Classification Coursework

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Introduction

The observations in the vertebral column dataset record measurements of six biomechanical features, with accompanying labels, 'normal' or 'abnormal'. In this report, we develop a kNN model (supervised) and a K-means clustering model (unsupervised). We showcase two methods of dimensionality reduction, observing correlations and eliminating features for the supervised model, then using PCA for the unsupervised model.

Data Pre-Processing and EDA

First, we attach the column names to the dataset; pelvic_incidence, pelvic_tilt, lumbar_lordosis_angle, sacral_slope, pelvic_radius, grade_of_spondylolisthesis and class. There are 310 observations in total.

There were 58 negative values in the grade_of_spondylolisthesis column. Spondylolisthesis grade is quantified by 'percentage of slip', which can range from 0% up to values exceeding 100%. Typically, one would try to identify why these negative values have occurred, then remove or impute them. Since the focus of this coursework is on classification algorithms, they have been kept in.

Two outliers were removed, one with high grade_of_spondylolisthesis (∼419%) and one with high lumbar_lordosis_angle (>120).

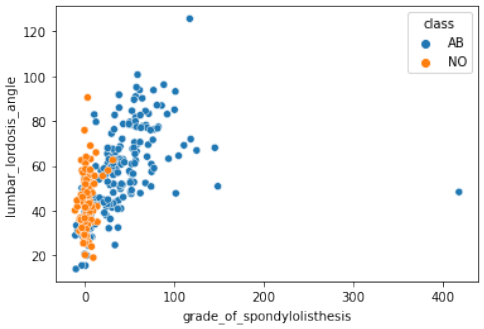


Figure 1: Scatter plot showing two outliers.

We can also see that grade_of_spondylolisthesis may be a useful feature. This is due to its concentrated peak around 2.187 for normal patients, in contrast to the more uniformly distributed density for abnormal patients.

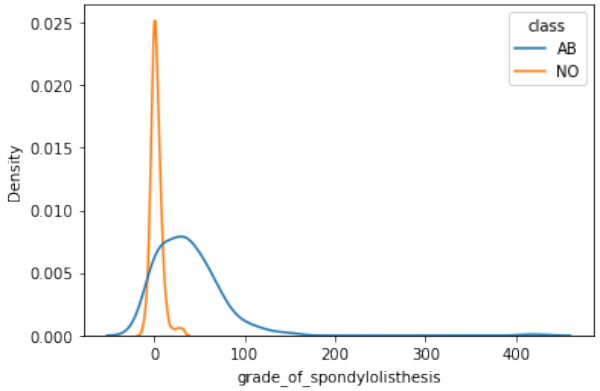


Figure 2: Distribution of grade_of_spondylolisthesis.

We observe that pelvic_incidence has high correlations with most of the other predictors, making it a candidate for removal.

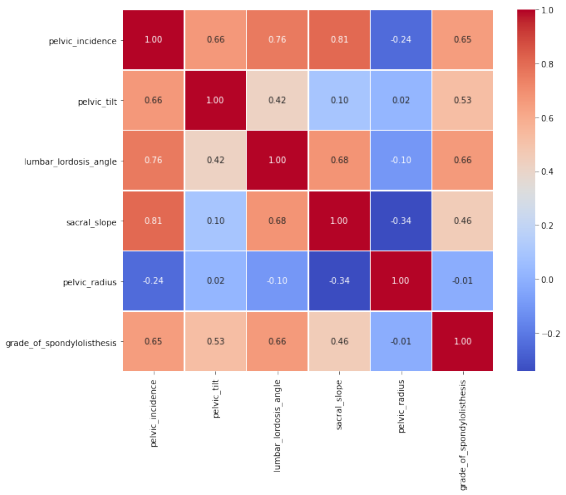


Figure 3: Heatmap showing correlations between variables.

There is a class imbalance in the distribution of labels, with 208 abnormal patients and 100 normal patients. This is addressed later using SMOTE (synthetic minority over-sampling technique) to oversample the minority 'NO' class, until the classes are of equal size. SMOTE uses a kNN algorithm to generate synthetic samples.

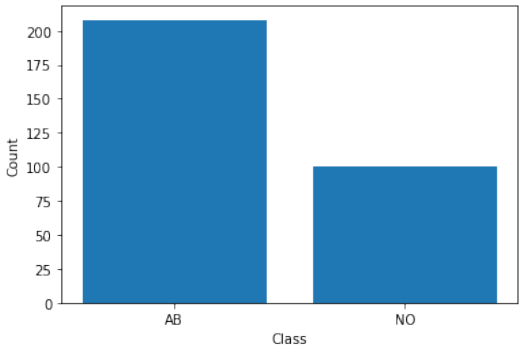


Figure 4: Bar chart showing label distribution.

We convert the 'NO' and 'AB' labels to binary values.

Please note that further pre-processing steps take place, to be brought up whenever relevant in the following sections.

kNN

The kNN algorithm classifies data point $\mathbf{x}$ by looking at the k data points closest to it, then assigning the most frequently occurring label. Distance between points is typically measured using Euclidean distance:

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{(x_1 - y_1)^2 + ... + (x_d - y_d)^2} \quad \text{for } \mathbf{x}, \mathbf{y} \text{ in } \mathbb{R}^d.$$

kNN is easy to understand and implement. However, calculating distances can become computationally expensive for larger datasets, and the hyperparameter k must be tuned.

We start building the model by separating the predictors as X, and the target variable as y. We run train_test_split to reserve 30% of the data for evaluation. We fit StandardScaler() on the training set only, before transforming both the train and test set. Doing so avoids data leakage. For the same reason, we apply SMOTE to the training set only. We use 5-fold cross-validation to calculate average model performance.

The initial model used all predictors, with $k = 5$ nearest neighbours. As alluded to earlier, removing pelvic_incidence improved performance. Testing different values of k, $k = 7$ had the highest average cross-validation accuracy score.

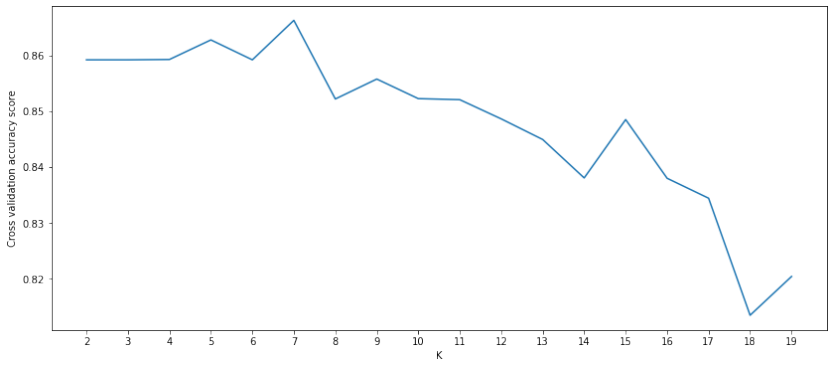


Figure 5: Line graph showing values of k and their accuracy scores.

The final model performed as follows:

- Accuracy: 0.7741935483870968
- Precision: 0.9245283018867925
- Recall: 0.7424242424242424
- F1-score: 0.823529411764706

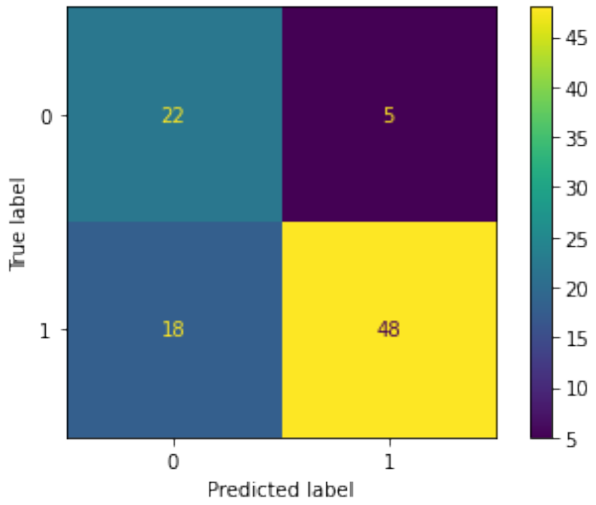


Figure 6: Confusion matrix for the final model.

PCA

PCA starts by standardising the dataset. We calculate the eigensystem for the covariance matrix of this standardised dataset:

$$\Sigma \mathbf{x}_i = \lambda_i \mathbf{x}_i$$

The eigenvectors $\mathbf{x}_i$ represent the principal components, and its corresponding eigenvalue λ_i indicates the variance it explains.

The original data is projected onto the vector space defined by these principal components. The resulting transformation is a set of orthogonal features that capture the maximum variance in the data.

We can see that the sixth principal component has very low explained variance, so it is dropped. Otherwise, there is no obvious elbow in this plot. For now, we use two principal components so we can visualise the classification results.

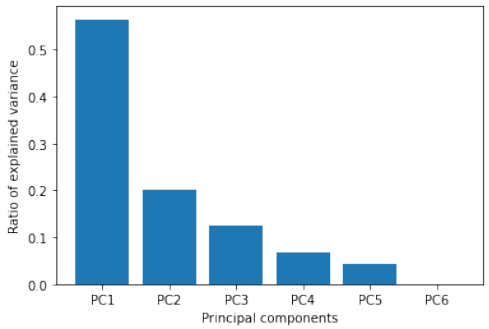


Figure 7: Principal components and their explained variances.

We can see that two principal components is not enough for distinct separation of classes.

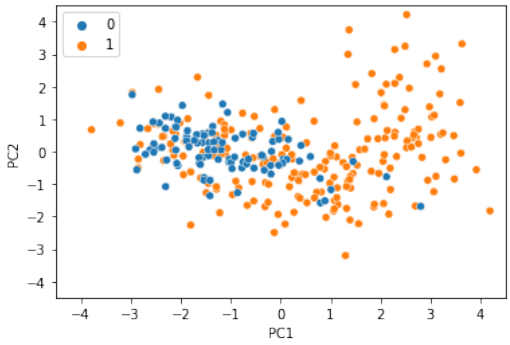


Figure 8: Distribution of classes using two principal components.

K-Means Clustering

K-means clustering selects k initial 'centroids' for the clusters. Each data point is assigned to the nearest centroid using some distance metric (typically Euclidean). After all points are assigned, the centroids are recalculated:

$$\boldsymbol{\mu}_j = \frac{1}{|C_j|} \sum_{\mathbf{x} \in C_j} \mathbf{x}$$

where $\mathbf{x}$ are the data points, and C_j is the jth cluster.

This repeats until some convergence criterion is met, or after $n = 10$ iterations in our case.

K-means clustering is efficient and easy to understand. However, it performs best when the classes are distinct and sphere-shaped. By figure 7 above, we can see that the two classes overlap each other in places, leading to poor classification, particularly of the abnormal class.

We standardise the principal components again, then apply SMOTE. We build models for different values of k. Each model is evaluated by sum of squares (inertia) and silhouette score.

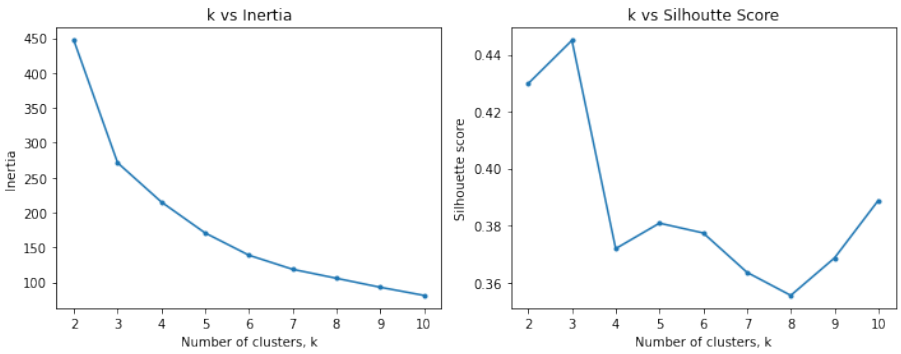


Figure 9: Line graphs showing the sums of squares and silhouette scores for different values of k.

Again, there is no clear elbow in the inertia plot. The silhouette score plot suggests $k = 3$ to be the best choice, followed by $k = 2$. In the original dataset, there are normal patients, and two types of abnormal patients (disc hernia or spondilolysthesis), totalling in three classes, making it plausible that $k = 3$ performs well.

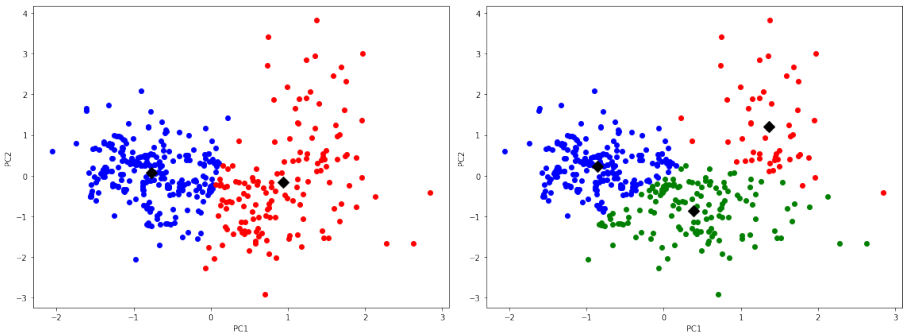


Figure 10: The clusterings with $k = 2$ and $k = 3$.

The optimal model was achieved using three principal components. This also made $k = 2$ the clear choice for number of clusters.

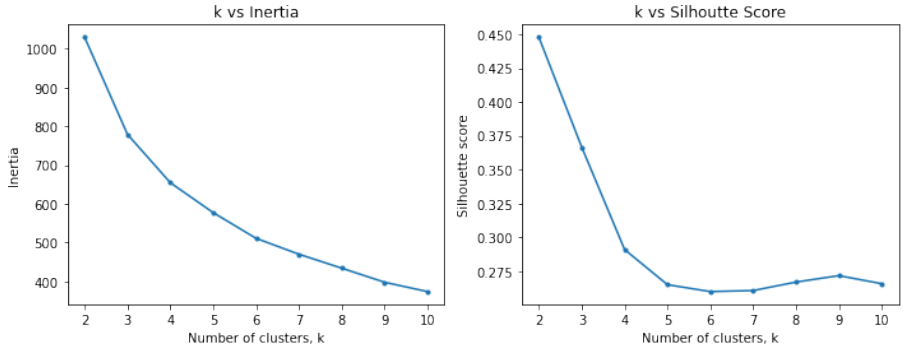


Figure 11: Inertia and silhouette plots, using three principal components.

In real scenarios, we do not have access to the true labels. Here, we do, so we can use them to better evaluate our model.

The following performance was achieved:

- Accuracy: 0.7427884615384616
- Precision: 0.8531468531468531
- Recall: 0.5865384615384616
- F1-score: 0.6951566951566952

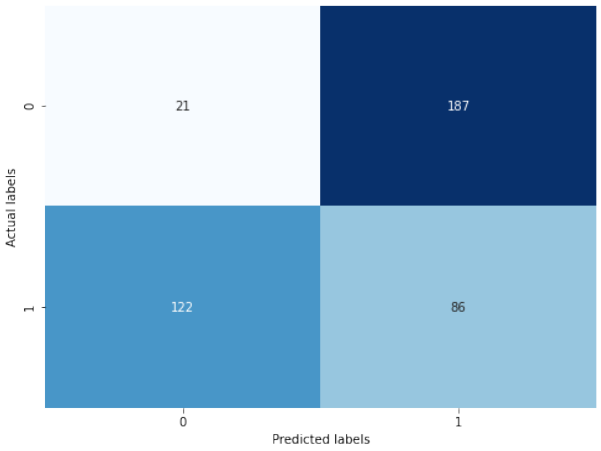


Figure 12: Confusion matrix for the final model.

In [1]:
```
# import packages
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
from imblearn.over_sampling import SMOTE
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import KFold, train_test_split, cross_val_score
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import confusion_matrix, accuracy_score, ConfusionMatrixDisplay
from sklearn.cluster import KMeans
```

In [2]:
```
# read the .txt file in
df = pd.read_csv("vertebral_column_data.txt", delim_whitespace = True, header = None
```

In [3]:
```
df.head()
```

Out[3]:

	0	1	2	3	4	5	6
0	63.03	22.55	39.61	40.48	98.67	-0.25	AB
1	39.06	10.06	25.02	29.00	114.41	4.56	AB
2	68.83	22.22	50.09	46.61	105.99	-3.53	AB
3	69.30	24.65	44.31	44.64	101.87	11.21	AB
4	49.71	9.65	28.32	40.06	108.17	7.92	AB

In [4]:
```
# add the column names
df.columns = ['pelvic_incidence', 'pelvic_tilt', 'lumbar_lordosis_angle', 'sacral_sl
'pelvic_radius', 'grade_of_spondylolisthesis', 'class']
```

In [5]:
```
# check for null values
df.isna().sum()
```

Out[5]:
```
pelvic_incidence             0
pelvic_tilt                  0
lumbar_lordosis_angle        0
sacral_slope                 0
pelvic_radius                0
grade_of_spondylolisthesis   0
class                        0
dtype: int64
```

In [6]:
```
# check there are no unusual values in the class column
df['class'].unique()
```

Out[6]:
```
array(['AB', 'NO'], dtype=object)
```

In [7]:
```
df.describe()
```

Out[7]:

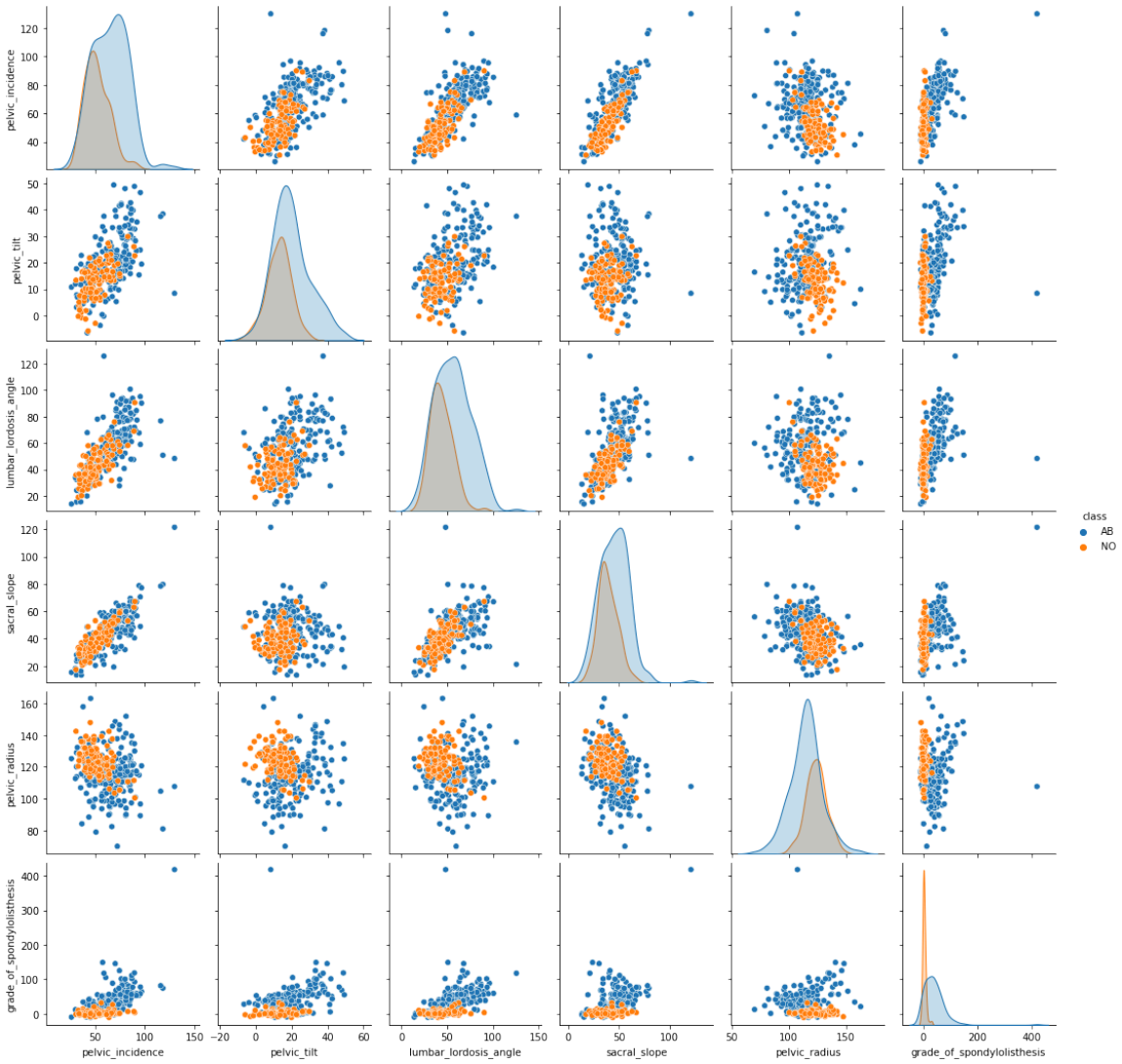
	pelvic_incidence	pelvic_tilt	lumbar_lordosis_angle	sacral_slope	pelvic_radius	grade_of_sponc
count	310.000000	310.000000	310.000000	310.000000	310.000000	
mean	60.496484	17.542903	51.930710	42.953871	117.920548	
std	17.236109	10.008140	18.553766	13.422748	13.317629	
min	26.150000	-6.550000	14.000000	13.370000	70.080000	
25%	46.432500	10.667500	37.000000	33.347500	110.710000	
50%	58.690000	16.360000	49.565000	42.405000	118.265000	
75%	72.880000	22.120000	63.000000	52.692500	125.467500	
max	129.830000	49.430000	125.740000	121.430000	163.070000	

In [8]:

```
# observe general patterns
sns.pairplot(df, hue = 'class')
```

Out[8]:

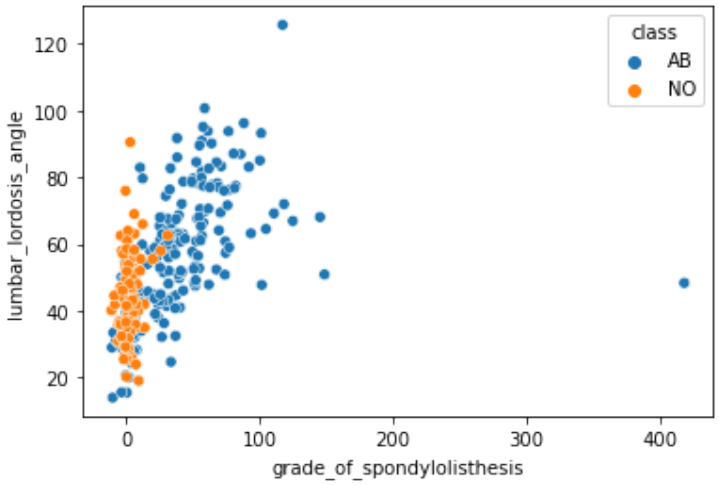
```
<seaborn.axisgrid.PairGrid at 0x23faa262fa0>
```



In [9]:

```
## a close up on plots with outliers
sns.scatterplot(data = df, x = 'grade_of_spondylolisthesis', y = 'lumbar_lordosis_an
```

Out[9]: <AxesSubplot:xlabel='grade_of_spondylolisthesis', ylabel='lumbar_lordosis_angle'>



In [10]:
```
# there is a clear outlier which has extremely high grade_of_spondylolisthesis
# another one with extremely high sacral_slope
# another one with high lumbar_lordosis_angle
# check their row indices

grade_of_spondylolisthesis_max = df['grade_of_spondylolisthesis'].max()
index = df[df['grade_of_spondylolisthesis'] == grade_of_spondylolisthesis_max].index
index
```

Out[10]: 115

In [11]:
```
sacral_slope_max = df['sacral_slope'].max()
index = df[df['sacral_slope'] == sacral_slope_max].index[0]
index
```

Out[11]: 115

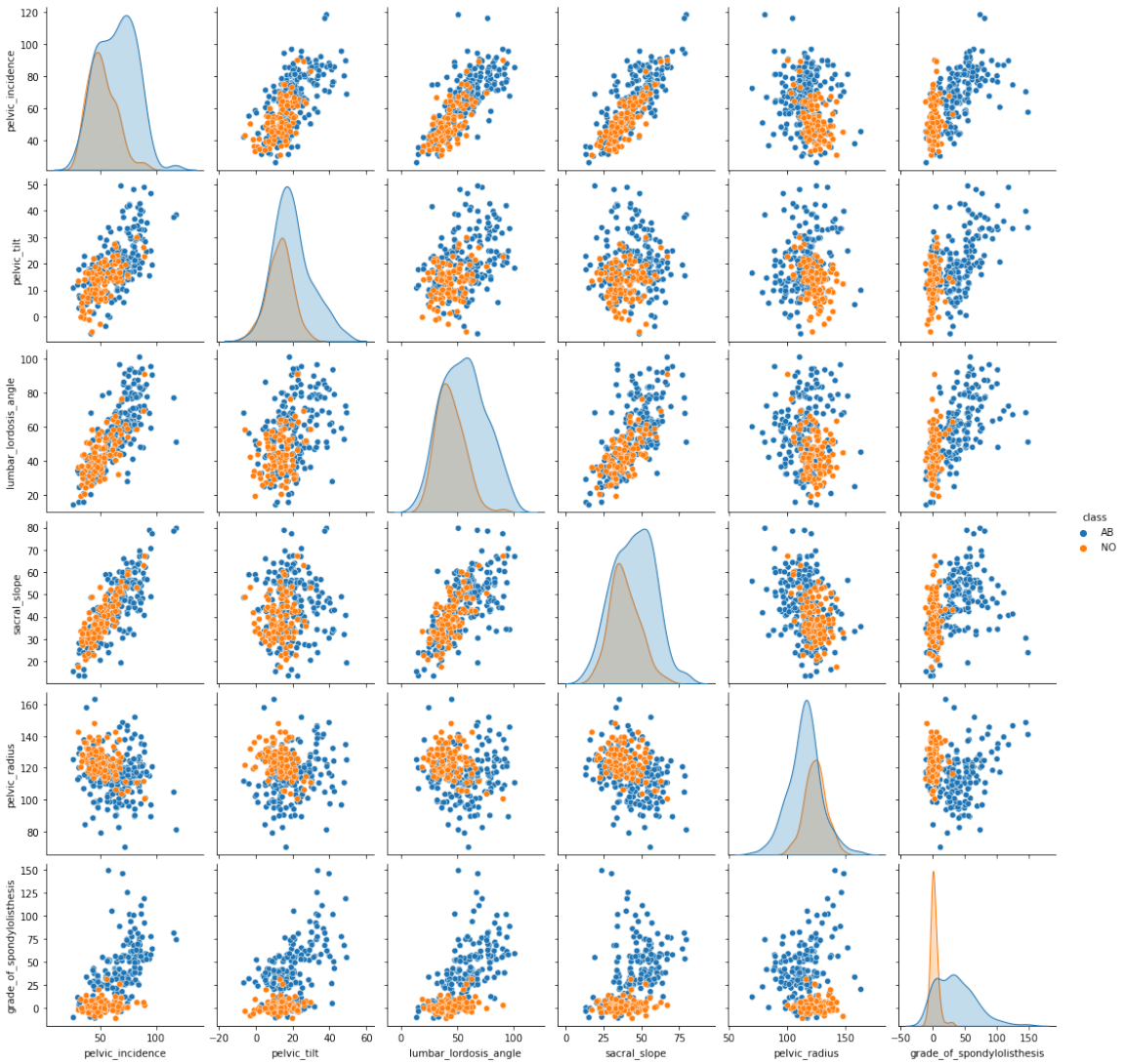
In [12]:
```
lumbar_lordosis_angle_max = df['lumbar_lordosis_angle'].max()
index = df[df['lumbar_lordosis_angle'] == lumbar_lordosis_angle_max].index[0]
index
```

Out[12]: 197

In [13]:
```
# remove these outliers
indices_to_remove = [115,197]
df.drop(indices_to_remove, inplace = True)
```

In [14]:
```
# observe again with outliers removed
sns.pairplot(df, hue = 'class')
```

Out[14]: <seaborn.axisgrid.PairGrid at 0x23fabb76fa0>



In [15]:
```
# high concentration around 0 for grade_of_spondylolisthesis
# check if there are zero values
(df['grade_of_spondylolisthesis'] == 0).sum()
```

Out[15]:
```
0
```

In [16]:
```
df[df['class'] == 'NO']['grade_of_spondylolisthesis'].mean()
```

Out[16]:
```
2.187000000000001
```

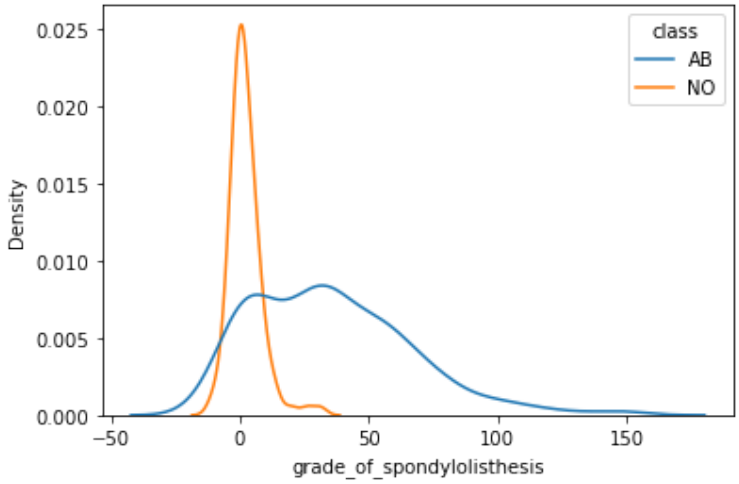
There are negative values in the pelvic_tilt column, which upon further research, makes sense.

There should not be negative values in the grade_of_spondylolisthesis column, however. Although these could be removed, since the focus of this coursework is classification algorithms, we will keep this data.

From the pairplots, we can see that the grade_of_spondylolisthesis predictor will be useful in classification. This is because of its large peak around 2.187. Those patients with values around this will likely be classified as 'normal'.

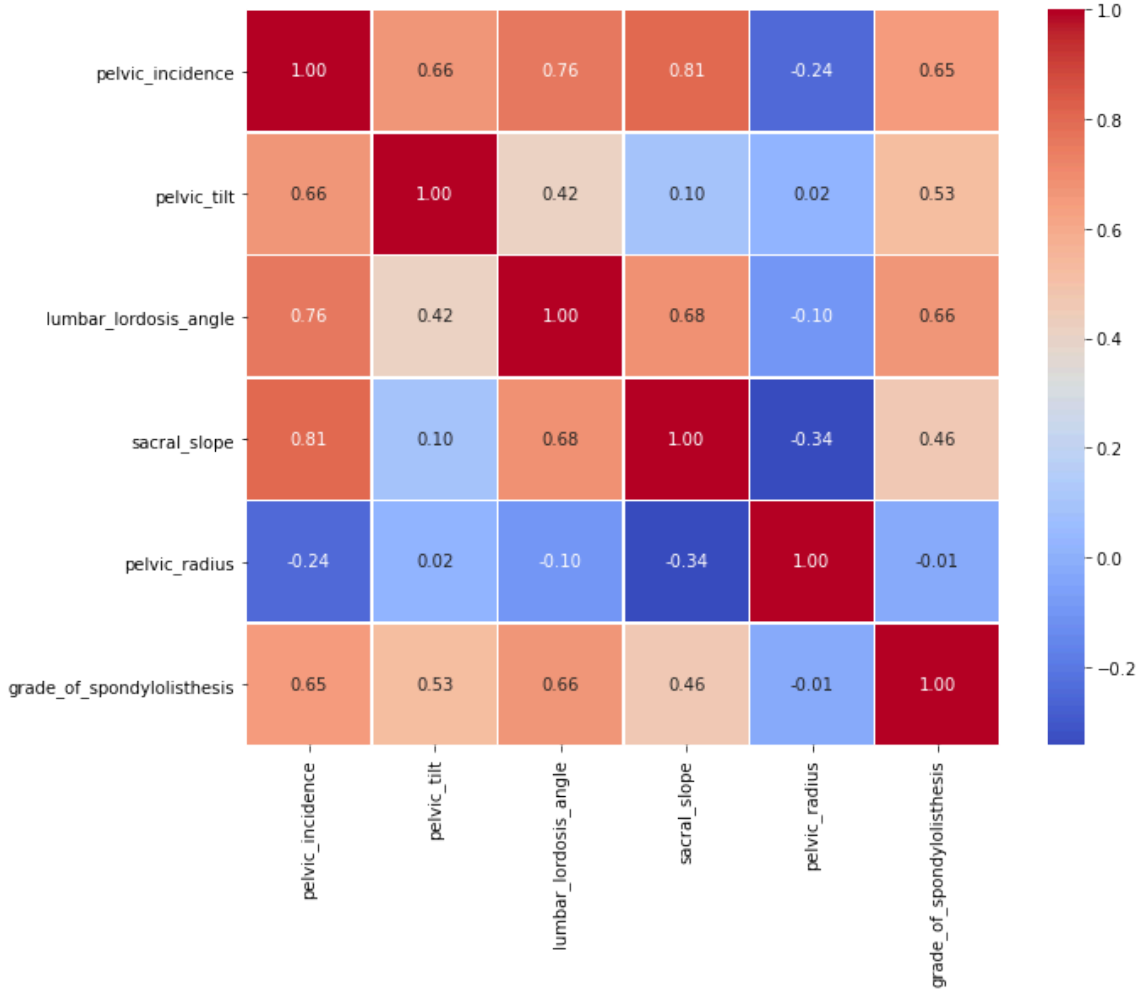
In [17]:
```
## closer look at grade_of_spondylolisthesis
sns.kdeplot(data = df, x = 'grade_of_spondylolisthesis', hue = 'class')
```

Out[17]: <AxesSubplot:xlabel='grade_of_spondylolisthesis', ylabel='Density'>



In [18]:

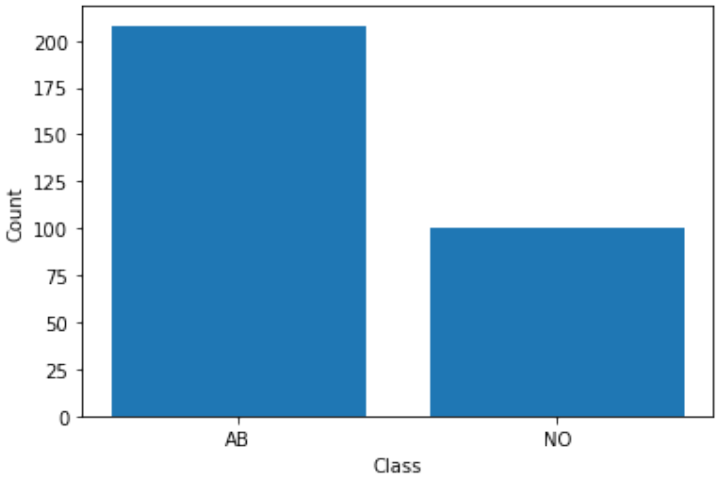
```
# observe correlations
plt.figure(figsize=(10, 8))
sns.heatmap(df.corr(), annot=True, cmap='coolwarm', fmt=".2f", linewidths=0.5)
plt.show()
```



pelvic_incidence has quite high correlations with most of the other variables, particularly sacral_slope and lumbar_lordosis_angle. This may be a candidate for removal.

In [19]:

```
# observe the total number of 'NO' and 'AB' instances
# there is some class imbalance
class_count = df['class'].value_counts()

# plot a bar chart
plt.bar(class_count.index, class_count.values)
plt.xlabel('Class')
plt.ylabel('Count')
plt.xticks(['NO','AB'])
plt.show()
```



In [20]:

```
# convert the 'NO' and 'AB' labels to 0s and 1s
df['class'] = df['class'].map({'AB': 1, 'NO': 0})
```

In [21]:

```
df.head()
```

Out[21]:

	pelvic_incidence	pelvic_tilt	lumbar_lordosis_angle	sacral_slope	pelvic_radius	grade_of_spondylolis
0	63.03	22.55	39.61	40.48	98.67	
1	39.06	10.06	25.02	29.00	114.41	
2	68.83	22.22	50.09	46.61	105.99	
3	69.30	24.65	44.31	44.64	101.87	
4	49.71	9.65	28.32	40.06	108.17	

Classification

Supervised

KNN

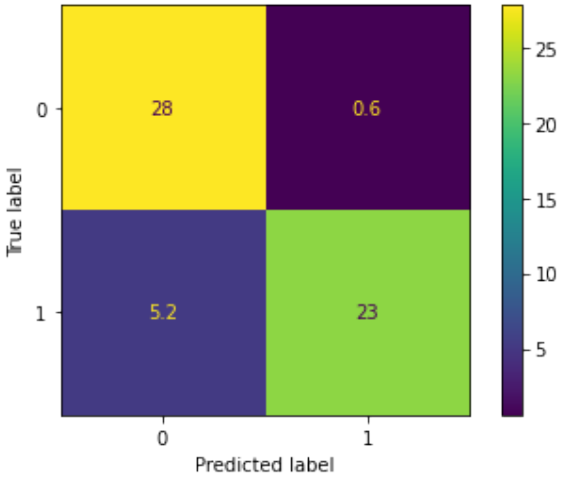
In [22]:

```
## initial KNN model, using 5 nearest neighbors

# predictors as X
X = df[['pelvic_incidence', 'pelvic_tilt', 'lumbar_lordosis_angle', 'sacral_slope',
'pelvic_radius', 'grade_of_spondylolisthesis']].values
```

```
# target variable as y
y = df[['class']].values

# reshape y
y = np.ravel(y)

# split into train and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.3, random_st

# initialise the standard scaler
scaler = StandardScaler()

# apply scaling
# fit on training data only to avoid data leakage
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)

# initialise the KNN classifier
knn = KNeighborsClassifier(n_neighbors=5)

# initialise K-fold CV object
kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)

# initialise lists to store evaluation metrics
val_accuracies = []
conf_matrices = []

# apply SMOTE to the training data only
# only applying to the training data avoids data leakage
# addresses class imbalance
smote = SMOTE(random_state = 1)
X_train, y_train = smote.fit_resample(X_train, y_train)

# fit the KNN model
knn.fit(X_train, y_train)

# iterate over the folds
for train_index, val_index in kfold.split(X_train, y_train):
    X_train_fold, X_val_fold = X_train[train_index], X_train[val_index]
    y_train_fold, y_val_fold = y_train[train_index], y_train[val_index]

    # predictions on the validation set
    y_pred_val = knn.predict(X_val_fold)

    # accuracy on the validation set
    val_accuracy = accuracy_score(y_val_fold, y_pred_val)
    val_accuracies.append(val_accuracy)

    # confusion matrix
    conf_matrix = confusion_matrix(y_val_fold, y_pred_val)
    conf_matrices.append(conf_matrix)


## following metrics are the averages based on the cross-validation process

# print average evaluation metrics
print("Average validation accuracy:", np.mean(val_accuracies))

# display the average confusion matrix
avg_conf_matrix = np.mean(conf_matrices, axis=0)
disp = ConfusionMatrixDisplay(confusion_matrix=avg_conf_matrix)
disp.plot()

# calculate additional metrics from the average confusion matrix
```

```
tn, fp, fn, tp = avg_conf_matrix.ravel()
# precision
precision = tp / (tp + fp)
# recall
recall = tp / (tp + fn)
# F1-score
f1_score = 2 * (precision * recall) / (precision + recall)

# display the metrics
print("Average precision:", precision)
print("Average recall:", recall)
print("Average F1-score:", f1_score)
print("Average confusion matrix:")
```

```
Average validation accuracy: 0.8979323308270676
Average precision: 0.9747899159663865
Average recall: 0.8169014084507042
Average F1-score: 0.888888888888889
Average confusion matrix:
```



In [23]:

```
## exactly the same code as above, but with pelvic_incidence removed
# performance improves slightly

# predictors as X
X = df[['pelvic_tilt', 'lumbar_lordosis_angle', 'sacral_slope',
'pelvic_radius', 'grade_of_spondylolisthesis']].values
# target variable as y
y = df[['class']].values

# reshape y
y = np.ravel(y)

# split into train and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.3, random_st

# initialise the standard scaler
scaler = StandardScaler()

# apply scaling
# fit on training data only to avoid data leakage
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)

# initialise the KNN classifier
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# initialise K-fold CV object
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```

```
# initialise lists to store evaluation metrics
val_accuracies = []
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# apply SMOTE to the training data only
# only applying to the training data avoids data leakage
# addresses class imbalance
smote = SMOTE(random_state = 1)
X_train, y_train = smote.fit_resample(X_train, y_train)

# fit the KNN model
knn.fit(X_train, y_train)

# iterate over the folds
for train_index, val_index in kfold.split(X_train, y_train):
    X_train_fold, X_val_fold = X_train[train_index], X_train[val_index]
    y_train_fold, y_val_fold = y_train[train_index], y_train[val_index]

    # predictions on the validation set
    y_pred_val = knn.predict(X_val_fold)

    # accuracy on the validation set
    val_accuracy = accuracy_score(y_val_fold, y_pred_val)
    val_accuracies.append(val_accuracy)

    # confusion matrix
    conf_matrix = confusion_matrix(y_val_fold, y_pred_val)
    conf_matrices.append(conf_matrix)


## following metrics are the averages based on the cross-validation process

# print average evaluation metrics
print("Average validation accuracy:", np.mean(val_accuracies))

# display the average confusion matrix
avg_conf_matrix = np.mean(conf_matrices, axis=0)
disp = ConfusionMatrixDisplay(confusion_matrix=avg_conf_matrix)
disp.plot()

# calculate additional metrics from the average confusion matrix
tn, fp, fn, tp = avg_conf_matrix.ravel()
# precision
precision = tp / (tp + fp)
# recall
recall = tp / (tp + fn)
# F1-score
f1_score = 2 * (precision * recall) / (precision + recall)

# display the metrics
print("Average precision:", precision)
print("Average recall:", recall)
print("Average F1-score:", f1_score)
print("Average confusion matrix:")
```
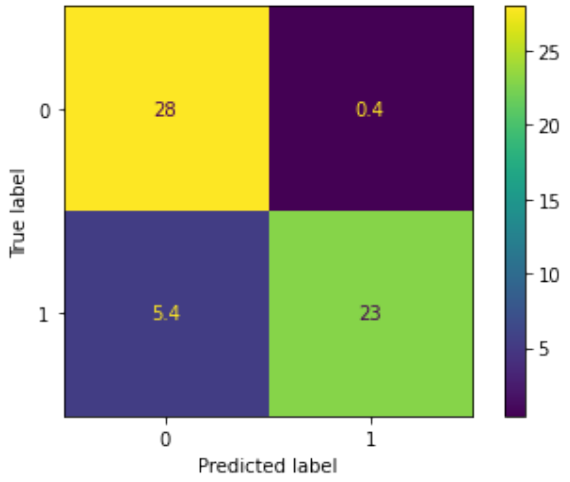

```
Average validation accuracy: 0.8978696741854637
Average precision: 0.982905982905983
Average recall: 0.8098591549295775
Average F1-score: 0.8880308880308881
Average confusion matrix:
```



In [24]:

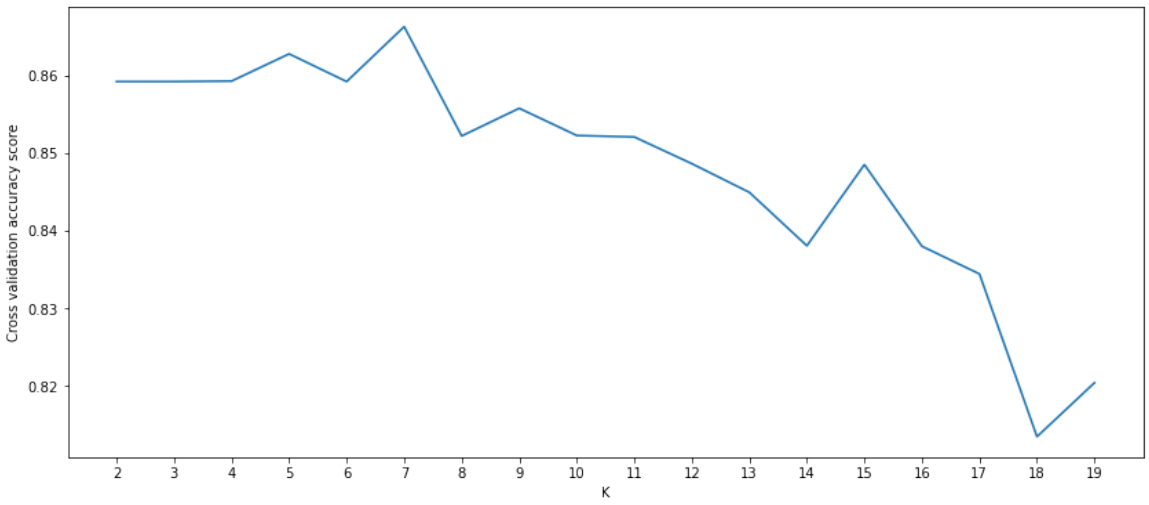
```
## finding the optimal value for k, the number of nearest neighbours
## this is based off of accuracy on the unseen test set


# predictors as X
X = df[['pelvic_tilt', 'lumbar_lordosis_angle', 'sacral_slope',
        'pelvic_radius', 'grade_of_spondylolisthesis']].values
# target variable as y
y = df[['class']].values

# reshape y
y = np.ravel(y)

# split into train and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_stat

# initialise the standard scaler
scaler = StandardScaler()

# apply scaling
# fit on training data only to avoid data leakage
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)

# initialise K-fold CV object
kfold = KFold(n_splits=5, shuffle=True, random_state=1)

# apply SMOTE to the training data only
# only applying to the training data avoids data leakage
# addresses class imbalance
smote = SMOTE(random_state=1)
X_train_resampled, y_train_resampled = smote.fit_resample(X_train, y_train)

from sklearn.model_selection import cross_val_score

# set up an array to keep track of the average cross-validation accuracies of each m
cv_accuracies = []
optimal_k = 0
highest_cv_accuracy = 0

# trying different values of k
for k in range(2, 20):
    # initialise KNN classifier
    knn = KNeighborsClassifier(n_neighbors=k)

    # compute cross-validation accuracy scores
```

```
    cv_scores = cross_val_score(knn, X_train_resampled, y_train_resampled, cv=kfold,

    # compute the average cross-validation accuracy
    avg_cv_accuracy = np.mean(cv_scores)
    cv_accuracies.append(avg_cv_accuracy)

    # update the optimal value of k if necessary
    if avg_cv_accuracy > highest_cv_accuracy:
        optimal_k = k
        highest_cv_accuracy = avg_cv_accuracy

# display the optimal k, along with its average cross-validation accuracy score
print("The optimal value of k is", optimal_k, ", which has average cross-validation
```

```
The optimal value of k is 7 , which has average cross-validation accuracy score 0.866
2907268170427
```

In [25]:

```
## show the performances of each value of k
plt.figure(figsize = (14,6))
plt.plot(range(2,20), cv_accuracies)
plt.xlabel("K")
plt.ylabel("Cross validation accuracy score")
plt.xticks(range(2,20))
plt.show()
```

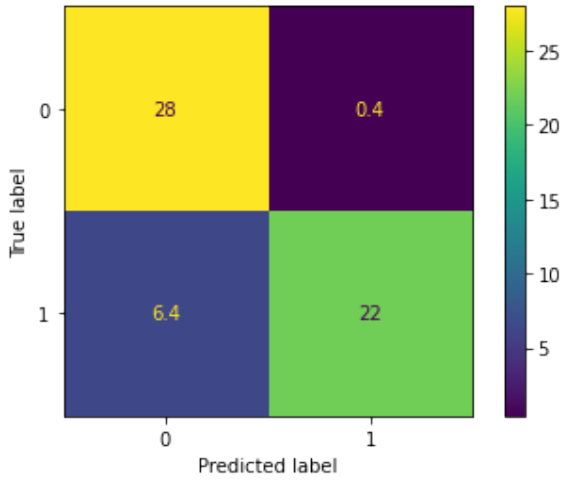


In [26]:

```
## final KNN model

# predictors as X
X = df[['pelvic_tilt', 'lumbar_lordosis_angle', 'sacral_slope',
'pelvic_radius', 'grade_of_spondylolisthesis']].values
# target variable as y
y = df[['class']].values

# reshape y
y = np.ravel(y)

# split into train and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.3, random_st

# initialise the standard scaler
scaler = StandardScaler()

# apply scaling
# fit on training data only to avoid data leakage
X_train = scaler.fit_transform(X_train)
```

```
X_test = scaler.transform(X_test)

# initialise the KNN classifier
final_knn = KNeighborsClassifier(n_neighbors=optimal_k)

# initialise K-fold CV object
kfold = KFold(n_splits = 5, shuffle = True, random_state = 1)

# initialise lists to store evaluation metrics
val_accuracies = []
conf_matrices = []

# apply SMOTE to the training data only
# only applying to the training data avoids data leakage
# addresses class imbalance
smote = SMOTE(random_state = 1)
X_train, y_train = smote.fit_resample(X_train, y_train)

# fit the KNN model
final_knn.fit(X_train, y_train)

# iterate over the folds
for train_index, val_index in kfold.split(X_train, y_train):
    X_train_fold, X_val_fold = X_train[train_index], X_train[val_index]
    y_train_fold, y_val_fold = y_train[train_index], y_train[val_index]

    # predictions on the validation set
    y_pred_val = final_knn.predict(X_val_fold)

    # accuracy on the validation set
    val_accuracy = accuracy_score(y_val_fold, y_pred_val)
    val_accuracies.append(val_accuracy)

    # confusion matrix
    conf_matrix = confusion_matrix(y_val_fold, y_pred_val)
    conf_matrices.append(conf_matrix)


## following metrics are the averages based on the cross-validation process

# print average evaluation metrics
print("Average validation accuracy:", np.mean(val_accuracies))

# display the average confusion matrix
avg_conf_matrix = np.mean(conf_matrices, axis=0)
disp = ConfusionMatrixDisplay(confusion_matrix=avg_conf_matrix)
disp.plot()

# calculate additional metrics from the average confusion matrix
tn, fp, fn, tp = avg_conf_matrix.ravel()
# precision
precision = tp / (tp + fp)
# recall
recall = tp / (tp + fn)
# F1-score
f1_score = 2 * (precision * recall) / (precision + recall)

# display the metrics
print("Average precision:", precision)
print("Average recall:", recall)
print("Average F1-score:", f1_score)
print("Average confusion matrix:")
```

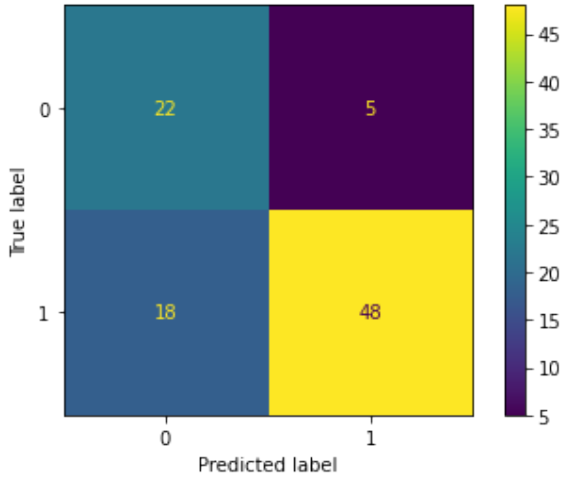
```
Average validation accuracy: 0.880325814536341
Average precision: 0.9821428571428572
Average recall: 0.7746478873239437
Average F1-score: 0.8661417322834647
Average confusion matrix:
```



In [27]:

```python
## evaluate performance of this model on the unseen test set

# use the model to predict the unseen labels
y_pred = final_knn.predict(X_test)

# display the test set confusion matrix
test_conf_matrix = confusion_matrix(y_test, y_pred)
disp = ConfusionMatrixDisplay(confusion_matrix=test_conf_matrix)
disp.plot()


# calculate additional metrics from the test set confusion matrix
tn, fp, fn, tp = test_conf_matrix.ravel()
# precision
precision = tp / (tp + fp)
# recall
recall = tp / (tp + fn)
# F1-score
f1_score = 2 * (precision * recall) / (precision + recall)

# display the metrics
print("Test set accuracy:", accuracy_score(y_test,y_pred))
print("Test set precision:", precision)
print("Test set recall:", recall)
print("Test set F1-score:", f1_score)
print("Test set confusion matrix:")
```

```
Test set accuracy: 0.7526881720430108
Test set precision: 0.9056603773584906
Test set recall: 0.7272727272727273
Test set F1-score: 0.8067226890756303
Test set confusion matrix:
```



Unsupervised

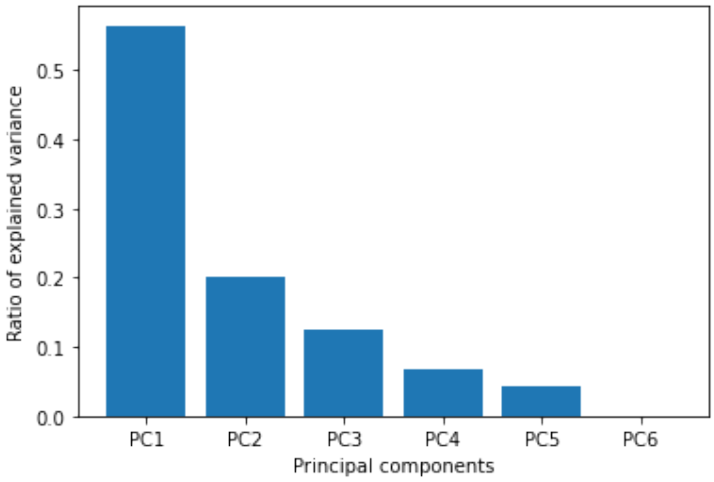
Applying PCA

In [28]:
```
df.head()
```

Out[28]:

	pelvic_incidence	pelvic_tilt	lumbar_lordosis_angle	sacral_slope	pelvic_radius	grade_of_spondylolis
0	63.03	22.55	39.61	40.48	98.67	
1	39.06	10.06	25.02	29.00	114.41	
2	68.83	22.22	50.09	46.61	105.99	
3	69.30	24.65	44.31	44.64	101.87	
4	49.71	9.65	28.32	40.06	108.17	

In [29]:
```
## decide how many components we want

# initialise scaler
scaler = StandardScaler()

# apply the scaler
# drop the class column, we do not want to include it in the PCA
scaled_data = scaler.fit_transform(df.drop(columns = ['class']))

# initialise PCA object
pca = PCA()

# fit to our data
pca_data = pca.fit_transform(scaled_data)

# prepare for elbow plot
per_var = pca.explained_variance_ratio_
labels = ['PC' + str(x) for x in range(1,len(per_var)+1)]

# plot elbow plot
plt.bar(x = range(1,len(per_var)+1), height = per_var, tick_label = labels)
plt.xlabel("Principal components")
plt.ylabel("Ratio of explained variance")
plt.show()
```



In [30]:

```
## there is not a very clear elbow in this plot
## we have reduced from 6 features to 5 for certain (PC6 explains virtually no varia
## but even PC5 explains a non-negligible amount of the variance

## we start by building models using 2, for the sake of visualisations
## later we look at using more, for the sake of  better performance

n_components = 3
reduced_data = pca_data[:, :n_components]
reduced_df = pd.DataFrame(reduced_data,
                          columns=[f"PC{i}" for i in range(1, n_components + 1)])

# Reassigning index from the original dataframe to the reduced dataframe
reduced_df.index = df.index

# Reattach the 'class' column
reduced_df['class'] = df['class']
```

In [31]:

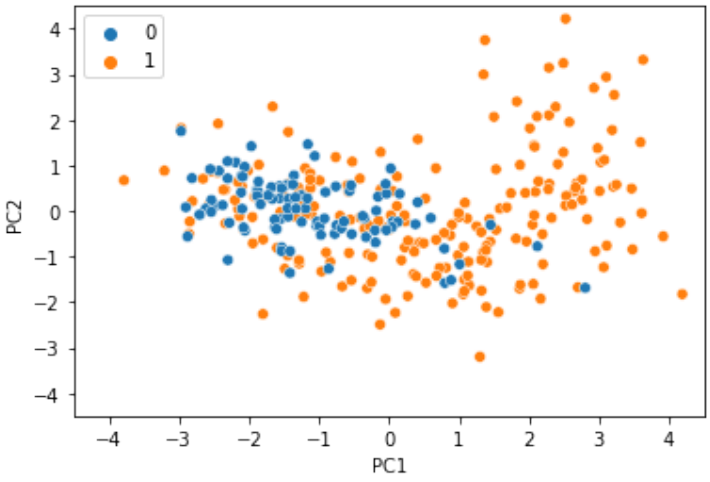
```
reduced_df.head()
```

Out[31]:

	PC1	PC2	PC3	class
0	-0.303390	-0.952249	1.535106	1
1	-2.336257	-0.274624	0.494357	1
2	0.226106	-0.799470	0.859675	1
3	0.361038	-0.716492	1.319662	1
4	-1.446155	-0.979529	0.408064	1

In [32]:

```
## visualise with the first two principal components only
sns.scatterplot(data = reduced_df, x = 'PC1', y = 'PC2', hue = 'class')
plt.xlabel("PC1")
plt.ylabel("PC2")
plt.xticks(range(-4,5));
plt.xlim([-4.5, 4.5]);
plt.ylim([-4.5, 4.5]);
plt.legend()
plt.show()
```



In [33]:
```
## the above plot reinforces that two principal components does not separate very we
```

K Means Clustering

In [34]:
```
# extract all the samples from the principal component dataframe we just created
samples = reduced_df[['PC1', 'PC2']].values

# save their labels so we can evaluate our unsupervised model later on
# in real scenarios, we often do not have these labels
actual_labels = reduced_df[['class']].values

# although we standardise before PCA, the PCs created are not standardised
# initialise scaler
scaler = StandardScaler()
# fit the scaler
samples = scaler.fit_transform(samples)

# apply SMOTE to balance the dataset
smote = SMOTE(random_state=42)
samples, actual_labels = smote.fit_resample(samples, actual_labels)

# iterate over different k
max_k = 10
# save the sums of squares for each model
sum_of_squares = []
# save the silhouette scores for each model
silhouette_scores = []
for k in range(2,max_k+1):
    # initialise KMeans model
    model = KMeans(n_clusters = k, n_init = 10)
    # fit the model
    model.fit(samples)
    # record the sum of squares
    sum_of_squares.append(model.inertia_)
    # calculate the silhouette scores
    silhouette_avg = silhouette_score(samples, model.labels_)
    silhouette_scores.append(silhouette_avg)
```

```
C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarni
ng: KMeans is known to have a memory leak on Windows with MKL, when there are less ch
unks than available threads. You can avoid it by setting the environment variable OMP
_NUM_THREADS=2.
  warnings.warn(
C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarni
```

```
ng: KMeans is known to have a memory leak on Windows with MKL, when there are less ch
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C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarni
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  warnings.warn(
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C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarni
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C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarni
ng: KMeans is known to have a memory leak on Windows with MKL, when there are less ch
unks than available threads. You can avoid it by setting the environment variable OMP
_NUM_THREADS=2.
  warnings.warn(
```
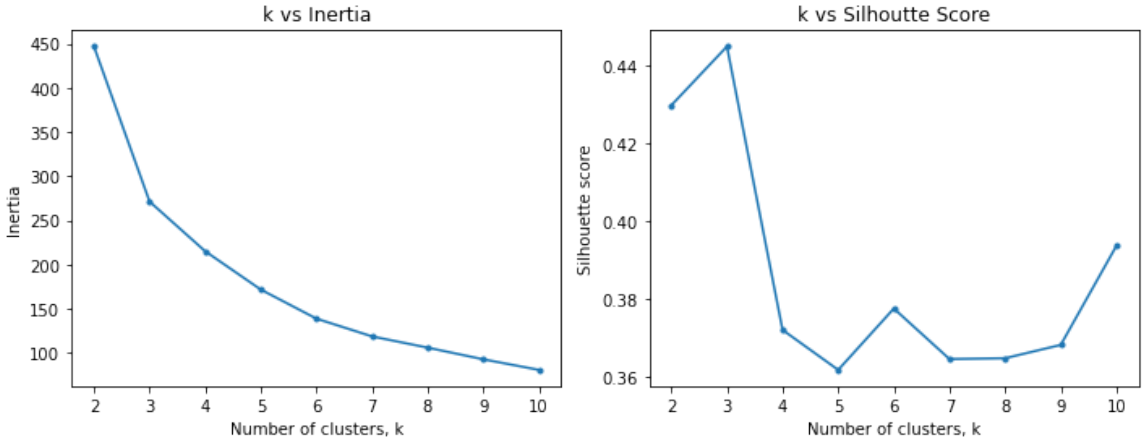

In [35]:

```python
# create subplots
fig, axes = plt.subplots(1, 2, figsize=(10,4))

# plot elbow plot of inertia for each k
axes[0].plot(list(range(2, max_k + 1)), sum_of_squares, marker=".")
axes[0].set_title("k vs Inertia")
axes[0].set_xlabel("Number of clusters, k")
axes[0].set_ylabel("Inertia")

# plot silhouette scores for each k
axes[1].plot(list(range(2, max_k + 1)), silhouette_scores, marker=".")
axes[1].set_title("k vs Silhoutte Score")
axes[1].set_xlabel("Number of clusters, k")
axes[1].set_ylabel("Silhouette score")

plt.tight_layout()
plt.show()
```



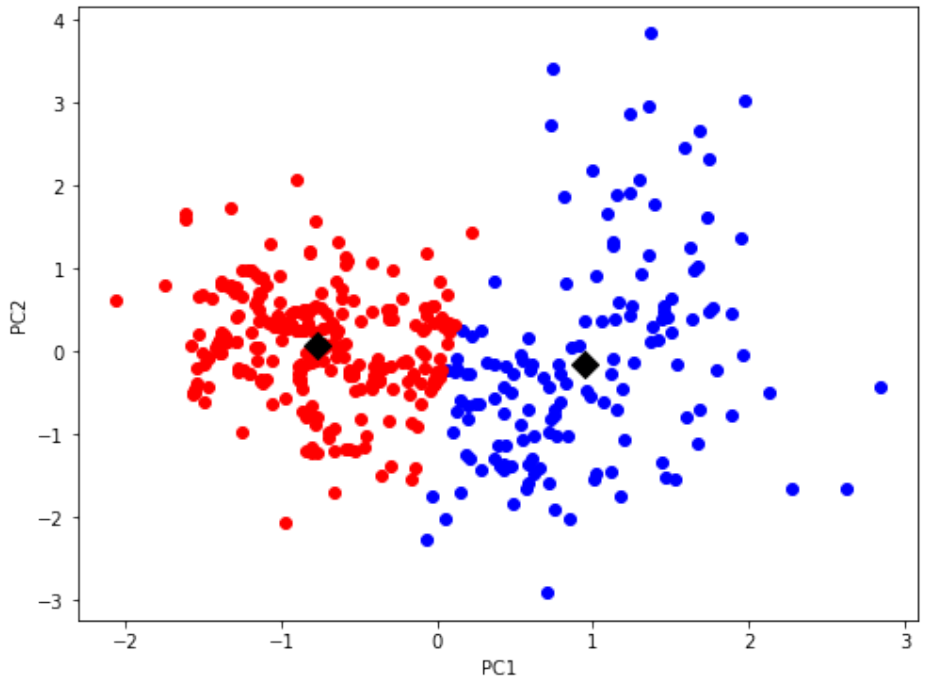
In [36]:
```
## build model with k = 2

# initialise model
two_model = KMeans(n_clusters = 2, n_init = 10)
# fit the model
two_model.fit(samples)
# make predictions
two_predicted_labels = two_model.predict(samples)
```

```
C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarni
ng: KMeans is known to have a memory leak on Windows with MKL, when there are less ch
unks than available threads. You can avoid it by setting the environment variable OMP
_NUM_THREADS=2.
  warnings.warn(
```

In [37]:
```
## build model with k = 3

# initialise model
three_model = KMeans(n_clusters = 3, n_init = 10)
# fit the model
three_model.fit(samples)
# make predictions
three_predicted_labels = three_model.predict(samples)
```

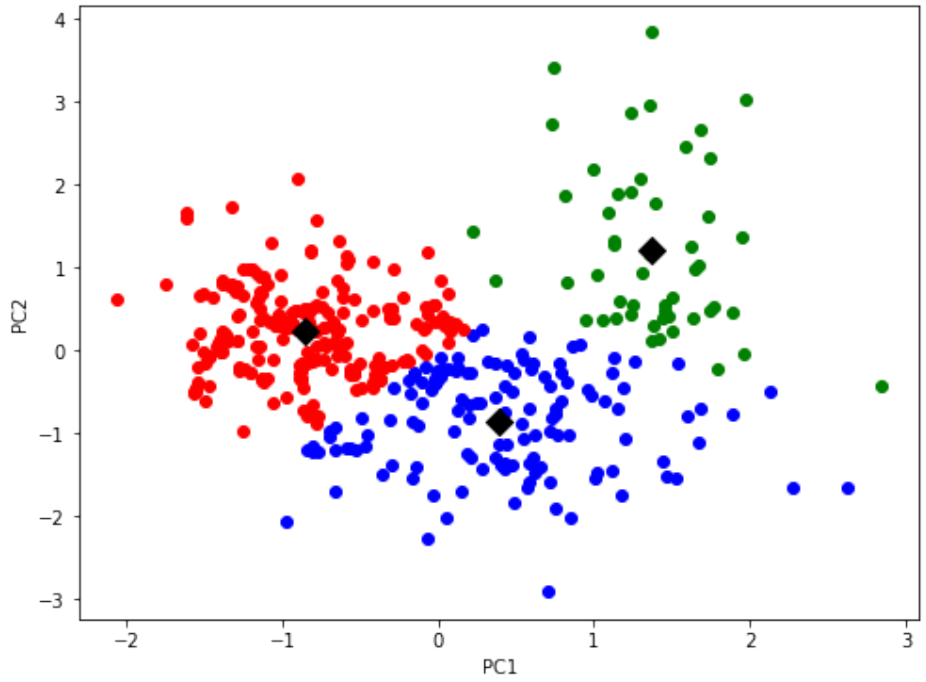
```
C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarni
ng: KMeans is known to have a memory leak on Windows with MKL, when there are less ch
unks than available threads. You can avoid it by setting the environment variable OMP
_NUM_THREADS=2.
  warnings.warn(
```

In [38]:
```
# define colors for each cluster
colors = ['blue', 'red']

# create a scatter plot of the data points
plt.figure(figsize=(8, 6))
for cluster_label in np.unique(two_model.labels_):
    cluster_samples = samples[two_model.labels_ == cluster_label]
    plt.scatter(cluster_samples[:, 0], cluster_samples[:, 1], color=colors[cluster_l

# plot centroids
centroids = two_model.cluster_centers_
plt.scatter(centroids[:, 0], centroids[:, 1], marker='D', s=100, color='black', labe

plt.xlabel('PC1')
plt.ylabel('PC2')
plt.show()
```



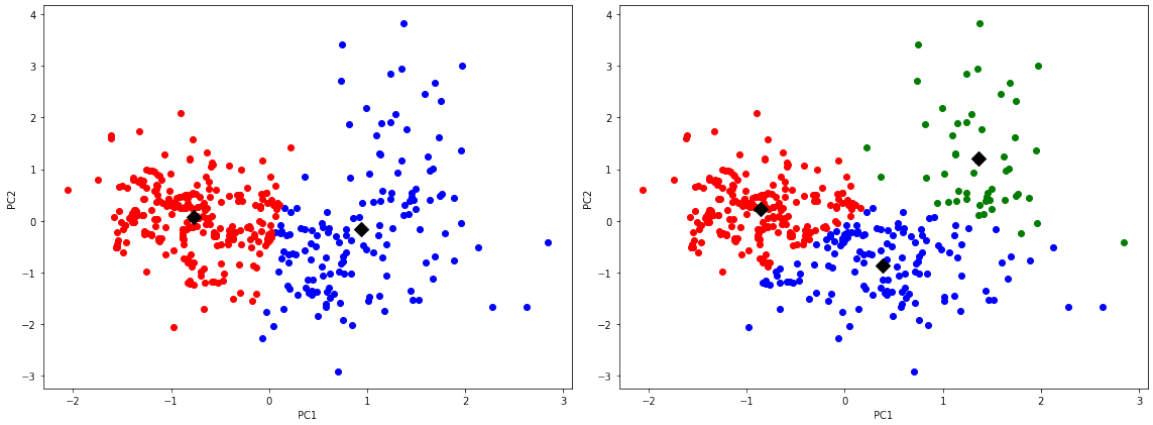
In [39]:

```
# define colors for each cluster
colors = ['blue', 'red', 'green']

# create a scatter plot of the data points
plt.figure(figsize=(8, 6))
for cluster_label in np.unique(three_model.labels_):
    cluster_samples = samples[three_model.labels_ == cluster_label]
    plt.scatter(cluster_samples[:, 0], cluster_samples[:, 1], color=colors[cluster_l

# plot centroids
centroids = three_model.cluster_centers_
plt.scatter(centroids[:, 0], centroids[:, 1], marker='D', s=100, color='black', labe

plt.xlabel('PC1')
plt.ylabel('PC2')
plt.show()
```



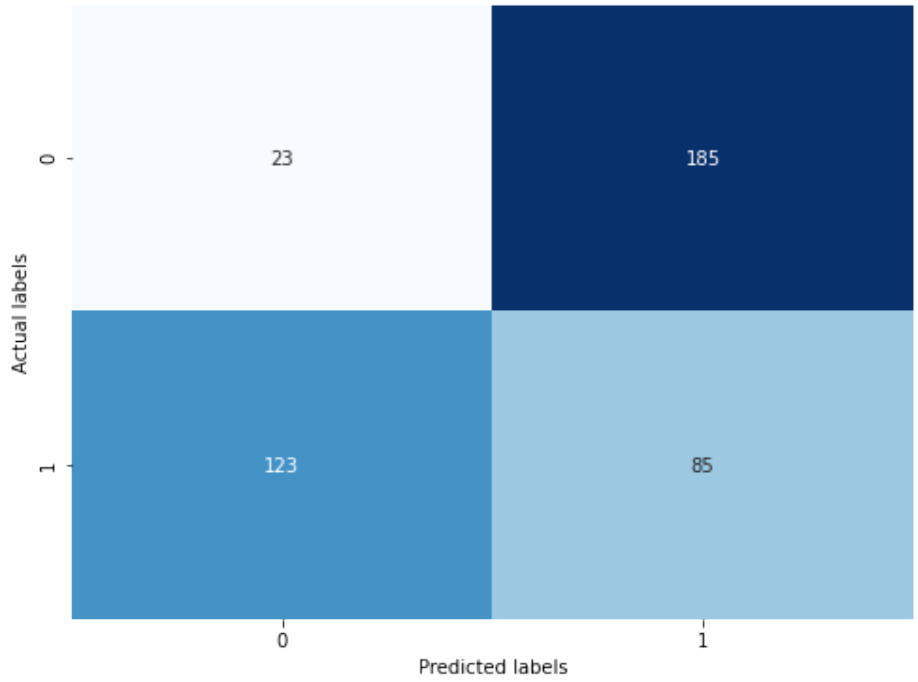
In [40]:

```
# define colors for each cluster
colors = ['blue', 'red']

# create figure and axes
fig, axes = plt.subplots(1, 2, figsize=(16, 6))

# scatter plot for two clusters
for cluster_label in np.unique(two_model.labels_):
    cluster_samples = samples[two_model.labels_ == cluster_label]
    axes[0].scatter(cluster_samples[:, 0], cluster_samples[:, 1], color=colors[clust

# plot centroids for two clusters
centroids = two_model.cluster_centers_
axes[0].scatter(centroids[:, 0], centroids[:, 1], marker='D', s=100, color='black')
axes[0].set_xlabel('PC1')
axes[0].set_ylabel('PC2')

# scatter plot for three clusters
colors = ['blue', 'red', 'green']
for cluster_label in np.unique(three_model.labels_):
    cluster_samples = samples[three_model.labels_ == cluster_label]
    axes[1].scatter(cluster_samples[:, 0], cluster_samples[:, 1], color=colors[clust

# plot centroids for three clusters
centroids = three_model.cluster_centers_
axes[1].scatter(centroids[:, 0], centroids[:, 1], marker='D', s=100, color='black')
axes[1].set_xlabel('PC1')
axes[1].set_ylabel('PC2')

plt.tight_layout()
plt.show()
```



In [41]:

```
## using the actual labels, for k = 2, we can use a crosstable to evaluate model per

# reshape predicted labels from (... , ) to (... , 1)
two_predicted_labels = two_predicted_labels.reshape(-1,1)

# create dataframe containing the actual labels and predicted labels
temp_df = pd.DataFrame({'actual_labels':actual_labels.flatten(),
                        'two_predicted_labels':two_predicted_labels.flatten()})

# form cross-table
two_ct = pd.crosstab(temp_df['actual_labels'], temp_df['two_predicted_labels'])

plt.figure(figsize=(8, 6))
sns.heatmap(two_ct, annot=True, cmap='Blues', fmt='g', cbar=False)
plt.xlabel('Predicted labels')
plt.ylabel('Actual labels')
plt.show()
```



In [42]:

```
# extract the TP,FP,TN,FN values from the cross table
TP = two_ct.iloc[1, 1]
FP = two_ct.iloc[0, 1]
TN = two_ct.iloc[0, 0]
FN = two_ct.iloc[1, 0]
```

```
# accuracy
accuracy = (TP + TN) / (TP + TN + FP + FN)

# precision
precision = TP / (TP + FP)

# recall
recall = TP / (TP + FN)

# F1-score
f1 = 2 * (precision * recall) / (precision + recall)

print("Accuracy:", accuracy)
print("Precision:", precision)
print("Recall:", recall)
print("F1-score:", f1)
```

```
Accuracy: 0.25961538461538464
Precision: 0.3148148148148148
Recall: 0.40865384615384615
F1-score: 0.3556485355648536
```

Improving the K-Means Model

In this following section, we are essentially copy and pasting the above code. The only difference is in increasing from 2 principal components, up to 4. With 4 principal components, however, we cannot make the same visualisations as before.

Increasing to 4 principal components improves performance.

In [43]:

```
## building a more robust model using more principal components

# extract samples
samples_v2 = reduced_df[['PC1', 'PC2', 'PC3']].values


actual_labels = reduced_df[['class']].values

# initialise scaler
scaler = StandardScaler()
# fit the scaler
samples = scaler.fit_transform(samples)

# apply SMOTE to balance the dataset
smote = SMOTE(random_state=42)
samples_v2, actual_labels = smote.fit_resample(samples_v2, actual_labels)

# iterate over different k
max_k = 10
# save the sums of squares for each model
sum_of_squares = []
# save the silhouette scores for each model
silhouette_scores = []
for k in range(2,max_k+1):
    # initialise KMeans model
    model = KMeans(n_clusters = k, n_init = 10)
    # fit the model
    model.fit(samples_v2)
    # record the sum of squares
    sum_of_squares.append(model.inertia_)
    # calculate the silhouette scores
```

```
    silhouette_avg = silhouette_score(samples_v2, model.labels_)
    silhouette_scores.append(silhouette_avg)
```

```
C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarning: KMeans is known to have a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by setting the environment variable OMP_NUM_THREADS=2.
  warnings.warn(
C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarning: KMeans is known to have a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by setting the environment variable OMP_NUM_THREADS=2.
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C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarning: KMeans is known to have a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by setting the environment variable OMP_NUM_THREADS=2.
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C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarning: KMeans is known to have a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by setting the environment variable OMP_NUM_THREADS=2.
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C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarning: KMeans is known to have a memory leak on Windows with MKL, when there are less chunks than available threads. You can avoid it by setting the environment variable OMP_NUM_THREADS=2.
  warnings.warn(
```
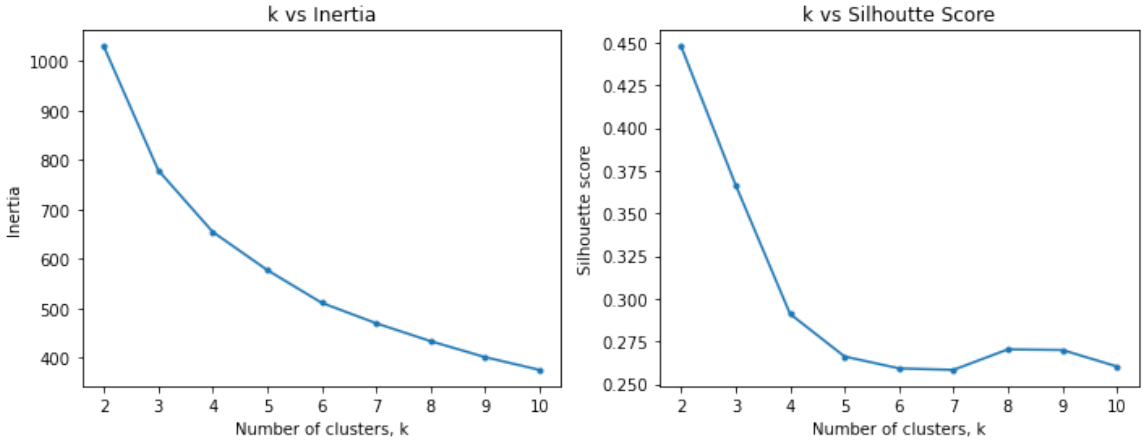

In [44]:

```
# create subplots
fig, axes = plt.subplots(1, 2, figsize=(10,4))

# plot elbow plot of inertia for each k
axes[0].plot(list(range(2, max_k + 1)), sum_of_squares, marker=".")
axes[0].set_title("k vs Inertia")
axes[0].set_xlabel("Number of clusters, k")
axes[0].set_ylabel("Inertia")

# plot silhouette scores for each k
axes[1].plot(list(range(2, max_k + 1)), silhouette_scores, marker=".")
axes[1].set_title("k vs Silhoutte Score")
axes[1].set_xlabel("Number of clusters, k")
axes[1].set_ylabel("Silhouette score")

plt.tight_layout()
plt.show()
```



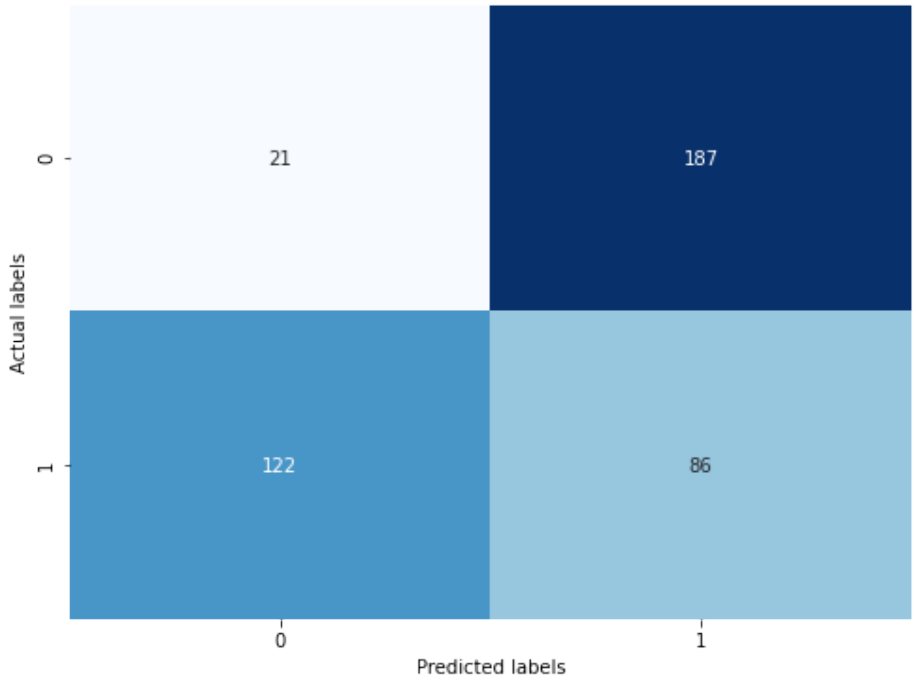
In [45]:

```
## build model with k = 2

# initialise model
two_model = KMeans(n_clusters = 2, n_init = 10)
# fit the model
two_model.fit(samples_v2)
# make predictions
two_predicted_labels = two_model.predict(samples_v2)
```

```
C:\Users\besso\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1440: UserWarni
ng: KMeans is known to have a memory leak on Windows with MKL, when there are less ch
unks than available threads. You can avoid it by setting the environment variable OMP
_NUM_THREADS=2.
  warnings.warn(
```

In [46]:

```
## using the actual labels, for k = 2, we can use a crosstable to evaluate model per

# reshape predicted labels from (... , ) to (... , 1)
two_predicted_labels = two_predicted_labels.reshape(-1,1)

# k-means clustering assigns 0s and 1s without knowing which is which in reality
# swap the labels round to reflect this
two_predicted_labels = 1 - two_predicted_labels

# create dataframe containing the actual labels and predicted labels
temp_df = pd.DataFrame({'actual_labels':actual_labels.flatten(),
                        'two_predicted_labels':two_predicted_labels.flatten()})

# form cross-table
two_ct = pd.crosstab(temp_df['actual_labels'], temp_df['two_predicted_labels'])

plt.figure(figsize=(8, 6))
sns.heatmap(two_ct, annot=True, cmap='Blues', fmt='g', cbar=False)
plt.xlabel('Predicted labels')
plt.ylabel('Actual labels')
plt.show()
```



In [47]:

```
# extract the TP,FP,TN,FN values from the cross table
TP = two_ct.iloc[1, 1]
FP = two_ct.iloc[0, 1]
TN = two_ct.iloc[0, 0]
FN = two_ct.iloc[1, 0]

# accuracy
accuracy = (TP + TN) / (TP + TN + FP + FN)

# precision
precision = TP / (TP + FP)

# recall
recall = TP / (TP + FN)

# F1-score
f1 = 2 * (precision * recall) / (precision + recall)

print("Accuracy:", accuracy)
print("Precision:", precision)
print("Recall:", recall)
print("F1-score:", f1)
```

```
Accuracy: 0.25721153846153844
Precision: 0.315018315018315
Recall: 0.41346153846153844
F1-score: 0.35758835758835755
```