A.3 Random Forest Method

A.3.1 Supplemental Information

Gini Impurity Calculation

Gini impurity measures how mixed the classes are within a node. It is computed as:

$$\text{Gini impurity}(S) = 1 - \sum_{i=1}^{k} p_i^2$$

Where:

- S = collection of features
- p_i = proportion of samples belonging to class (i)
- k = total number of classes

A Gini value of 0 indicates a perfectly pure node (all samples belong to one class), while higher values indicate more class mixing.

Information Gain (Split Criterion)

Decision trees choose the split that produces the largest reduction in impurity. Information gain is defined as:

$$\text{Gain}(S, A) = \text{Impurity}(S) - \sum_{v \in Value(A)} \frac{|S_v|}{|S|} \text{Impurity}(S_v)$$

Where:

- S is a collection of features
- A is a feature in S
- Value(A) is the set of all possible values for attribute A
- S_v is the subset of S for which attribute A has value v.

The split with the highest information gain is selected.

A.3.2 Pipelines

In [1]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

```
from sklearn.model_selection import train_test_split, GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.ensemble import RandomForestClassifier
from sklearn.metrics import accuracy_score,f1_score, classification_report,
from sklearn.pipeline import Pipeline as SkPipeline

from imblearn.pipeline import Pipeline as ImbPipeline
from imblearn.over_sampling import SMOTE
```

In [2]:

```
# load data
raw_path = "../../data/raw/winequality-red.csv"

with open(raw_path, "r") as f:
    header_line = f.readline().strip()

header_clean = header_line.replace('""', '"').replace('"', '')
columns = [col.strip() for col in header_clean.split(';')]

df_raw = pd.read_csv(raw_path, sep=";", skiprows=1, names=columns)

X = df_raw.drop(columns=["quality"])
y = df_raw["quality"]

# split
X_train, X_test, y_train, y_test = train_test_split(
    X,
    y,
    test_size=0.2,
    random_state=42,
    stratify=y,
)
```

A.3.2.1 Normalized Pipeline & Results

In [3]:

```
pipe_normalized = SkPipeline([
    ("scaler", StandardScaler()),
    ("rf", RandomForestClassifier(random_state=42)),
])

param_grid_normalized = {
    "rf__n_estimators": [50, 100, 150, 200],
    "rf__max_depth": [None, 15, 25, 50],
    "rf__max_features": ["sqrt", "log2", None],
    "rf__class_weight": [None, "balanced"],
}

grid_norm = GridSearchCV(
    pipe_normalized,
    param_grid=param_grid_normalized,
    scoring="f1_macro",
    cv=5,
```

```python
    n_jobs=-1,
    return_train_score=True,
)

print("Running normalized pipeline")
grid_norm.fit(X_train, y_train)

best_idx = grid_norm.best_index_
best_params = grid_norm.best_params_

# cv metrics
train_cv_macro_f1_mean = grid_norm.cv_results_["mean_train_score"][best_idx
train_cv_macro_f1_std  = grid_norm.cv_results_["std_train_score"][best_idx]

val_cv_macro_f1_mean = grid_norm.best_score_
val_cv_macro_f1_std  = grid_norm.cv_results_["std_test_score"][best_idx]

print("Best parameters:", best_params)
print(f"Train CV Macro F1 (mean): {train_cv_macro_f1_mean:.4f}")
print(f"Train CV Macro F1 (std):  {train_cv_macro_f1_std:.4f}")
print(f"Val   CV Macro F1 (mean): {val_cv_macro_f1_mean:.4f}")
print(f"Val   CV Macro F1 (std):  {val_cv_macro_f1_std:.4f}")

# test metrics
best_norm = grid_norm.best_estimator_
y_pred_norm = best_norm.predict(X_test)

test_macro_f1 = f1_score(y_test, y_pred_norm, average="macro")
test_acc = accuracy_score(y_test, y_pred_norm)

print(f"\nTest Macro F1: {test_macro_f1:.4f}")
print(f"Test Accuracy: {test_acc:.4f}")
print("\nClassification Report:")
print(classification_report(y_test, y_pred_norm, zero_division=0))

# confusion matrix
ConfusionMatrixDisplay.from_predictions(
    y_test, y_pred_norm, normalize="true", values_format=".2f"
)
plt.title("Normalized Data — RF")
plt.show()
```

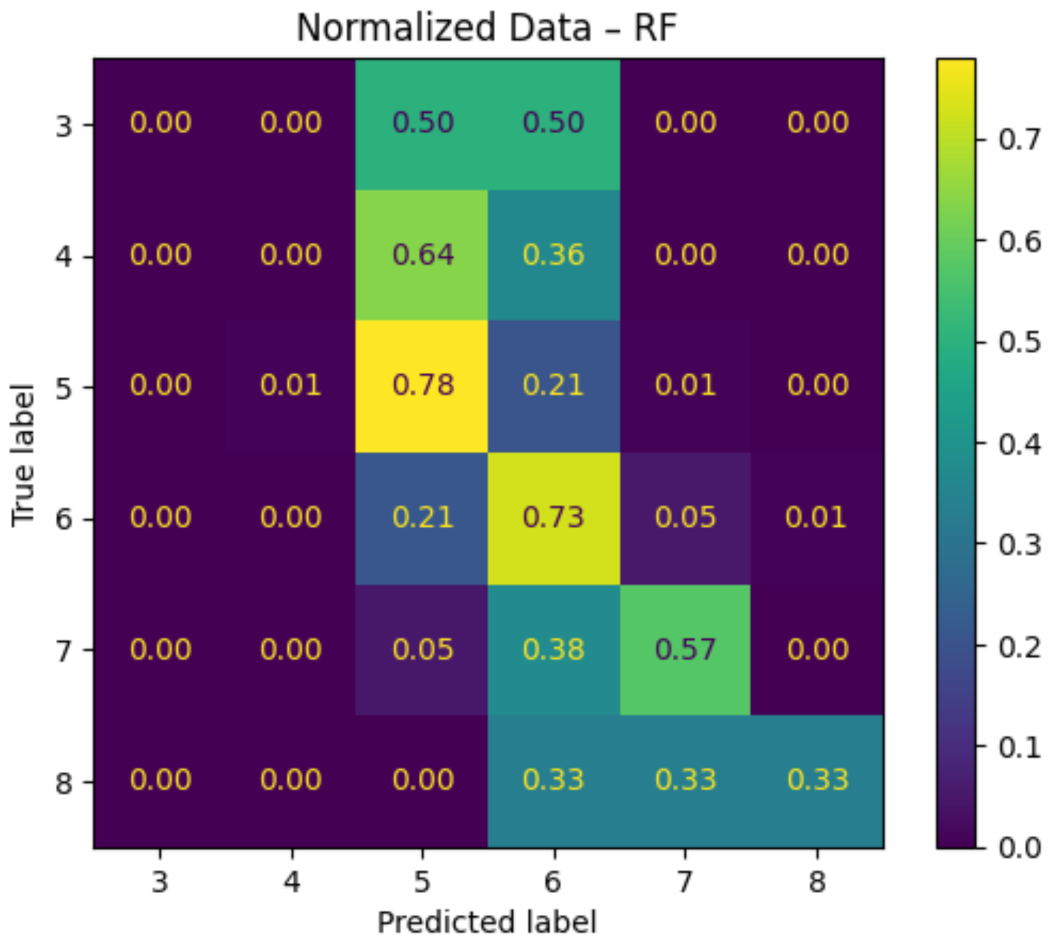
```
Running normalized pipeline
Best parameters: {'rf__class_weight': 'balanced', 'rf__max_depth': 25, 'rf__
max_features': None, 'rf__n_estimators': 100}
Train CV Macro F1 (mean): 1.0000
Train CV Macro F1 (std):  0.0000
Val   CV Macro F1 (mean): 0.3510
Val   CV Macro F1 (std):  0.0333

Test Macro F1: 0.4146
Test Accuracy: 0.6969

Classification Report:
              precision    recall  f1-score   support

           3       0.00      0.00      0.00         2
           4       0.00      0.00      0.00        11
           5       0.74      0.78      0.76       136
           6       0.65      0.73      0.69       128
           7       0.72      0.57      0.64        40
           8       0.50      0.33      0.40         3

    accuracy                           0.70       320
   macro avg       0.44      0.40      0.41       320
weighted avg       0.67      0.70      0.68       320
```



A.3.2.2 PCA Pipeline & Results

In [4]:
```python
pipe_pca = SkPipeline([
    ("scaler", StandardScaler()),
    ("pca", PCA(n_components=5)),
    ("rf", RandomForestClassifier(random_state=42)),
])

param_grid_pca = {
    "rf__n_estimators": [50, 100, 150, 200],
    "rf__max_depth": [None, 15, 25, 50],
    "rf__max_features": ["sqrt", "log2", None],
    "rf__class_weight": [None, "balanced"],
}

grid_pca = GridSearchCV(
    pipe_pca,
    param_grid=param_grid_pca,
    scoring="f1_macro",
    cv=5,
    n_jobs=-1,
    return_train_score=True,
)

print("Running PCA pipeline")
grid_pca.fit(X_train, y_train)

best_idx = grid_pca.best_index_
best_params_pca = grid_pca.best_params_

# cv metrics
train_cv_macro_f1_mean = grid_pca.cv_results_["mean_train_score"][best_idx]
train_cv_macro_f1_std  = grid_pca.cv_results_["std_train_score"][best_idx]
val_cv_macro_f1_mean   = grid_pca.best_score_
val_cv_macro_f1_std    = grid_pca.cv_results_["std_test_score"][best_idx]

print("Best parameters:", best_params_pca)
print(f"Train CV Macro F1 (mean): {train_cv_macro_f1_mean:.4f}")
print(f"Train CV Macro F1 (std):  {train_cv_macro_f1_std:.4f}")
print(f"Val   CV Macro F1 (mean): {val_cv_macro_f1_mean:.4f}")
print(f"Val   CV Macro F1 (std):  {val_cv_macro_f1_std:.4f}")

# test metrics
best_pca = grid_pca.best_estimator_
y_pred_pca = best_pca.predict(X_test)

test_macro_f1_pca = f1_score(y_test, y_pred_pca, average="macro")
test_acc_pca = accuracy_score(y_test, y_pred_pca)

print(f"\nTest Macro F1: {test_macro_f1_pca:.4f}")
print(f"Test Accuracy: {test_acc_pca:.4f}")
print("\nClassification Report:")
print(classification_report(y_test, y_pred_pca, zero_division=0))

ConfusionMatrixDisplay.from_predictions(
    y_test, y_pred_pca, normalize="true", values_format=".2f"
)
plt.title("PCA (5 components) — RF")
plt.show()
```

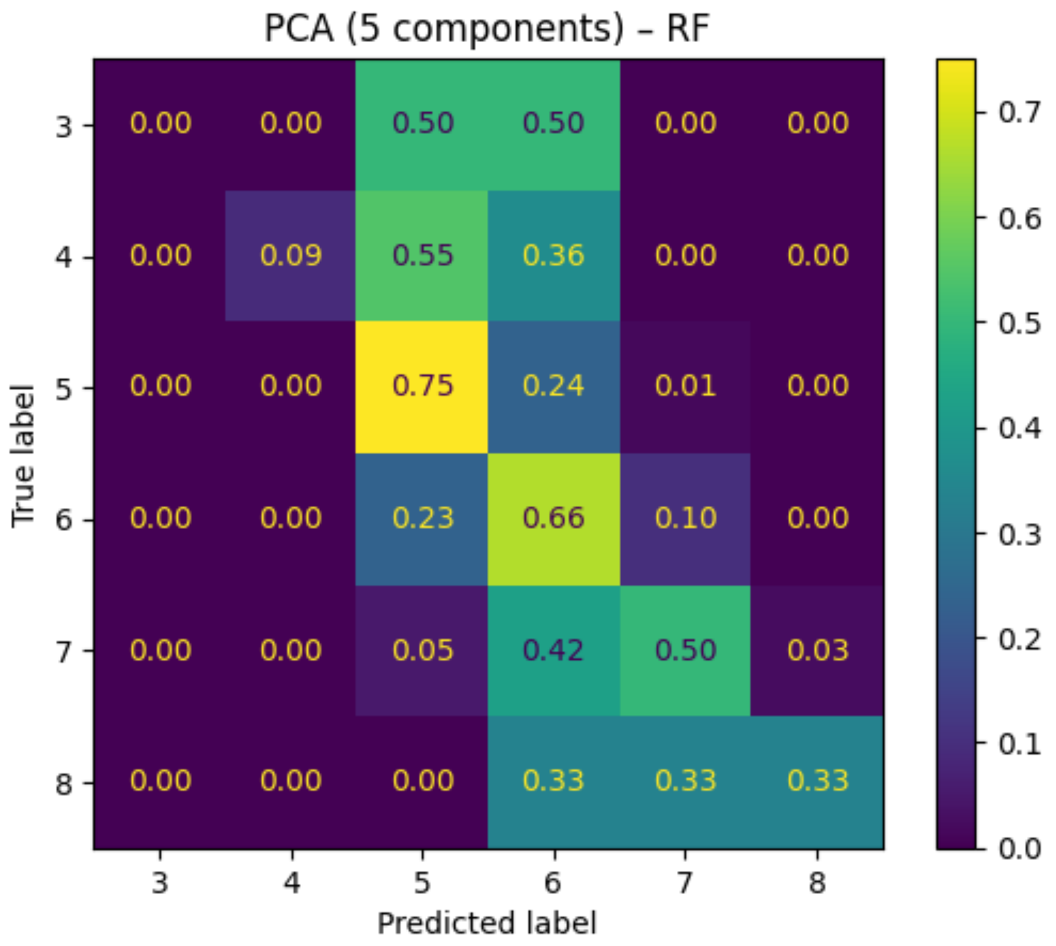
```
Running PCA pipeline
Best parameters: {'rf__class_weight': None, 'rf__max_depth': 25, 'rf__max_fe
atures': 'sqrt', 'rf__n_estimators': 50}
Train CV Macro F1 (mean): 1.0000
Train CV Macro F1 (std):  0.0000
Val   CV Macro F1 (mean): 0.3734
Val   CV Macro F1 (std):  0.0685

Test Macro F1: 0.4106
Test Accuracy: 0.6531

Classification Report:
              precision    recall  f1-score   support

           3       0.00      0.00      0.00         2
           4       1.00      0.09      0.17        11
           5       0.72      0.75      0.74       136
           6       0.61      0.66      0.63       128
           7       0.56      0.50      0.53        40
           8       0.50      0.33      0.40         3

    accuracy                           0.65       320
   macro avg       0.56      0.39      0.41       320
weighted avg       0.66      0.65      0.64       320
```



A.3.2.3 SMOTE Pipeline & Results

In [5]:
```
pipe_smote = ImbPipeline([
    ("scaler", StandardScaler()),
    ("smote", SMOTE(random_state=42, k_neighbors=3)),
    ("rf", RandomForestClassifier(random_state=42)),
])

param_grid_smote = {
    "rf__n_estimators": [50, 100, 150, 200],
    "rf__max_depth": [None, 15, 25, 50],
    "rf__max_features": ["sqrt", "log2", None],
    "rf__class_weight": [None, "balanced"],
}

grid_smote = GridSearchCV(
    pipe_smote,
    param_grid=param_grid_smote,
    scoring="f1_macro",
    cv=5,
    n_jobs=-1,
    return_train_score=True,
)

print("Running SMOTE pipeline")
grid_smote.fit(X_train, y_train)

best_idx_smote = grid_smote.best_index_
best_params_smote = grid_smote.best_params_

# cv metrics
train_cv_macro_f1_mean_sm = grid_smote.cv_results_["mean_train_score"][best
train_cv_macro_f1_std_sm  = grid_smote.cv_results_["std_train_score"][best_
val_cv_macro_f1_mean_sm   = grid_smote.best_score_
val_cv_macro_f1_std_sm    = grid_smote.cv_results_["std_test_score"][best_i

print("Best parameters:", best_params_smote)
print(f"Train CV Macro F1 (mean): {train_cv_macro_f1_mean_sm:.4f}")
print(f"Train CV Macro F1 (std):  {train_cv_macro_f1_std_sm:.4f}")
print(f"Val   CV Macro F1 (mean): {val_cv_macro_f1_mean_sm:.4f}")
print(f"Val   CV Macro F1 (std):  {val_cv_macro_f1_std_sm:.4f}")

# test metrics
best_smote = grid_smote.best_estimator_
y_pred_smote = best_smote.predict(X_test)

test_macro_f1_smote = f1_score(y_test, y_pred_smote, average="macro")
test_acc_smote = accuracy_score(y_test, y_pred_smote)

print(f"\nTest Macro F1: {test_macro_f1_smote:.4f}")
print(f"Test Accuracy: {test_acc_smote:.4f}")
print("\nClassification Report:")
print(classification_report(y_test, y_pred_smote, zero_division=0))

ConfusionMatrixDisplay.from_predictions(
    y_test, y_pred_smote, normalize="true", values_format=".2f"
)
```

```
plt.title("SMOTE – RF")
plt.show()
```

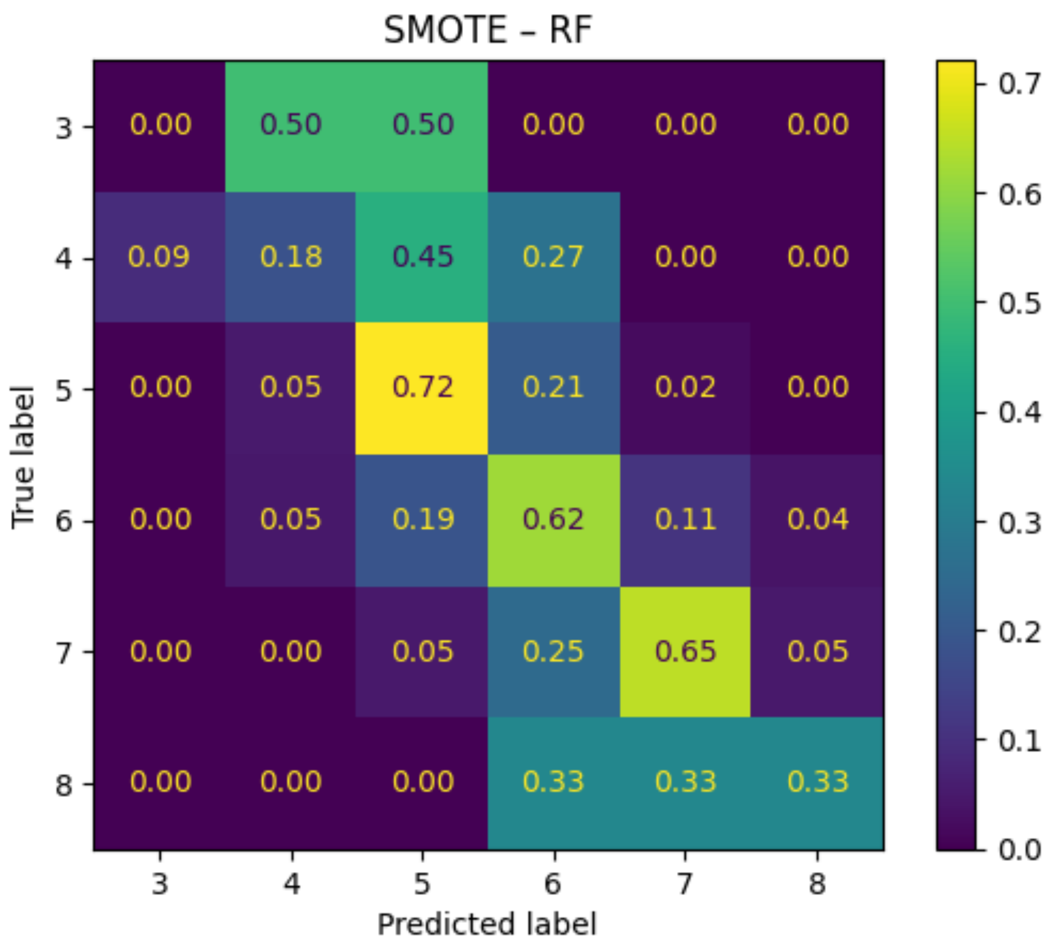
```
Running SMOTE pipeline
Best parameters: {'rf__class_weight': None, 'rf__max_depth': 15, 'rf__max_fe
atures': 'sqrt', 'rf__n_estimators': 150}
Train CV Macro F1 (mean): 1.0000
Train CV Macro F1 (std):  0.0000
Val   CV Macro F1 (mean): 0.3802
Val   CV Macro F1 (std):  0.0453

Test Macro F1: 0.3867
Test Accuracy: 0.6438

Classification Report:
              precision    recall  f1-score   support

           3       0.00      0.00      0.00         2
           4       0.12      0.18      0.15        11
           5       0.75      0.72      0.74       136
           6       0.65      0.62      0.63       128
           7       0.59      0.65      0.62        40
           8       0.12      0.33      0.18         3

    accuracy                           0.64       320
   macro avg       0.37      0.42      0.39       320
weighted avg       0.66      0.64      0.65       320
```


SMOTE – RF
True label
Predicted label