Home Assignment 1

Group 3

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In [141…

```python
import numpy as np
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
from time import time

from scipy.sparse import dok_matrix
from scipy.sparse.linalg import svds

from sklearn.pipeline import Pipeline
from sklearn.decomposition import PCA
from sklearn.preprocessing import LabelEncoder, StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.naive_bayes import GaussianNB
from sklearn.tree import DecisionTreeClassifier, DecisionTreeRegressor
from sklearn.metrics import mean_squared_error, max_error, ConfusionMatrixDisplay, confusion_matı

np.seterr(divide='ignore', invalid='ignore');
```

In [2]:

```python
# Merge the two datasets
df = pd.read_csv("train.csv").merge(
    pd.read_csv("unique_m.csv"),
    left_index=True,
    right_index=True
)
df.head()
```

Out[2]:

	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atomic_mass	wtd_gmean_atomic_mass
0	4	88.944468	57.862692	66.361592	36.116612
1	5	92.729214	58.518416	73.132787	36.396602
2	4	88.944468	57.885242	66.361592	36.122509
3	4	88.944468	57.873967	66.361592	36.119560
4	4	88.944468	57.840143	66.361592	36.110716

5 rows × 170 columns

In [3]:

```python
# Separate dependent and independent sets
X = df.drop(columns=["critical_temp_x", "critical_temp_y", "material"])
y = df.critical_temp_x
```

In [4]:

```python
# Create training and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.1, random_state=22)
```

In [79]:
```
X_train.head()
```

Out[79]:

	number_of_elements	mean_atomic_mass	wtd_mean_atomic_mass	gmean_atomic_mass	wtd_gmean_atomic_
2915	5	95.891840	54.218519	73.468530	35.68
3532	5	68.975310	52.166945	54.601832	35.69
4002	5	38.834940	35.215547	35.512542	31.78
10044	1	112.411000	112.411000	112.411000	112.41
3553	5	88.936744	52.703157	70.358975	35.89

5 rows × 167 columns

Objective 1 - Dimensionality reduction

In [20]:
```
print(f"Percentage of 0's in the X matrix = {(X_train==0).sum().sum() / np.prod(X_train.shape):.
```
```
Percentage of 0's in the X matrix = 0.495
```

Roughly half of the data contains non-null elements.
We will use PCA for the dimensionality reduction, as the majority of the matrix is dense.

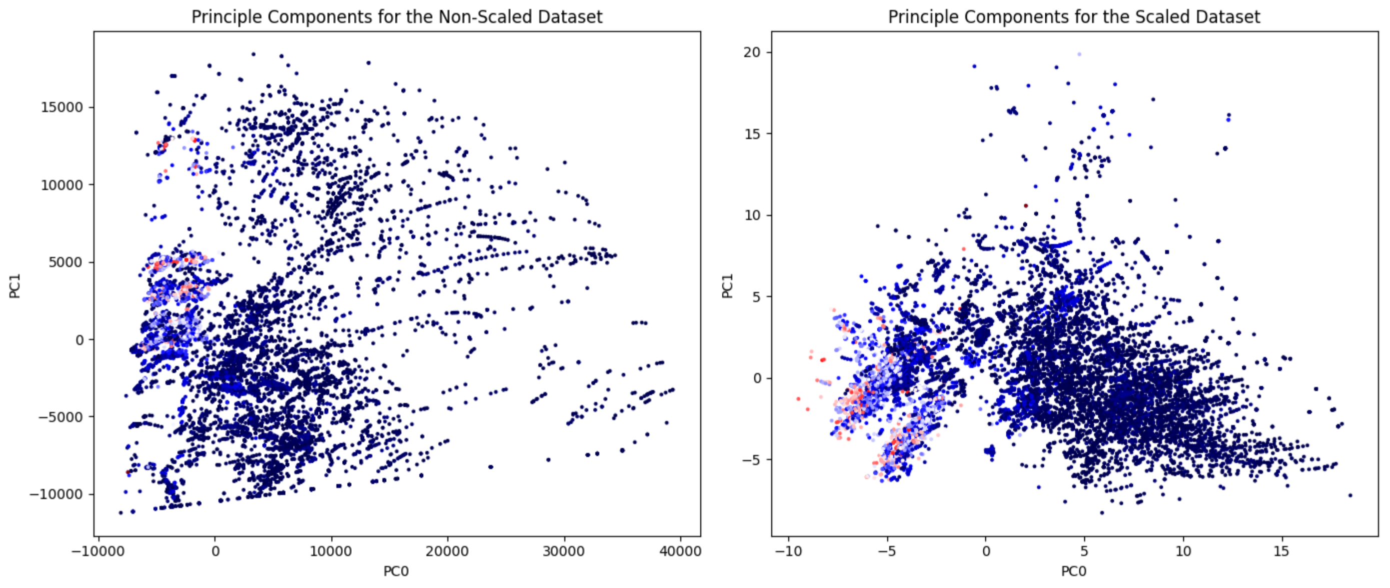
In [21]:
```
#create a scaler to compare data with and without scaling
scaler = StandardScaler().fit(X_train)
```

In [24]:
```
n_elements_pca = len(PCA(n_components=0.9, svd_solver='full').fit(X_train).explained_variance_)
n_scaled_elements_pca = len(PCA(n_components=0.9, svd_solver='full').fit(
    scaler.transform(X_train)
).explained_variance_)

print(f"Number of components to reach 90% explainability with non-scaled dataset = {n_elements_p
print(f"Number of components to reach 90% explainability with scaled dataset = {n_scaled_element
```
```
Number of components to reach 90% explainability with non-scaled dataset = 2
Number of components to reach 90% explainability with scaled dataset = 66
```

Both scenarios have a good decrease in the number of features. Originally there were 170.

In [70]:
```
#function to scatter in pre-defined axis
def scatter(x, y, c, ax, xlabel="", ylabel="", title="", cmap="seismic"):
    ax.scatter(x,y,c=c, cmap=cmap, s=3)
    ax.set_xlabel(xlabel)
    ax.set_ylabel(ylabel)
    ax.set_title(title)
```

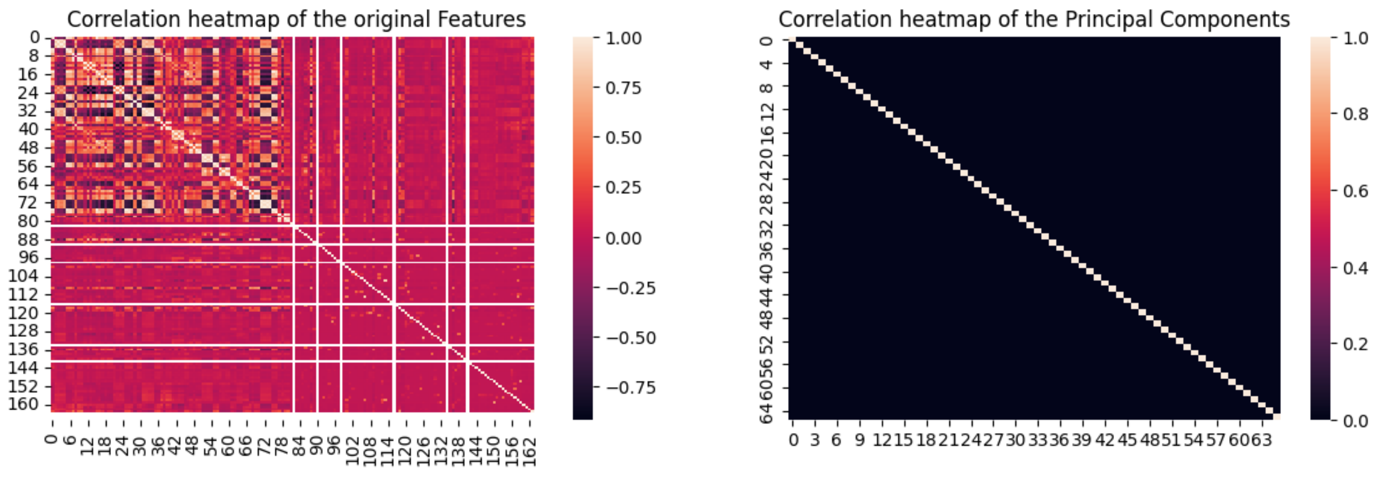
In [74]:
```
f, ax = plt.subplots(1,2, figsize=(14,6))

X_train_reduced = PCA(n_components=0.9, svd_solver='full').fit_transform(X_train)
X_train_scaled_reduced = PCA(n_components=0.9, svd_solver='full').fit_transform(
    scaler.transform(X_train)
)

scatter(X_train_reduced[:,0], X_train_reduced[:, 1], y_train, ax[0], "PC0", "PC1", "Principle Co
scatter(X_train_scaled_reduced[:,0], X_train_scaled_reduced[:, 1], y_train, ax[1], "PC0", "PC1",

f.tight_layout()
```



From the figure above, it seems that even though the original dataset has only 2 components to explain all the variance, the scaled dataset clusters the data better with it's 2 main components.

```
In [123…  f, ax = plt.subplots(1,2, figsize=(14,4))

          sns.heatmap(
              np.corrcoef(scaler.transform(X_train).T),
              ax=ax[0]
          )
          ax[0].set_title("Correlation heatmap of the original Features")
          sns.heatmap(
              np.corrcoef(
                  PCA(n_components=0.9, svd_solver="full").fit_transform(
                      scaler.transform(X_train)
                  ).T
              ),
              ax=ax[1]
          )
          ax[1].set_title("Correlation heatmap of the Principal Components");
```

```
Out[123]:  Text(0.5, 1.0, 'Correlation heatmap of the Principal Components')
```



In the left plot we can see that in the full dataset there are some features that are redundant. Overall it seems that some independent variables are related to other independent variables.
On the plot presented on the right, as expected, we can see that the components are not correlated with each other.

Objective 2 - Create a Regression and a Classification Model

2.1 Regression Model

For this section we will use Decision Tree, as PCA components are decorrelated between themselves. With no linear relation between components we do not expect Linear Regression to have a good performance.

In [89]:
```
t =time()
dtr = Pipeline([
    ("scaler", StandardScaler()),
    ("regressor", DecisionTreeRegressor())
]).fit(X_train, y_train)
print(f"Train time without PCA = {time() - t:.3f}")

t = time()
dtr_pca = Pipeline([
    ("scaler", StandardScaler()),
    ("dim", PCA(n_components=0.9, svd_solver="full")),
    ("regressor", DecisionTreeRegressor())
]).fit(X_train, y_train)
print(f"Train time with PCA = {time() - t:.3f}")
```

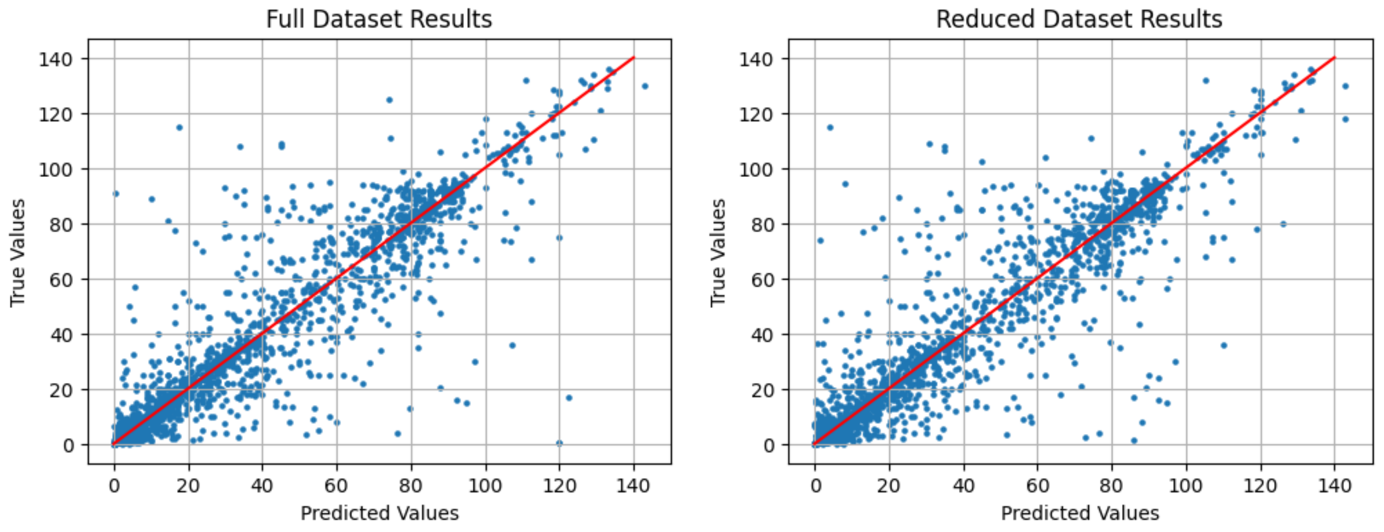
```
Fit time without PCA = 1.877
Fit time with PCA = 1.939
```

We can see that PCA didn't create much overhead. The complexity is mainly in training the tree model.

In [104…
```
def scatter(y_test, preds, ax, ylabel="True Values", xlabel="Predicted Values", title=""):
    ax.scatter(preds,y_test, s=5)
    ax.set_xlabel(xlabel)
    ax.set_ylabel(ylabel)
    ax.set_title(title)
    ax.plot([0,140],[0,140], "r")
    ax.grid()
```

In [109…
```
t = time()
preds = dtr.predict(X_test)
print(f"Prediction time without PCA = {time() - t:.3f}")
t=time()
preds_pca = dtr_pca.predict(X_test)
print(f"Prediction time with PCA = {time() - t:.3f}", end="\n"+"-"*120+"\n")
#Compute RMSE
rmse = mean_squared_error(y_test, preds, squared=False)
rmse_pca = mean_squared_error(y_test, preds_pca, squared=False)
#Compute Maximum Error
max_err = max_error(y_test, preds)
max_err_pca = max_error(y_test, preds_pca)
#Compute Pearson Correlation between predictions and original data
pearson_r = np.corrcoef(y_test, preds)[0,1]
pearson_r_pca = np.corrcoef(y_test, preds_pca)[0,1]

print(f"Full Dataset RMSE = {rmse:.3f}", "\t"*5,  f"| Reduced Dataset RMSE = {rmse_pca:.3f}")
print(f"Full Dataset Max. Error = {max_err:.3f}", "\t"*4, f"| Reduced Dataset Max. Error = {max_
print(f"Full Dataset Pearson Corr. = {pearson_r:.3f}", "\t"*4, f"| Reduced Dataset Pearson Corr =
f, ax = plt.subplots(1,2,figsize=(12,4))

scatter(y_test, preds, ax[0], title="Full Dataset Results")
scatter(y_test, preds_pca, ax[1],title="Reduced Dataset Results")
```

```
Prediction time without PCA = 0.008
Prediction time with PCA = 0.011
--------------------------------------------------------------------------------------------------
------------------------
Full Dataset RMSE = 12.799                                         | Reduced Dataset RMSE = 12.836
Full Dataset Max. Error = 119.620                                  | Reduced Dataset Max. Error =
111.000
Full Dataset Pearson Corr. = 0.928                                 | Reduced Dataset Pearson Corr
= 0.928
```



In [114…
```python
print(
    "Full dataset number of elements = ",
    np.prod(X_train.shape),
    "\nReduced dataset number of elements = ",
    np.prod(
        PCA(n_components=0.9, svd_solver="full").fit_transform(
            StandardScaler().fit_transform(X_train)
        ).shape
    ),
)
```

```
Full dataset number of elements =  3195712
Reduced dataset number of elements =  1262976
```

We can see that the regression difference is minimal using full dataset or reduced dataset. In fact, while the RMSE stayed almost the same, the maximum error obtained in the reduced dataset is reduced.

There is almost no overhead in the prediction time, using PCA.

With this results, it is much better to use the reduced dataset, as the total size is reduced from 3195712 elements to 1262976, which is around 2.5 less space.

2.2 Classification Model

It is requested to use both NaiveBayes and DecisionTrees for Full Dataset and the Reduced Dataset.
First we will compare the models on the full dataset. Afterwards compare both models using the reduced dataset.

In [117…
```python
def to_class(x: float) -> str:
    if 0 <= x < 1.0:
        return "VeryLow"
    elif 1 <= x < 5.0:
        return "Low"
    elif 5 <= x < 20.0:
        return "Medium"
    elif 20 <= x < 100.0:
        return "High"
    elif x >= 100:
        return "VeryHigh"
    return np.nan


y_train_class = y_train.apply(to_class)
y_test_class = y_test.apply(to_class)
```

- Full Dataset

In [137…

```
t = time()
dtc = Pipeline([
    ("scaler", StandardScaler()),
    ("classifier", DecisionTreeClassifier())
]).fit(X_train, y_train_class)
print(f"Decision Tree train time (no PCA) = {time() - t:.3f}")

t = time()
nb = Pipeline([
    ("scaler", StandardScaler()),
    ("classifier", GaussianNB())
]).fit(X_train, y_train_class)
print(f"Naive Bayes train time (no PCA) = {time() - t:.3f}")
```

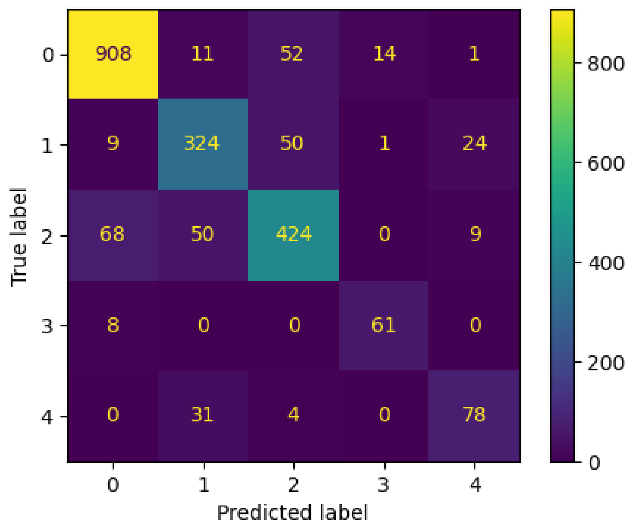
```
Decision Tree train time (no PCA) = 2.595
Naive Bayes train time (no PCA) = 0.192
```

For this small dataset, we can already see big differences in the training time of Naive Bayes model and Decision Trees.

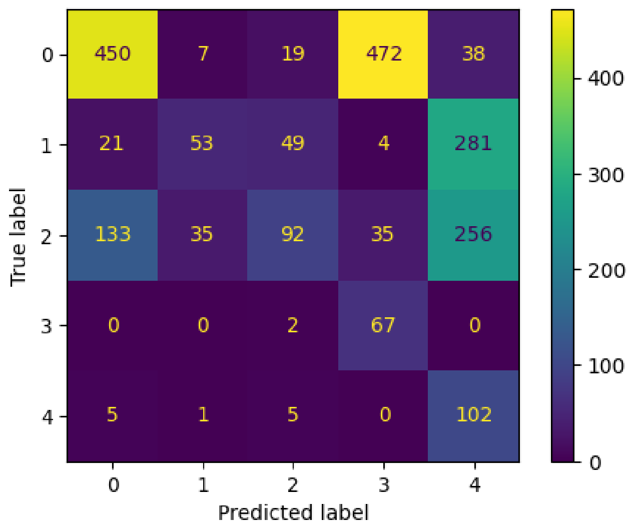
In [138…

```
t = time()
dtc_preds = dtc.predict(X_test)
print(f"Decision Tree predict time (no PCA) = {time() - t:.3f}")
t=time()
nb_preds = nb.predict(X_test)
print(f"Naive Bayes predict time (no PCA) = {time() - t:.3f}")

#Compute MFCC
dtc_mfcc = matthews_corrcoef(y_test_class,dtc_preds)
nb_mfcc= matthews_corrcoef(y_test_class, nb_preds)

print(f"Decision Tree MFCC = {dtc_mfcc:.3f}", "\t"*5,  f"| Naive Bayes MFCC = {nb_mfcc:.3f}")

f, ax = plt.subplots(1,2, figsize=(12,4))
ConfusionMatrixDisplay(
    confusion_matrix(y_test_class, dtc_preds)
).plot(ax=ax[0]);

ConfusionMatrixDisplay(
    confusion_matrix(y_test_class, nb_preds)
).plot(ax=ax[1]);
```

```
Decision Tree predict time (no PCA) = 0.013
Naive Bayes predict time (no PCA) = 0.033
Decision Tree MFCC = 0.770                                      | Naive Bayes MFCC = 0.243
```



	0	1	2	3	4
0	908	11	52	14	1
1	9	324	50	1	24
2	68	50	424	0	9
3	8	0	0	61	0
4	0	31	4	0	78



	0	1	2	3	4
0	450	7	19	472	38
1	21	53	49	4	281
2	133	35	92	35	256
3	0	0	2	67	0
4	5	1	5	0	102

We can see that the decision tree (DT) was actually faster making the predictions than naive bayes (NB). The DT model when making predictions only parses the Tree, which means complexity of $O(d)$, where d is the depth of the tree. Parsing a tree is faster than calculating probabilities/likelihoods.

The DT also obtained better mfcc score and in the confusion matrix we can visualize why. As we have seen previously the features of the full dataset have high correlations. This could indicate some variable dependency, which is what NB discards, as it assumes the features are independent.

- Reduced Dataset

In [139…

```
t = time()
dtc = Pipeline([
    ("scaler", StandardScaler()),
    ("dim", PCA(n_components=0.9, svd_solver="full")),
    ("classifier", DecisionTreeClassifier())
]).fit(X_train, y_train_class)
print(f"Decision Tree train time (with PCA) = {time() - t:.3f}")

t = time()
nb = Pipeline([
    ("scaler", StandardScaler()),
    ("dim", PCA(n_components=0.9, svd_solver="full")),
    ("classifier", GaussianNB())
]).fit(X_train, y_train_class)
print(f"Naive Bayes train time (with PCA) = {time() - t:.3f}")
```

```
Decision Tree train time (with PCA) = 2.547
Naive Bayes train time (with PCA) = 0.428
```

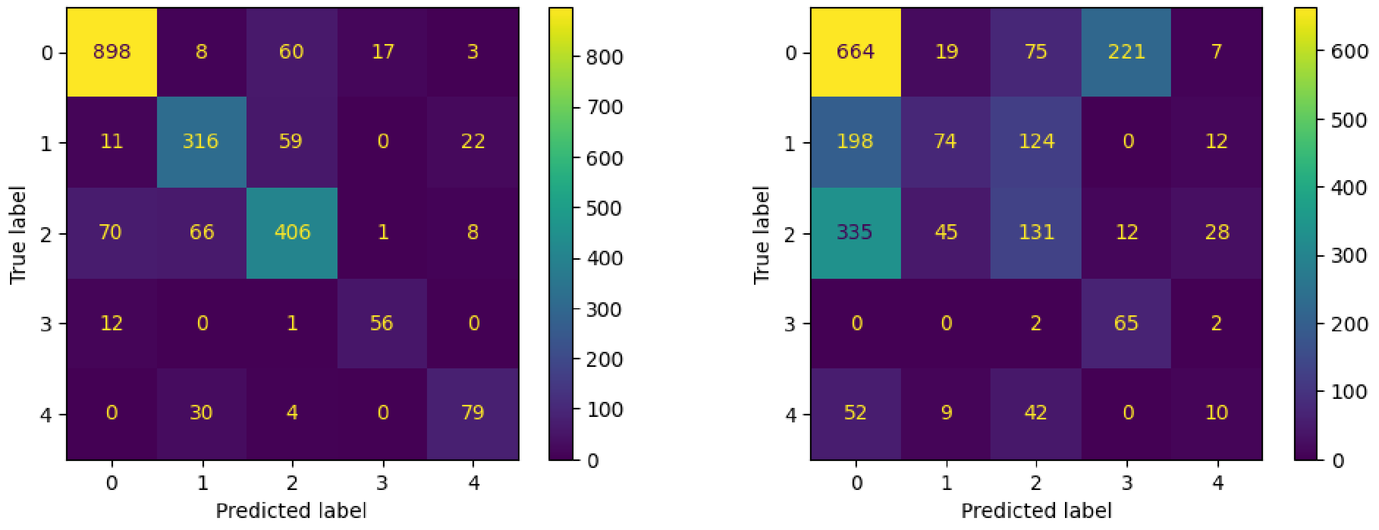
We can see that reducing the dimension with PCA had a bigger impact in the NB model. While DT took the same time to train, NB took significant more time.

In [140…

```
t = time()
dtc_preds = dtc.predict(X_test)
print(f"Decision Tree predict time (with PCA) = {time() - t:.3f}")
t=time()
nb_preds = nb.predict(X_test)
print(f"Naive Bayes predict time (with PCA) = {time() - t:.3f}")

#Compute MFCC
dtc_mfcc = matthews_corrcoef(y_test_class,dtc_preds)
nb_mfcc= matthews_corrcoef(y_test_class, nb_preds)
```

```python
print(f"Decision Tree MFCC = {dtc_mfcc:.3f}", "\t"*5,  f"| Naive Bayes MFCC = {nb_mfcc:.3f}")

f, ax = plt.subplots(1,2, figsize=(12,4))
ConfusionMatrixDisplay(
    confusion_matrix(y_test_class, dtc_preds)
).plot(ax=ax[0]);

ConfusionMatrixDisplay(
    confusion_matrix(y_test_class, nb_preds)
).plot(ax=ax[1]);
```

```
Decision Tree predict time (with PCA) = 0.014
Naive Bayes predict time (with PCA) = 0.019
Decision Tree MFCC = 0.742                                  | Naive Bayes MFCC = 0.168
```



Even with the independence of the variables, NB did not have a good performance. Has DT are universal function approximaters they performed better, as they can adapt more to every kind of relation with the data.

Comparing both decision trees, as with the regression, we see similar results on both datasets. Therefore, using the reduced dataset is advisable.