaled, y_dev)
```

Q8. Plot confusion matrices on the test set for all four models above. Comment on your result.

[19]:
```
from sklearn.metrics import plot_confusion_matrix
import warnings

warnings.filterwarnings("ignore")
```

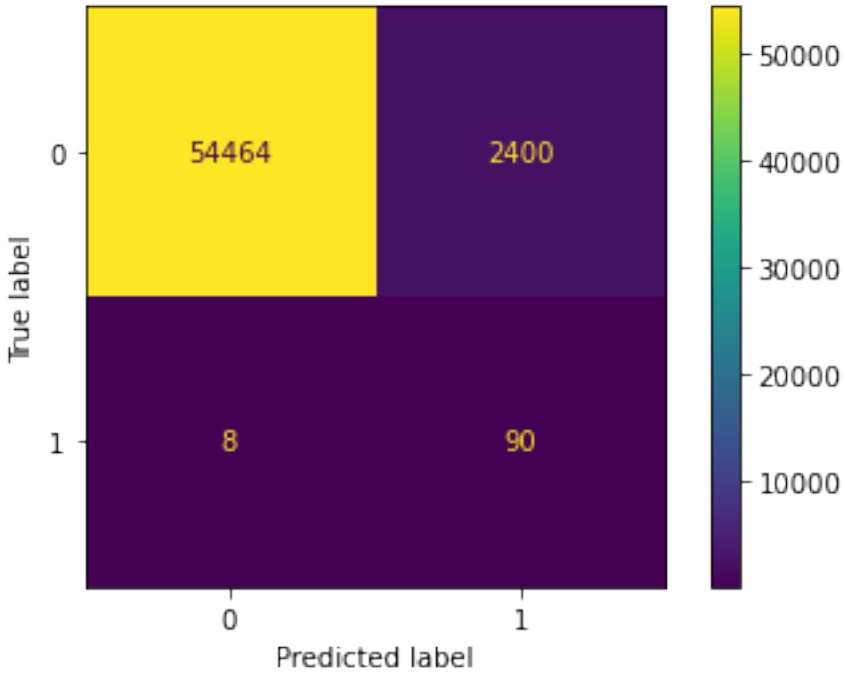
[20]:
```
print(f"The Confusion Matrix for default Logistic Regression Model without any␣
 ↪sampling used: ")
plot_confusion_matrix(lr_default_model, X_test_scaled, y_test)
plt.show()
```

```
The Confusion Matrix for default Logistic Regression Model without any sampling
used:
```



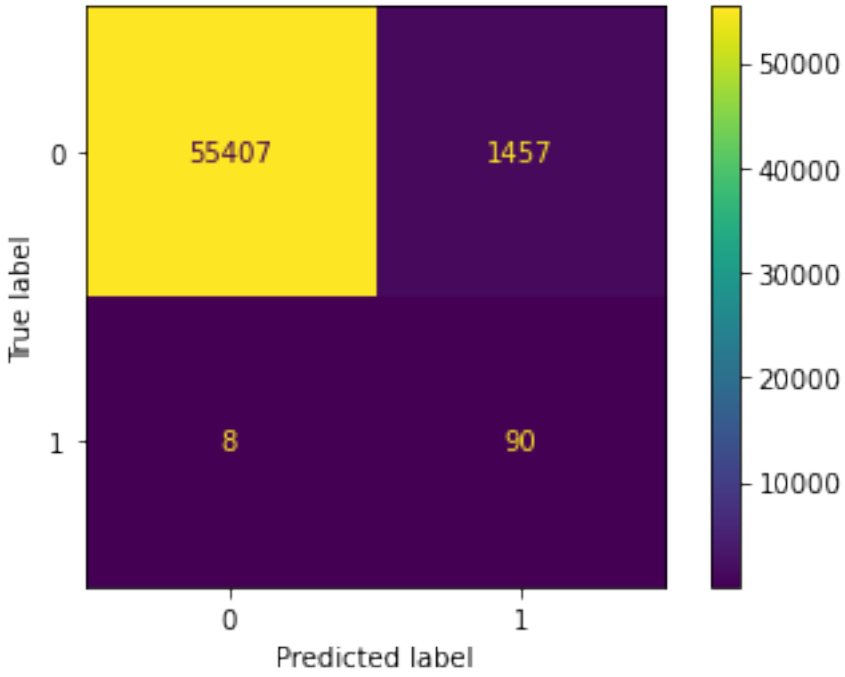
[21]:
```
print(f"The Confusion Matrix for default Logistic Regression Model with Under␣
 ↪Sampling used: ")
plot_confusion_matrix(lr_under_sampled_model, X_test_scaled, y_test)
plt.show()
```

The Confusion Matrix for default Logistic Regression Model with Under Sampling used:



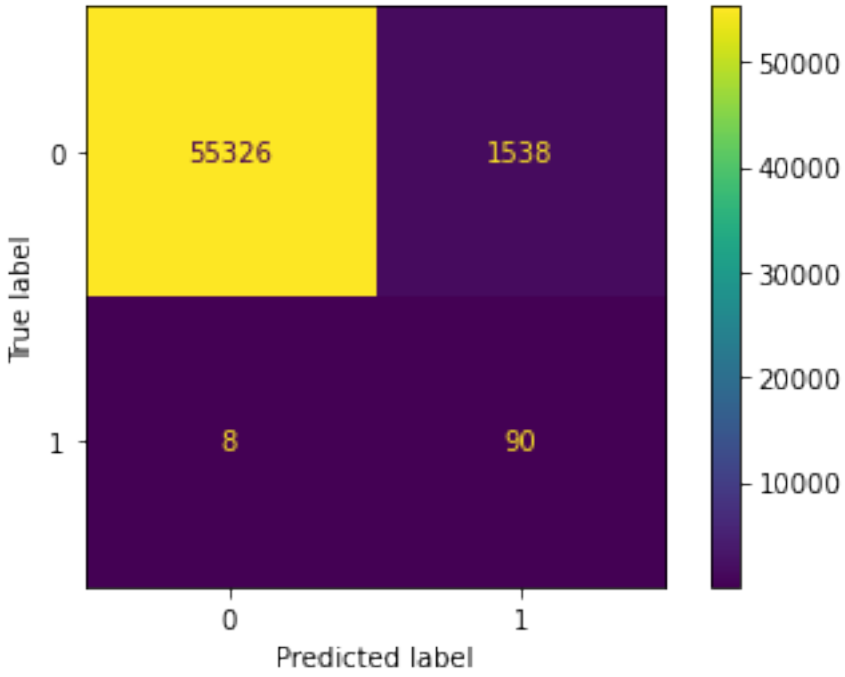
[22]:
```
print(f"The Confusion Matrix for default Logistic Regression Model with Over␣
 ↪Sampling used: ")
plot_confusion_matrix(lr_over_sampled_model, X_test_scaled, y_test)
plt.show()
```

```
The Confusion Matrix for default Logistic Regression Model with Over Sampling
used:
```



[23]:
```
print(f"The Confusion Matrix for default Logistic Regression Model with SMOTE␣
↪used: ")
plot_confusion_matrix(lr_smote_model, X_test_scaled, y_test)
plt.show()
```

```
The Confusion Matrix for default Logistic Regression Model with SMOTE used:
```



Analysis of the Results: As our dataset is related to credit card fraud detection, recall matters more here in comparison to the precision. Recall for all the models above can be calculated by the confusion matrices shown above as follows: 1. Default Logistic Regression: Recall: (62/62+36) = 0.633 2. Logistic Regression with Random Under Sampling: Recall: (89/89+9) = 0.908 3. Logistic Regression with Random Over Sampling: Recall: (90/90+8) = 0.918 4. Logistic Regression with SMOTE: Recall: (90/90+8) = 0.918

As we can see above, the Default Logistic Regression model has the least recall amongst all the 4 models above and the Logistic Regression model with Over Sampling and SMOTE has the highest recall (the same for both).

Also, the default logistic regression model makes very good predictions for the majority class with class label 0 as most of the class labels 0 are correctly classified by it. However, the default logistic regression model has a low recall and thus, would not suit our use case very well.

Furthermore, although the recall is the highest for the models with Over Sampling and SMOTE, the model with under sampling has a comparable recall. But, when we see the false positives, we see that the model with under sampling gives a lot more false positives in comparison to the over sampling and SMOTE cases. Although false positives does not pose a heavy threat to our use case, but still classifying a lot more transactions as fraud can be a hassle for the users and thus, we would try to keep it down as much as possible.

The results according to the confusion matrix for both the Logistic Regression models with SMOTE and over sampling are comprabale in terms of: 1. Both of them have the same recall. 2. Both of them have less false positives when the recall is quite high (which we want). 3. Both have decent precision as well.

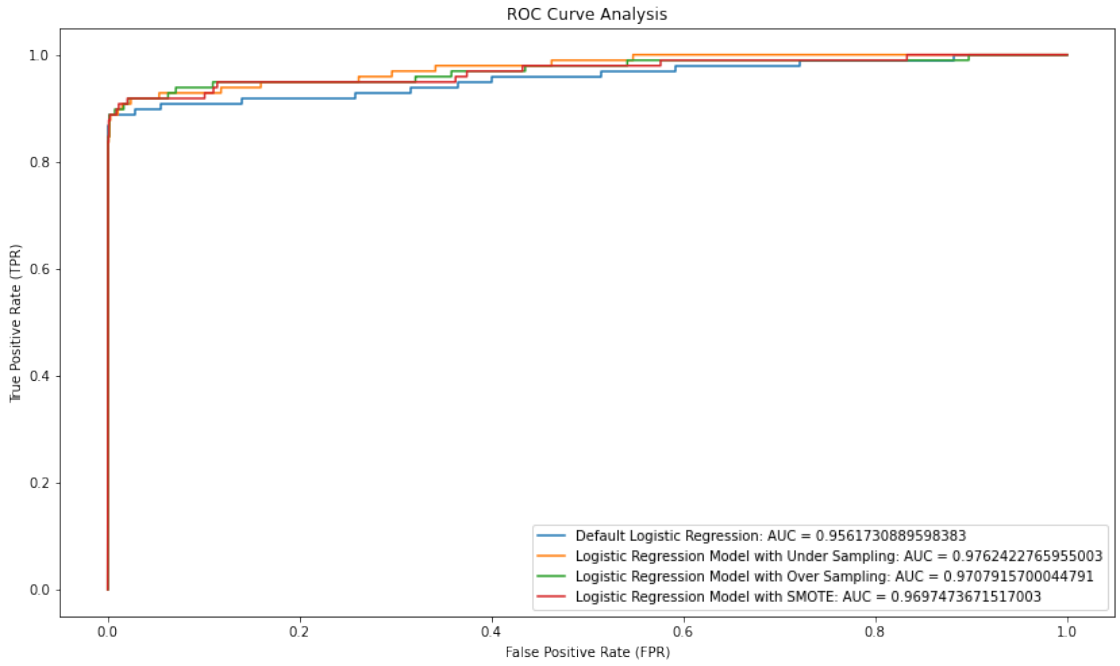
Thus, we can choose any of these 2 models based on the confusion matrices. However, I would go with the model training with over sampling as that has even less false positives with the same recall and nearly the same precision. This analysis is completely based on the confusion matrices above.

Q9. Plot the ROC for all four models above in a single plot. Make sure to label the axes and legend. Comment on your result.

[24]:
```
from sklearn.metrics import roc_curve
from sklearn.metrics import roc_auc_score
```

[25]:
```
models_trained = {"Default Logistic Regression": lr_default_model,
                  "Logistic Regression Model with Under Sampling":␣
 ↪lr_under_sampled_model,
                  "Logistic Regression Model with Over Sampling":␣
 ↪lr_over_sampled_model,
                  "Logistic Regression Model with SMOTE": lr_smote_model}
```

[26]:
```
# Making predictions and plotting the ROC for all the models trained above...
fig = plt.figure(figsize = (14, 8))

for model_name, model in models_trained.items():
    y_pred_proba = model.predict_proba(X_test_scaled)[:, 1]
    fpr, tpr, thresholds = roc_curve(y_test, y_pred_proba, pos_label = 1)
    auc_score = roc_auc_score(y_test, y_pred_proba)
    plt.plot(fpr, tpr, label = f"{model_name}: AUC = {auc_score}")

plt.xlabel("False Positive Rate (FPR)")
plt.ylabel("True Positive Rate (TPR)")
plt.title("ROC Curve Analysis")
plt.legend(loc = "lower right")
plt.show()
```



ROC Curve Analysis: Looking at the ROC above for all the models trained, I can clearly see that the Default Logistic Regression will have the least AUROC and would have larger number of false positives (recall lesser) in comparison to the other models and thus, I wouldn't take this model as the final one. Furthermore, the other 3 models (Logistic Regression with under sampling, over sampling and SMOTE) are quite comparable w.r.t the ROC plot above. All of them perform quite similarly with the Logistic Regression with Under sampling being the marginally best one. All of them have higher number of true positives than false negatives and also have quite a high recall. Thus, according to the ROC curve, I can choose any of the 3 models.

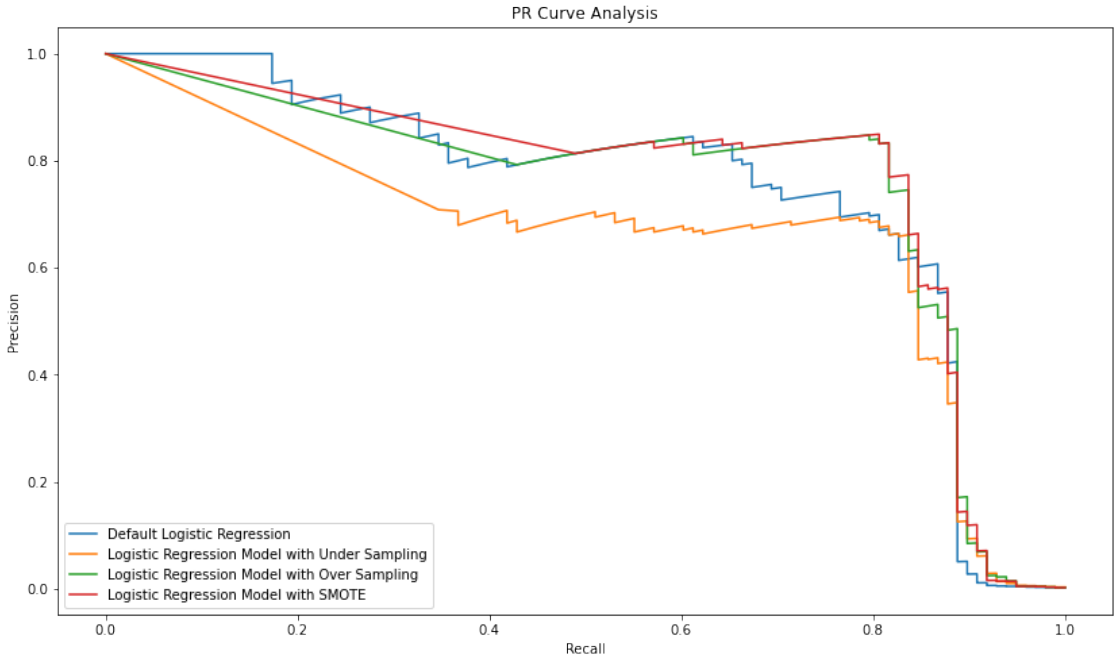
Q10. Plot the precision-recall curve for all four models above in a single plot. Make sure to label the axes and legend. Comment on your result.

[27]:
```
from sklearn.metrics import precision_recall_curve
```

[28]:
```
models_trained = {"Default Logistic Regression": lr_default_model,
                  "Logistic Regression Model with Under Sampling":␣
 ↪lr_under_sampled_model,
                  "Logistic Regression Model with Over Sampling":␣
 ↪lr_over_sampled_model,
                  "Logistic Regression Model with SMOTE": lr_smote_model}
```

[29]:
```
# Making predictions and plotting the PR Curve for all the models trained above.
 ↪..
fig = plt.figure(figsize = (14, 8))

for model_name, model in models_trained.items():
```

```
    y_pred_proba = model.predict_proba(X_test_scaled)[:, 1]
    precision, recall, thresholds = precision_recall_curve(y_test,␣
↪y_pred_proba, pos_label = 1)

    plt.plot(recall, precision, label = f"{model_name}")

plt.xlabel("Recall")
plt.ylabel("Precision")
plt.title("PR Curve Analysis")
plt.legend(loc = "lower left")
plt.show()
```



PR Curve Analysis: As shown in the curve above, the Logistic Regression model with under sampling is performing not quite well as the curve is quite close to that of a random classifier. The other 3 models seems to perform fine. However, the Default Logistic Regression model seems to give more preference to precision than recall. Furthermore, the other two models perform quite comparably and have quite the similar PR curves as shown above. Lastly, it seems that marginally the Logistic Regression with SMOTE gives more preference to recall and thus, I would consider it to be the case with which I would move forward in general.

Q11. Adding class weights to a logistic regression model. Print the AUC and average precision of 5-fold cross validation. Also, plot its confusion matrix on test set.

[30]:
```
scores = cross_validate(LogisticRegression(class_weight = 'balanced'),
                        X_dev_scaled, y_dev, cv = 5,
                        scoring = ['roc_auc', 'average_precision'],
```

```
                                return_estimator = True)
```

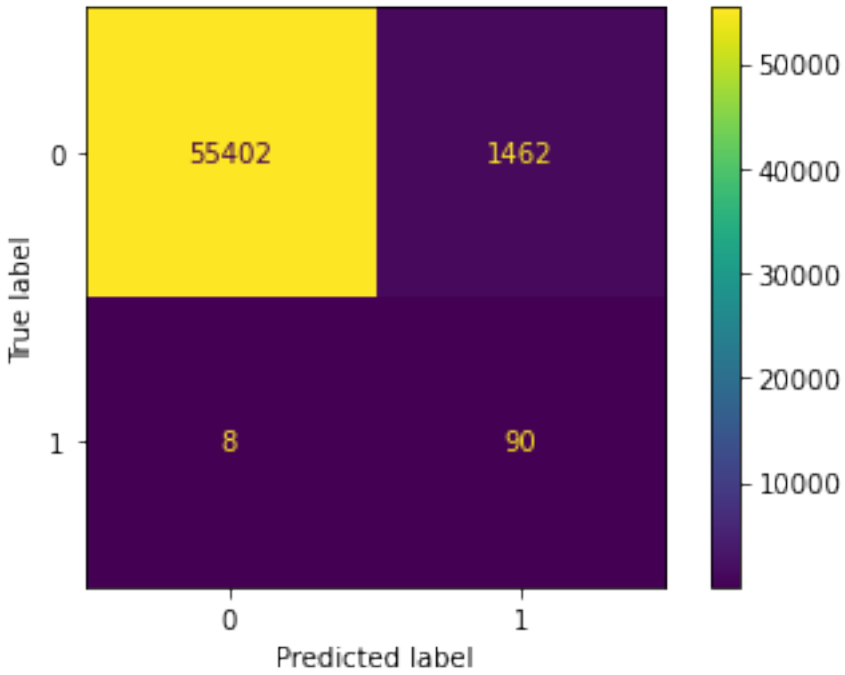
[31]:
```
print(f"The AUC values are as follows: {scores['test_roc_auc']}")
print(f"The AUC of the Logistic Regression model with balanced class weights is:
 ↪ " + \
      f"{scores['test_roc_auc'].mean()}")
print(f"The Average Precision of the Logistic Regression model with balanced␣
 ↪class weights is: " + \
      f"{scores['test_average_precision'].mean()}")
```

```
The AUC values are as follows: [0.95940194 0.9812208  0.98718789 0.98181545
0.9934096 ]
The AUC of the Logistic Regression model with balanced class weights is:
0.9806071364184955
The Average Precision of the Logistic Regression model with balanced class
weights is: 0.7521264537120119
```

[32]:
```
lr_class_weights_model = LogisticRegression(class_weight = 'balanced')
lr_class_weights_model = lr_class_weights_model.fit(X_dev_scaled, y_dev)
```

[33]:
```
print(f"The Confusion Matrix for Logistic Regression model with balanced class␣
 ↪weights: ")
plot_confusion_matrix(lr_class_weights_model, X_test_scaled, y_test)
plt.show()
```

```
The Confusion Matrix for Logistic Regression model with balanced class weights:
```

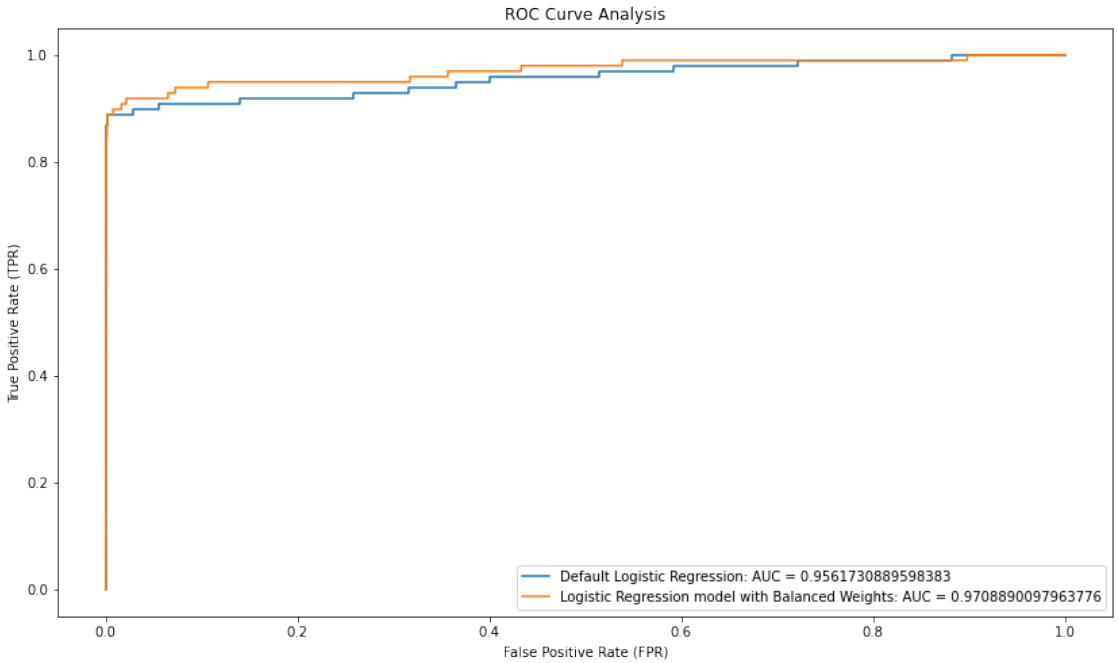


Looking at the confusion matrix above, we can see that a Logistic Regression model with balanced class weights has a higher recall of 90/(90+8) = 0.918 and has lower precision 90/(90+1462) in comparison to the default logistic regression model. As for our use case, recall matters more so, we would consider the logistic regression model with balanced class weights.

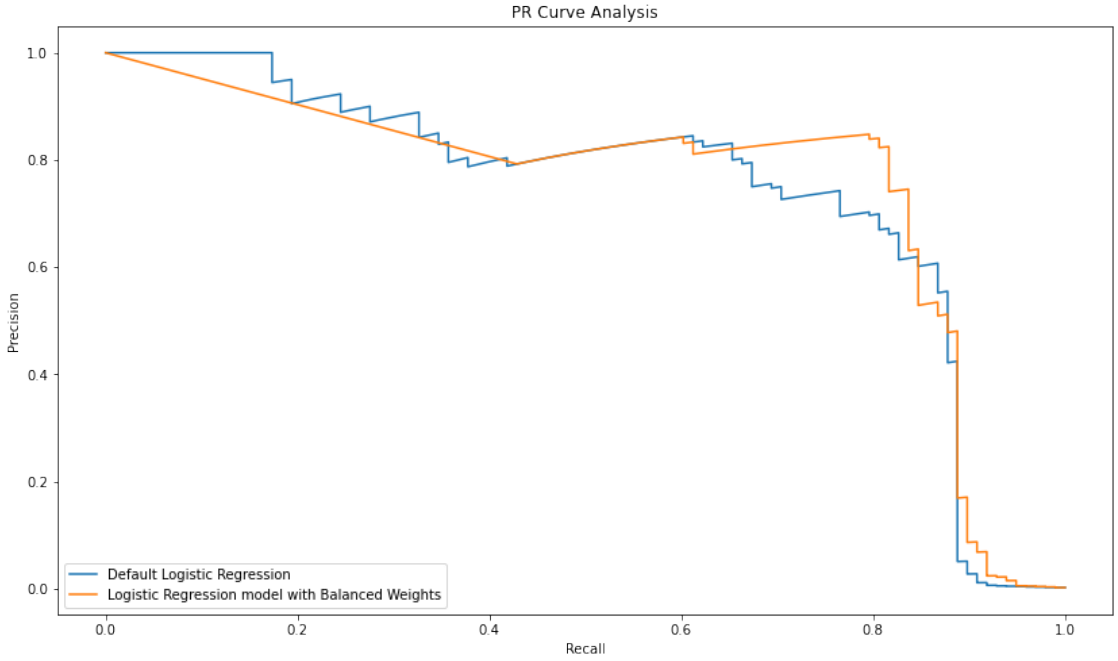
Q12. Plot the ROC and the precision-recall curve for default Logistic without any sampling method and this balanced Logistic model in two single plots. Make sure to label the axes and legend. Comment on your result.

[34]:
```
models_to_plot = {"Default Logistic Regression": lr_default_model,
                  "Logistic Regression model with Balanced Weights":␣
 ↪lr_class_weights_model}
```

[35]:
```
# Making predictions and plotting the ROC for 2 models above...
fig = plt.figure(figsize = (14, 8))

for model_name, model in models_to_plot.items():
    y_pred_proba = model.predict_proba(X_test_scaled)[:, 1]
    fpr, tpr, thresholds = roc_curve(y_test, y_pred_proba, pos_label = 1)
    auc_score = roc_auc_score(y_test, y_pred_proba)
    plt.plot(fpr, tpr, label = f"{model_name}: AUC = {auc_score}")

plt.xlabel("False Positive Rate (FPR)")
plt.ylabel("True Positive Rate (TPR)")
plt.title("ROC Curve Analysis")
plt.legend(loc = "lower right")
plt.show()
```



[36]:
```
# Making predictions and plotting the PR Curve for 2 models above...
fig = plt.figure(figsize = (14, 8))

for model_name, model in models_to_plot.items():
    y_pred_proba = model.predict_proba(X_test_scaled)[:, 1]
    precision, recall, thresholds = precision_recall_curve(y_test,␣
 ↪y_pred_proba, pos_label = 1)

    plt.plot(recall, precision, label = f"{model_name}")

plt.xlabel("Recall")
plt.ylabel("Precision")
plt.title("PR Curve Analysis")
plt.legend(loc = "lower left")
plt.show()
```



Curve Analysis: Looking at both the curves above, we can clearly see that the Logistic Regression model with balanced weights performs better in comparison to the default Logistic Regression model. As Area under the ROC curve is higher for the logistic regression model with balanced weights and the PR curve also does give more preference to recall for the same, it is clearly visible that this model performs better than the default logistic regression model.

1.4 Part 2: Unsupervised Learning

In this part, we will be applying unsupervised learning approaches to a problem in computational biology. Specifically, we will be analyzing single-cell genomic sequencing data. Single-cell genomics is a set of revolutionary new technologies which can profile the genome of a specimen (tissue, blood, etc.) at the resolution of individual cells. This increased granularity can help capture intercellular heterogeneity, key to better understanding and treating complex genetic diseases such as cancer and Alzheimer's.

Source: 10xgenomics.com/blog/single-cell-rna-seq-an-introductory-overview-and-tools-for-getting-started

A common challenge of genomic datasets is their high-dimensionality: a single observation (a cell, in the case of single-cell data) may have tens of thousands of gene expression features. Fortunately, biology offers a lot of structure - different genes work together in pathways and are co-regulated by gene regulatory networks. Unsupervised learning is widely used to discover this intrinsic structure and prepare the data for further analysis.

1.4.1 Dataset: single-cell RNASeq of mouse brain cells

We will be working with a single-cell RNASeq dataset of mouse brain cells. In the following gene expression matrix, each row represents a cell and each column represents a gene. Each entry in the matrix is a normalized gene expression count - a higher value means that the gene is expressed more in that cell. The dataset has been pre-processed using various quality control and normalization methods for single-cell data.

Data source is on Coursework.

[37]:
```
cell_gene_counts_df = pd.read_csv('data/mouse_brain_cells_gene_counts.csv',␣
↪index_col='cell')
cell_gene_counts_df
```

[37]:

cell	0610005C13Rik	0610007C21Rik	0610007L01Rik	\
A1.B003290.3_38_F.1.1	-0.08093	0.7856	1.334	
A1.B003728.3_56_F.1.1	-0.08093	-1.4840	-0.576	
A1.MAA000560.3_10_M.1.1	-0.08093	0.6300	-0.576	
A1.MAA000564.3_10_M.1.1	-0.08093	0.3809	1.782	
A1.MAA000923.3_9_M.1.1	-0.08093	0.5654	-0.576	
…	…	…	…	
E2.MAA000902.3_11_M.1.1	14.98400	1.1550	-0.576	
E2.MAA000926.3_9_M.1.1	-0.08093	-1.4840	-0.576	
E2.MAA000932.3_11_M.1.1	-0.08093	0.5703	-0.576	
E2.MAA000944.3_9_M.1.1	-0.08093	0.3389	-0.576	
E2.MAA001894.3_39_F.1.1	-0.08093	0.3816	-0.576	

cell	0610007N19Rik	0610007P08Rik	0610007P14Rik	\
A1.B003290.3_38_F.1.1	-0.2727	-0.4153	-0.8310	
A1.B003728.3_56_F.1.1	-0.2727	-0.4153	1.8350	

```
A1.MAA000560.3_10_M.1.1        -0.2727        -0.4153        -0.2084
A1.MAA000564.3_10_M.1.1        -0.2727        -0.4153         1.0300
A1.MAA000923.3_9_M.1.1         -0.2727        -0.4153        -0.8310
…                                 …              …              …
E2.MAA000902.3_11_M.1.1        -0.2727        -0.4153         0.7530
E2.MAA000926.3_9_M.1.1         -0.2727        -0.4153         1.4720
E2.MAA000932.3_11_M.1.1        -0.2727        -0.4153        -0.8310
E2.MAA000944.3_9_M.1.1         -0.2727        -0.4153        -0.2434
E2.MAA001894.3_39_F.1.1        -0.2727        -0.4153        -0.8310

                          0610007P22Rik  0610009B14Rik  0610009B22Rik  \
cell
A1.B003290.3_38_F.1.1           -0.4692       -0.03146        -0.6035
A1.B003728.3_56_F.1.1           -0.4692       -0.03146        -0.6035
A1.MAA000560.3_10_M.1.1         -0.4692       -0.03146        -0.6035
A1.MAA000564.3_10_M.1.1         -0.4692       -0.03146         1.2640
A1.MAA000923.3_9_M.1.1          -0.4692       -0.03146        -0.6035
…                                  …             …              …
E2.MAA000902.3_11_M.1.1         -0.4692       -0.03146        -0.6035
E2.MAA000926.3_9_M.1.1          -0.4692       -0.03146         1.8120
E2.MAA000932.3_11_M.1.1         -0.4692       -0.03146        -0.6035
E2.MAA000944.3_9_M.1.1          -0.4692       -0.03146        -0.6035
E2.MAA001894.3_39_F.1.1         -0.4692       -0.03146        -0.6035

                          0610009D07Rik  …   Zwint    Zxda    Zxdb    Zxdc  \
cell                                     …
A1.B003290.3_38_F.1.1        -1.021000  … -0.7227 -0.2145 -0.1927 -0.4163
A1.B003728.3_56_F.1.1        -1.021000  … -0.7227 -0.2145 -0.1927 -0.4163
A1.MAA000560.3_10_M.1.1       1.253000  …  1.3150 -0.2145 -0.1927 -0.4163
A1.MAA000564.3_10_M.1.1      -1.021000  … -0.7227 -0.2145 -0.1927 -0.4163
A1.MAA000923.3_9_M.1.1       -1.021000  … -0.7227 -0.2145 -0.1927 -0.4163
…                                  …  …     …        …       …       …
E2.MAA000902.3_11_M.1.1      -1.021000  …  1.4260 -0.2145 -0.1927 -0.4163
E2.MAA000926.3_9_M.1.1        1.079000  … -0.7227 -0.2145 -0.1927 -0.4163
E2.MAA000932.3_11_M.1.1      -0.003473  … -0.7227 -0.2145 -0.1927 -0.4163
E2.MAA000944.3_9_M.1.1        1.281000  …  1.2160 -0.2145 -0.1927 -0.4163
E2.MAA001894.3_39_F.1.1       1.106000  … -0.7227 -0.2145 -0.1927 -0.4163

                          Zyg11b     Zyx  Zzef1    Zzz3        a  l7Rn6
cell
A1.B003290.3_38_F.1.1   -0.5923 -0.5913 -0.553 -0.5654 -0.04385  1.567
A1.B003728.3_56_F.1.1   -0.5923 -0.5913 -0.553 -0.5654 -0.04385 -0.681
A1.MAA000560.3_10_M.1.1 -0.5923 -0.5913  2.072 -0.5654 -0.04385  1.260
A1.MAA000564.3_10_M.1.1 -0.5923  2.3900 -0.553  0.1697 -0.04385 -0.681
A1.MAA000923.3_9_M.1.1   2.3180 -0.5913 -0.553 -0.5654 -0.04385 -0.681
…                           …     …    …     …       …    …
E2.MAA000902.3_11_M.1.1 -0.5923 -0.5913 -0.553 -0.5654 -0.04385  1.728
```

```
E2.MAA000926.3_9_M.1.1   0.2422 -0.5913 -0.553  1.6060 -0.04385 -0.681
E2.MAA000932.3_11_M.1.1 -0.5923 -0.5913 -0.553 -0.5654 -0.04385  2.074
E2.MAA000944.3_9_M.1.1  -0.5923 -0.5913 -0.553  1.3070 -0.04385 -0.681
E2.MAA001894.3_39_F.1.1 -0.5923 -0.5913 -0.553 -0.5654 -0.04385  1.628

[1000 rows x 18585 columns]
```

Note the dimensionality - we have 1000 cells (observations) and 18,585 genes (features)!

We are also provided a metadata file with annotations for each cell (e.g. cell type, subtissue, mouse sex, etc.)

[38]:
```
cell_metadata_df = pd.read_csv('data/mouse_brain_cells_metadata.csv')
cell_metadata_df
```

[38]:
```
                       cell cell_ontology_class    subtissue mouse.sex  \
0      A1.B003290.3_38_F.1.1           astrocyte     Striatum         F
1      A1.B003728.3_56_F.1.1           astrocyte     Striatum         F
2    A1.MAA000560.3_10_M.1.1     oligodendrocyte       Cortex         M
3    A1.MAA000564.3_10_M.1.1    endothelial cell     Striatum         M
4     A1.MAA000923.3_9_M.1.1           astrocyte  Hippocampus         M
..                       …                   …         …       …
995  E2.MAA000902.3_11_M.1.1           astrocyte     Striatum         M
996   E2.MAA000926.3_9_M.1.1     oligodendrocyte       Cortex         M
997  E2.MAA000932.3_11_M.1.1    endothelial cell  Hippocampus         M
998   E2.MAA000944.3_9_M.1.1     oligodendrocyte       Cortex         M
999  E2.MAA001894.3_39_F.1.1     oligodendrocyte       Cortex         F

    mouse.id plate.barcode  n_genes   n_counts
0     3_38_F       B003290     3359   390075.0
1     3_56_F       B003728     1718   776436.0
2     3_10_M     MAA000560     3910  1616084.0
3     3_10_M     MAA000564     4352   360004.0
4      3_9_M     MAA000923     2248   290282.0
..       …           …      …         …
995   3_11_M     MAA000902     3026  3134463.0
996    3_9_M     MAA000926     3085   744301.0
997   3_11_M     MAA000932     2277   519257.0
998    3_9_M     MAA000944     3234  1437895.0
999   3_39_F     MAA001894     3375   885166.0

[1000 rows x 8 columns]
```

Different cell types

[39]:
```
cell_metadata_df['cell_ontology_class'].value_counts()
```

[39]:
```
oligodendrocyte                 385
endothelial cell                264
```

```
astrocyte                          135
neuron                              94
brain pericyte                      58
oligodendrocyte precursor cell      54
Bergmann glial cell                 10
Name: cell_ontology_class, dtype: int64
```

Different subtissue types (parts of the brain)

[40]:
```
cell_metadata_df['subtissue'].value_counts()
```

[40]:
```
Cortex         364
Hippocampus    273
Striatum       220
Cerebellum     143
Name: subtissue, dtype: int64
```

Our goal in this exercise is to use dimensionality reduction and clustering to visualize and better understand the high-dimensional gene expression matrix. We will use the following pipeline, which is common in single-cell analysis: 1. Use PCA to project the gene expression matrix to a lower-dimensional linear subspace. 2. Cluster the data using K-means on the first 20 principal components. 3. Use t-SNE to project the first 20 principal components onto two dimensions. Visualize the points and color by their clusters from (2).

1.5 1 PCA

Q1. Perform PCA and project the gene expression matrix onto its first 50 principal components. You may use `sklearn.decomposition.PCA`.

[41]:
```
from sklearn.decomposition import PCA
```

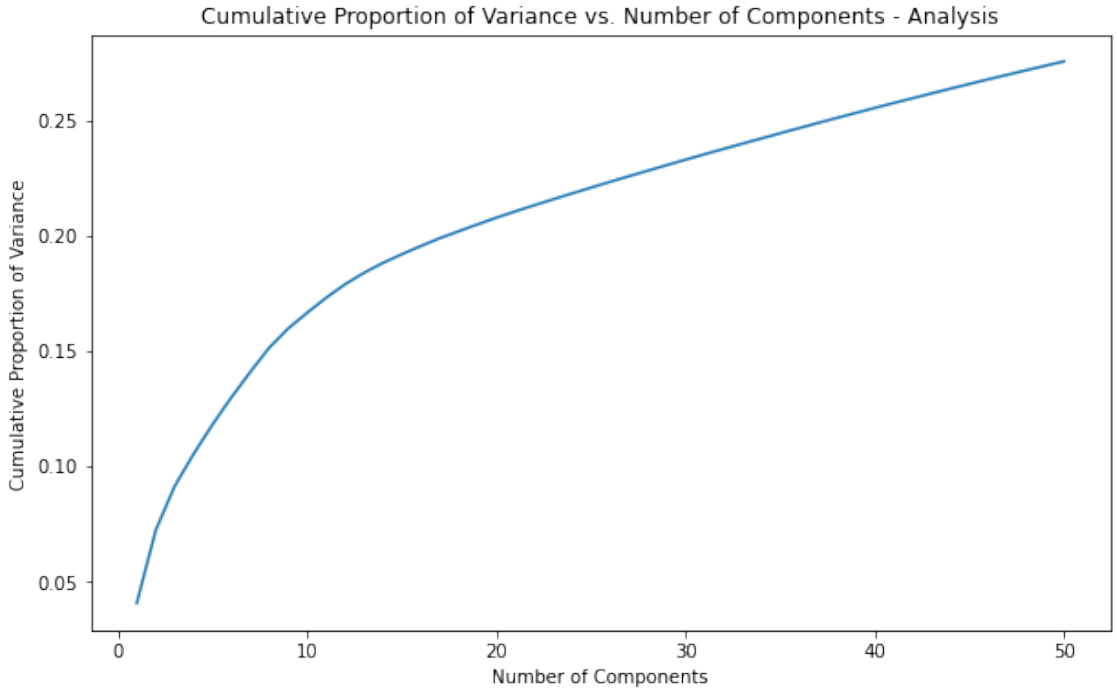
[42]:
```
# As the data has already been normalized we can directly perform PCA on it.
pca_obj = PCA(n_components = 50)
pcs_cell_gene_counts = pca_obj.fit_transform(cell_gene_counts_df)
print(pcs_cell_gene_counts.shape)
```

```
(1000, 50)
```

Q2. Plot the cumulative proportion of variance explained as a function of the number of principal components. How much of the total variance in the dataset is explained by the first 20 principal components?

[43]:
```
fig = plt.figure(figsize = (10, 6))
variances = pca_obj.explained_variance_ratio_
cdf_variance = np.cumsum(variances)
plt.plot(list(range(1, len(cdf_variance) + 1)), cdf_variance)
plt.xlabel("Number of Components")
plt.ylabel("Cumulative Proportion of Variance")
plt.title("Cumulative Proportion of Variance vs. Number of Components -␣
 ↪Analysis")
```

```
plt.show()
```



[44]:
```
print(f"The Cumulative Proportion of Variance captured by the first 20␣
↪principal components is: " + \
      f"{cdf_variance[19]}")
```

```
The Cumulative Proportion of Variance captured by the first 20 principal
components is: 0.20765340847459496
```

Q3. For the first principal component, report the top 10 loadings (weights) and their corresponding gene names. In other words, which 10 genes are weighted the most in the first principal component?

[45]:
```
feature_name_first_pc_map = list(zip(cell_gene_counts_df.columns, pca_obj.
↪components_[0]))
top_10_weights_first_pc = sorted(feature_name_first_pc_map, key = lambda x :␣
↪x[1])
top_10_weights_first_pc.reverse()
```

[46]:
```
print(f"Top 10 gene weights with their corresponding gene names are as follows:␣
↪")
top_10_loadings_df = pd.DataFrame(top_10_weights_first_pc[:10], columns =␣
↪["Feature name", "Weight"])
top_10_loadings_df
```

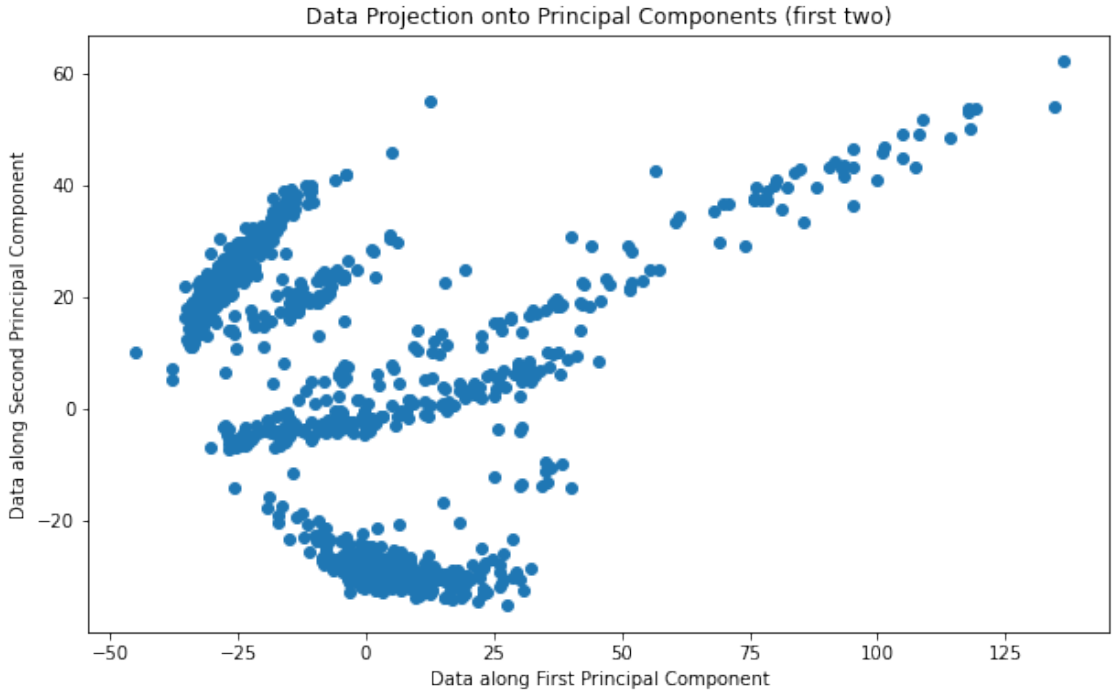
Top 10 gene weights with their corresponding gene names are as follows:

[46]:

	Feature name	Weight
0	Nsg2	0.026673
1	St8sia3	0.026595
2	Ptpn5	0.026588
3	Kcnj4	0.026539
4	Rasgef1a	0.026347
5	Camkv	0.026221
6	Hpca	0.026173
7	Cpne5	0.026022
8	Nrsn2	0.025979
9	Erc2	0.025853

Q4. Plot the projection of the data onto the first two principal components using a scatter plot.

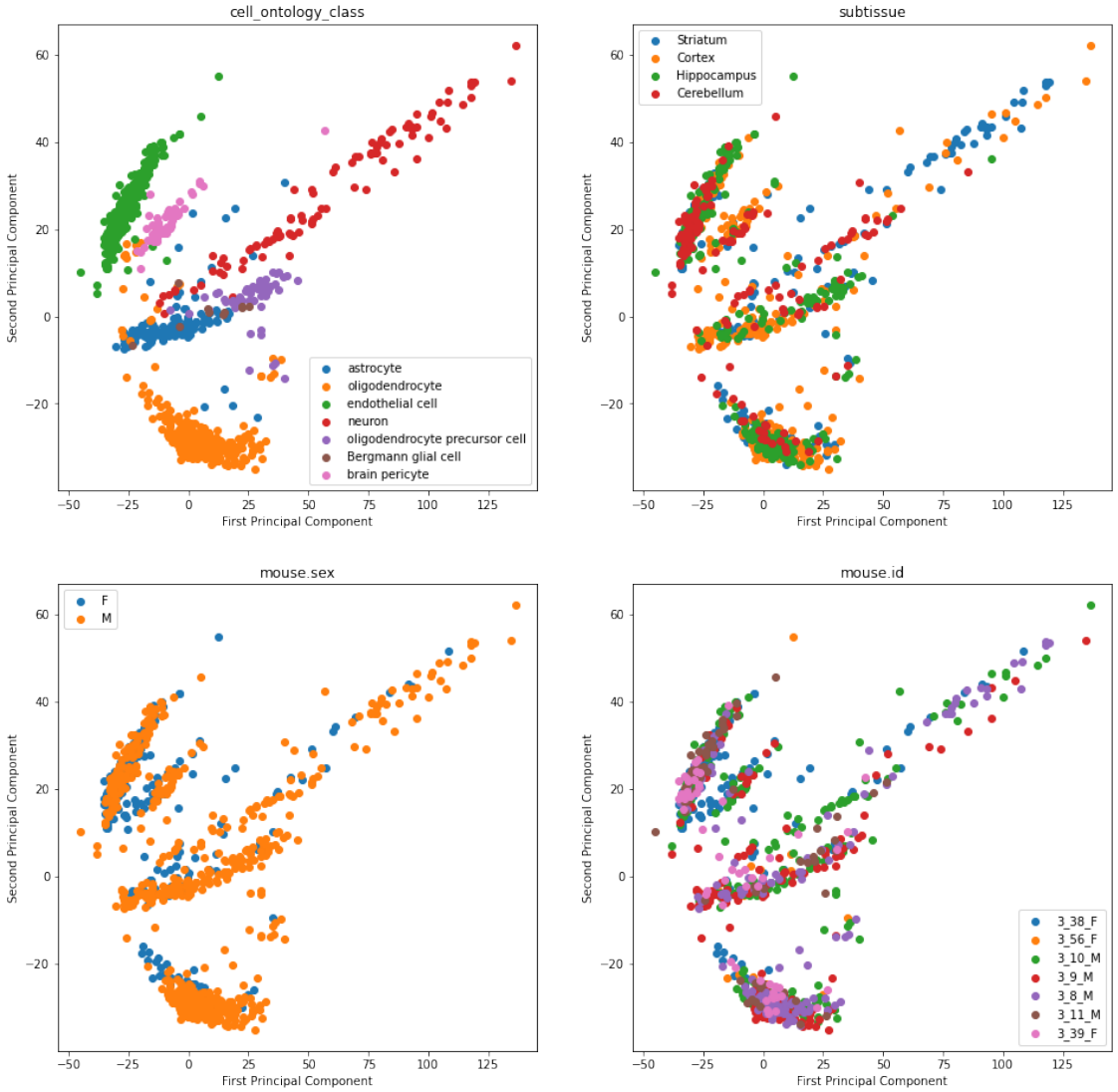
[47]:
```
fig = plt.figure(figsize = (10, 6))

plt.scatter(pcs_cell_gene_counts[:, 0], pcs_cell_gene_counts[:, 1])
plt.xlabel("Data along First Principal Component")
plt.ylabel("Data along Second Principal Component")
plt.title("Data Projection onto Principal Components (first two)")
plt.show()
```



Q5. Now, use a small multiple of four scatter plots to make the same plot as above,

but colored by four annotations in the metadata: cell_ontology_class, subtissue, mouse.sex, mouse.id. Include a legend for the labels. For example, one of the plots should have points projected onto PC 1 and PC 2, colored by their cell_ontology_class.

[48]:
```
fig, axes = plt.subplots(2, 2, figsize = (16, 16))
metadata_col_names = ['cell_ontology_class', 'subtissue', 'mouse.sex', 'mouse.
 ↪id']
metadata_col_idx = 0

for row_idx in range(0, 2):
    for col_idx in range(0, 2):
        curr_col_vals = cell_metadata_df[metadata_col_names[metadata_col_idx]].
 ↪unique()
        for col_value in curr_col_vals:
            pc1 =␣
 ↪pcs_cell_gene_counts[cell_metadata_df[metadata_col_names[metadata_col_idx]]␣
 ↪== col_value, 0]
            pc2 =␣
 ↪pcs_cell_gene_counts[cell_metadata_df[metadata_col_names[metadata_col_idx]]␣
 ↪== col_value, 1]
            axes[row_idx, col_idx].scatter(pc1, pc2, label = col_value)
        axes[row_idx, col_idx].legend()
        axes[row_idx, col_idx].set_title(metadata_col_names[metadata_col_idx])
        axes[row_idx, col_idx].set_xlabel("First Principal Component")
        axes[row_idx, col_idx].set_ylabel("Second Principal Component")
        metadata_col_idx += 1

plt.show()
```



Q6. Based on the plots above, the first two principal components correspond to which aspect of the cells? What is the intrinsic dimension that they are describing?

The first two principal components seem to correspond to the "cell_ontology" aspect of the cells. Intrinsic Dimension: As we can cluster them quite visible looking at the scatter plot above based on the "cell_ontology" feature of the cell in 2 dimenions or 2 principal component, then the intrinsic dimension that it descibes is the "cell_ontology feature having 2 dimenions.

1.6 2 K-means

While the annotations provide high-level information on cell type (e.g. cell_ontology_class has 7 categories), we may also be interested in finding more granular subtypes of cells. To achieve this, we will use K-means clustering to find a large number of clusters in the gene expression dataset. Note that the original gene expression matrix had over 18,000 noisy features, which is not ideal for clustering. So, we will perform K-means clustering on the first 20 principal components of the

dataset.

Q7. Implement a `kmeans` function which takes in a dataset `X` and a number of clusters `k`, and returns the cluster assignment for each point in `X`. You may NOT use sklearn for this implementation. Use lecture 6, slide 14 as a reference.

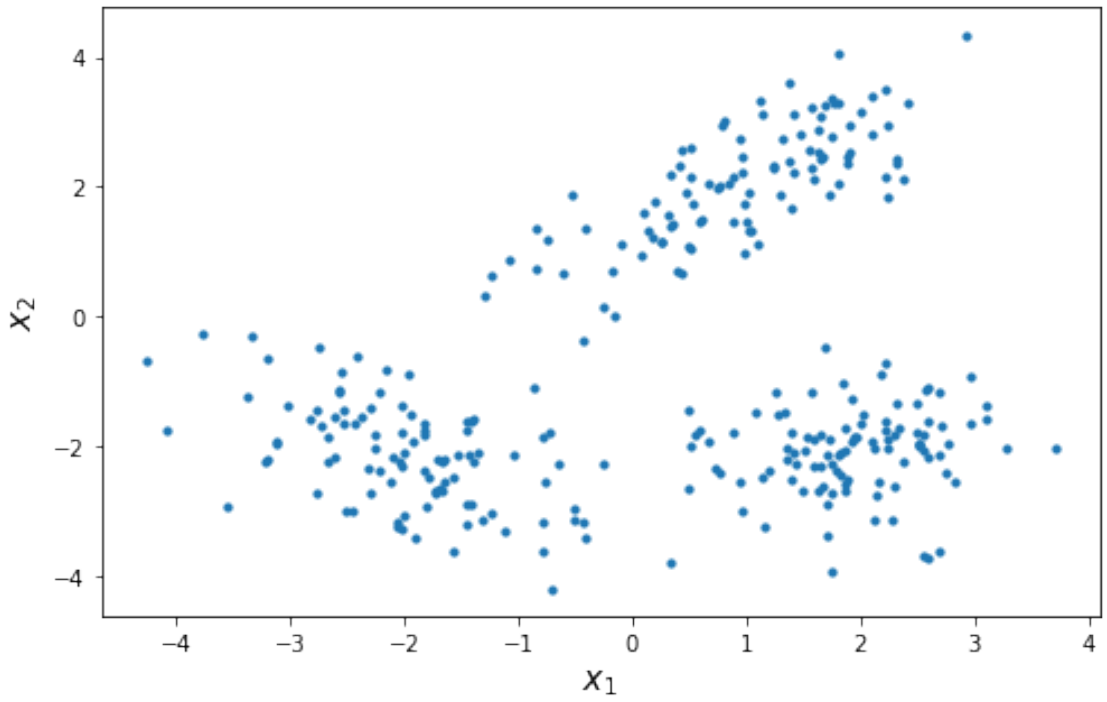
[49]:
```
def kmeans(X, k, iters=10):
    '''Groups the points in X into k clusters using the K-means algorithm.

    Parameters
    ----------
    X : (m x n) data matrix
    k: number of clusters
    iters: number of iterations to run k-means loop

    Returns
    -------
    y: (m x 1) cluster assignment for each point in X
    '''
    # Randomly choose initial centroids
    centroid_indices = np.random.choice(len(X), k, replace = False)
    centroids = X[centroid_indices, :]
    iteration = 0

    while iteration <= iters:
        distances = compute_distances(X, centroids)
        new_clusters = np.array([np.argmin(distance) for distance in distances])
        prev_centroids = centroids

        # finding new centroids
        centroids = []
        for cluster_idx in range(k):
            new_centroid = X[new_clusters == cluster_idx].mean(axis = 0)
            centroids.append(new_centroid)

        centroids = np.vstack(centroids)
        iteration += 1

        if prev_centroids.tolist() == centroids.tolist():
            return new_clusters

    distances = compute_distances(X, centroids)
    new_clusters = np.array([np.argmin(distance) for distance in distances])

    return new_clusters

def compute_distances(data, centroids):
    distances = list()
```

```
    for point in data:
        distances_from_centroids = list()
        for centroid_idx in range(len(centroids)):
            distances_from_centroids.append(np.linalg.norm(point -␣
↪centroids[centroid_idx]))
        distances.append(distances_from_centroids)

    return distances
```

Before applying K-means on the gene expression data, we will test it on the following synthetic dataset to make sure that the implementation is working.

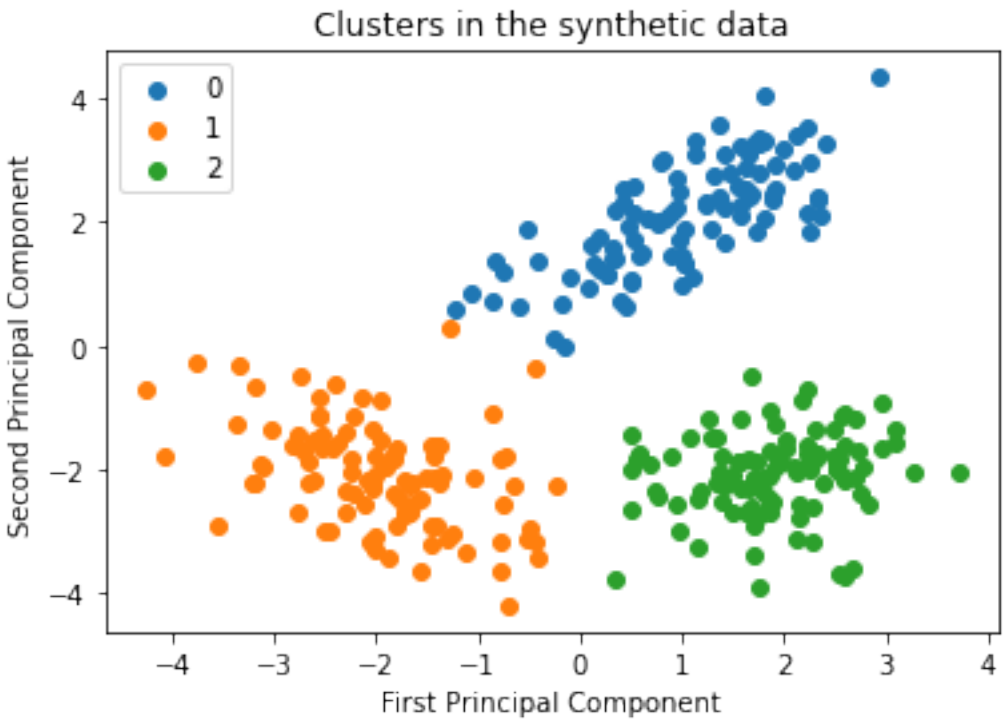
[50]:
```
np.random.seed(0)
x_1 = np.random.multivariate_normal(mean=[1, 2], cov=np.array([[0.8, 0.6], [0.
↪6, 0.8]]), size=100)
x_2 = np.random.multivariate_normal(mean=[-2, -2], cov=np.array([[0.8, -0.4],␣
↪[-0.4, 0.8]]), size=100)
x_3 = np.random.multivariate_normal(mean=[2, -2], cov=np.array([[0.4, 0], [0, 0.
↪4]]), size=100)
X = np.vstack([x_1, x_2, x_3])

plt.figure(figsize=(8, 5))
plt.scatter(X[:, 0], X[:, 1], s=10)
plt.xlabel('$x_1$', fontsize=15)
plt.ylabel('$x_2$', fontsize=15)
```

[50]:
```
Text(0, 0.5, '$x_2$')
```



Q8. Apply K-means with k=3 to the synthetic dataset above. Plot the points colored by their K-means cluster assignments to verify that your implementation is working.

[51]:
```
k = 3
labels_found = kmeans(X, k, 25)
labeled_synthetic_data = np.column_stack([X, labels_found])

for idx in range(k):
    pc1 = labeled_synthetic_data[labeled_synthetic_data[:, -1] == idx][:, 0]
    pc2 = labeled_synthetic_data[labeled_synthetic_data[:, -1] == idx][:, 1]
    plt.scatter(pc1, pc2, label = idx)

plt.xlabel("First Principal Component", fontsize = 10)
plt.ylabel("Second Principal Component", fontsize = 10)
plt.title("Clusters in the synthetic data")
plt.legend()
plt.show()
```



Q9. Use K-means with k=20 to cluster the first 20 principal components of the gene expression data.

[52]:
```
k = 20
gene_labels = kmeans(pcs_cell_gene_counts[:, :20], k, 200)
print(gene_labels[:200])
```

```
[13  0 16  6  0  0 15 12  5  2 15  3 13  3  9 16 16 14  2  4  2  3  3 12
 14  6 13 14  9 12  0  4  6 15 14  5 12  3 13 16 10 14 14  2  2 11 13 16
 18  0 16  9  6 16  6  2 16 10 18 19 16 19 12  4 19  5 13 19 15  5  9 12
  0  2  7 14 11  3  9  4 13  5  3 12  1  0  7 12 13 12  9  2 14  1 14  5
 16  5 14 10  9 10 16  2  5 10 16  1 19 13  0  5  0  9 16  9 14  4 15 16
 12  3 16 19  5 11 19 11  3  5 16  7  6 13 12  5 14  0 10  9 14  7  6  2
  4  6 14 15 10 14 16  0 16 19  5  3 19 14 13 14  9  0 14 10 19 15  3  3
  4 16 14  6  2 10 13  5  5  0  0  9 14 10  9  0 15 15  5 14 13 17  9 10
 12  0  2  2  5 10 14 14]
```

As we can see above, using K-means with k = 20, we can cluster the gene expresssion data with the first 20 principal components. Now, we will visualize the same by projecting it into 2 dimensions using t-SNE.

1.7 3 t-SNE

In this final section, we will visualize the data again using t-SNE - a non-linear dimensionality reduction algorithm. You can learn more about t-SNE in this interactive tutorial:

https://distill.pub/2016/misread-tsne/.

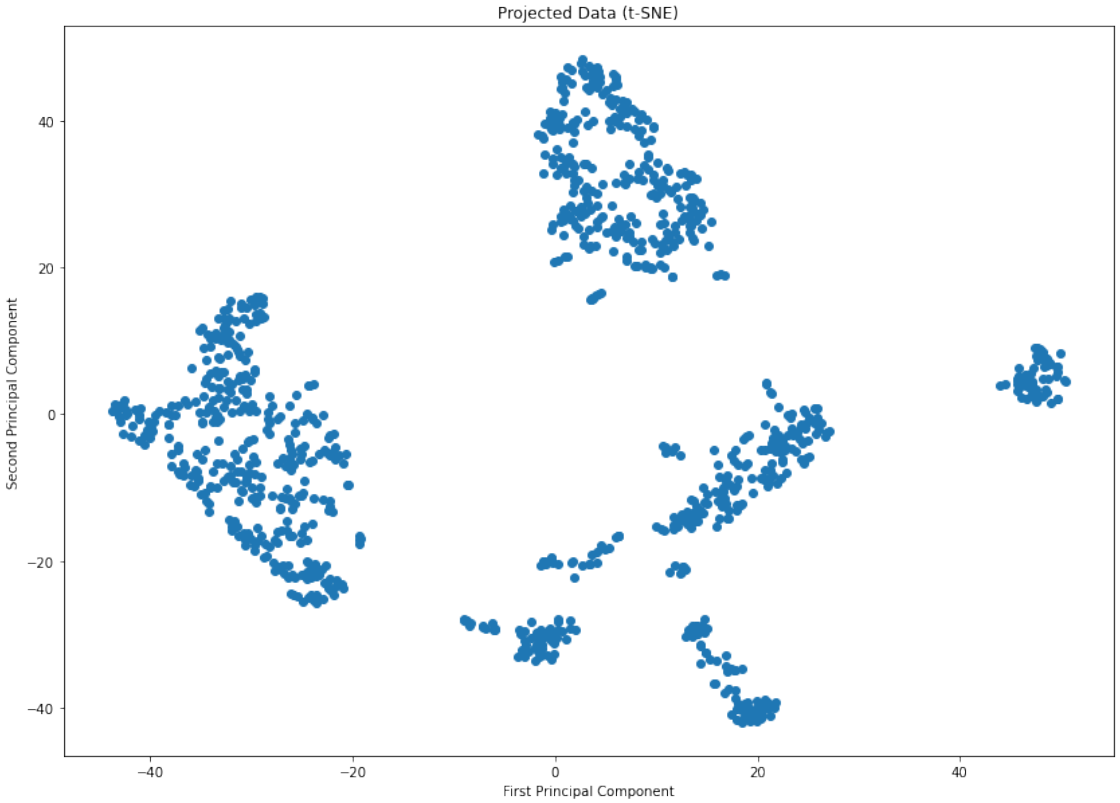
Q10. Use t-SNE to reduce the first 20 principal components of the gene expression dataset to two dimensions. You may use `sklearn.manifold.TSNE`. Note that it is recommended to first perform PCA before applying t-SNE to suppress noise and speed up computation.

[53]:
```
from sklearn.manifold import TSNE
```

[54]:
```
tsne_obj = TSNE(n_components = 2, random_state = 42)
X_transformed_data = tsne_obj.fit_transform(pcs_cell_gene_counts[:, :20])
```

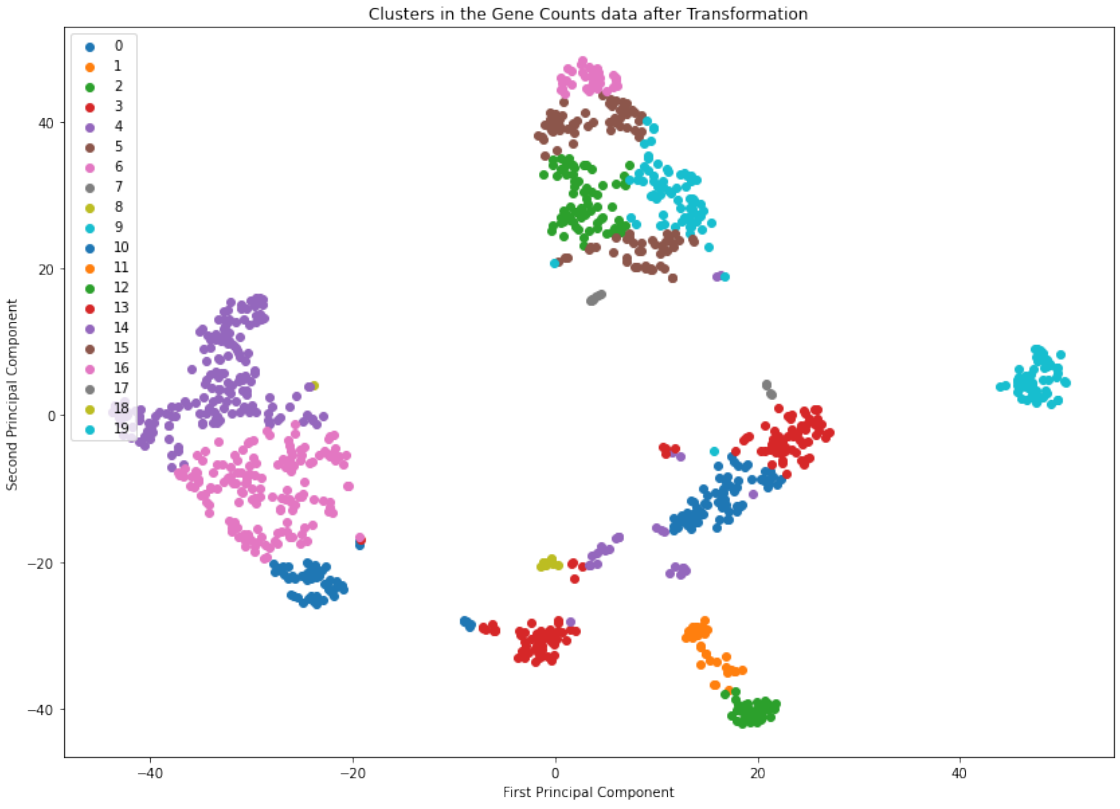
Q11. Plot the data (first 20 principal components) projected onto the first two t-SNE dimensions.

[55]:
```
fig = plt.figure(figsize = (14, 10))
plt.scatter(X_transformed_data[:, 0], X_transformed_data[:, 1])
plt.xlabel("First Principal Component")
plt.ylabel("Second Principal Component")
plt.title("Projected Data (t-SNE)")
plt.show()
```



Q12. Plot the data (first 20 principal components) projected onto the first two t-SNE dimensions, with points colored by their cluster assignments from part 2.

[56]:
```
k = 20

fig = plt.figure(figsize = (14, 10))
X_labeled_gene_counts_data = np.column_stack([X_transformed_data, gene_labels])

for idx in range(k):
    pc1 = X_labeled_gene_counts_data[X_labeled_gene_counts_data[:, -1] == idx][:
 ↪, 0]
    pc2 = X_labeled_gene_counts_data[X_labeled_gene_counts_data[:, -1] == idx][:
 ↪, 1]
    plt.scatter(pc1, pc2, label = idx)

plt.xlabel("First Principal Component", fontsize = 10)
plt.ylabel("Second Principal Component", fontsize = 10)
plt.title("Clusters in the Gene Counts data after Transformation")
plt.legend()
plt.show()
```



Q13. Why is there overlap between points in different clusters in the t-SNE plot above?

Analysis: As we can see above, there is quite some overlap between the points in different clusters

in the t-SNE plot above because as we are projecting down 20 principal components (or 20 different dimensions or axes of change) to just 2 dimensions, we can't keep all the information intact and it's not perfectly projectable in just 2 dimenions. Also, initially gene expression data had more than 18000 dimensions, coming down to just 20 principal components is a very big leap in terms of dimensionality reduction and it makes quite a lot of sense that we can see some overlap in the clusters formed above in the t-SNE plot.

These 20 clusters may correspond to various cell subtypes or cell states. They can be further investigated and mapped to known cell types based on their gene expressions (e.g. using the K-means cluster centers). The clusters may also be used in downstream analysis. For instance, we can monitor how the clusters evolve and interact with each other over time in response to a treatment.