# notebook

October 20, 2025

## 1 Compétition 1 : Prédiction de la Qualité de la Bière

Ce notebook fournit du code de démarrage pour la compétition de prédiction de la qualité de la bière. Pour les instructions complètes, l'énoncé du problème et les critères de notation, veuillez vous référer au fichier **README.md**.

**Résumé rapide** : Vous allez construire un modèle de classification pour prédire la qualité de la bière (scores 1-10) basé sur des propriétés chimiques. Soumettez vos prédictions sur Kaggle.

### 1.1 Importer les Dépendances

[471]:
```
# Importer les bibliothèques requises
import pandas as pd
import numpy as np
from sklearn.preprocessing import StandardScaler, LabelEncoder
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
from sklearn.metrics import accuracy_score, classification_report,␣
↪confusion_matrix
import matplotlib.pyplot as plt
import seaborn as sns
```

### 1.2 Charger et Explorer les Données

[472]:
```
# Charger les données d'entraînement
train_df = pd.read_csv('data/train.csv', delimiter=';')

print(f"Forme des données d'entraînement : {train_df.shape}")
print(f"Nombre d'échantillons (n) : {train_df.shape[0]}")
print(f"Nombre de caractéristiques (d) : {train_df.shape[1] - 1}")  #␣
↪Soustraire 1 pour la colonne cible
print(f"Colonnes : {list(train_df.columns)}")
print("\nPremières lignes :")
print(train_df.head())

# Vérifier les types de données et informations de base
```

```python
print("\nTypes de données et informations :")
print(train_df.info())

#########################################################################
###############   À compléter   ###################################
#########################################################################
```

```
Forme des données d'entraînement : (4469, 15)
Nombre d'échantillons (n) : 4469
Nombre de caractéristiques (d) : 14
Colonnes : ['id', 'beer_style', 'bitterness_IBU', 'diacetyl_concentration',
'lactic_acid', 'final_gravity', 'sodium', 'free_CO2', 'dissolved_oxygen',
'original_gravity', 'pH', 'gypsum_level', 'alcohol_ABV',
'fermentation_strength', 'quality']

Premières lignes :
   id beer_style  bitterness_IBU  diacetyl_concentration  lactic_acid  \
0   0       Pale           7.997                   0.446        0.280
1   1       Pale           6.906                   0.222        0.303
2   2      Brown           7.183                   0.636        0.071
3   3       Pale           6.403                   0.242        0.260
4   4      Brown           7.917                   0.182        0.347

   final_gravity  sodium  free_CO2  dissolved_oxygen  original_gravity     pH  \
0         10.803   0.052    24.999           157.026             0.995  3.057
1          6.305   0.034    40.993           130.993             1.012  3.083
2          2.495   0.080    16.998            84.003             1.013  3.509
3          1.506   0.043    34.999           105.001             0.994  3.137
4          1.700   0.053     7.011            14.999             1.002  3.326

   gypsum_level  alcohol_ABV  fermentation_strength  quality
0         0.466        5.436                  9.545        7
1         0.476        5.137                  9.847        6
2         0.545        4.618                  8.771        5
3         0.308        5.909                 10.504        6
4         0.805        5.674                  9.748        7

Types de données et informations :
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 4469 entries, 0 to 4468
Data columns (total 15 columns):
 #   Column                 Non-Null Count  Dtype
---  ------                 --------------  -----
 0   id                     4469 non-null   int64
 1   beer_style             4469 non-null   object
 2   bitterness_IBU         4469 non-null   float64
 3   diacetyl_concentration  4469 non-null   float64
 4   lactic_acid            4469 non-null   float64
```

```
 5   final_gravity           4469 non-null   float64
 6   sodium                  4469 non-null   float64
 7   free_CO2                4469 non-null   float64
 8   dissolved_oxygen        4469 non-null   float64
 9   original_gravity        4469 non-null   float64
 10  pH                      4469 non-null   float64
 11  gypsum_level            4469 non-null   float64
 12  alcohol_ABV             4469 non-null   float64
 13  fermentation_strength   4469 non-null   float64
 14  quality                 4469 non-null   int64
dtypes: float64(12), int64(2), object(1)
memory usage: 523.8+ KB
None
```

### 1.3 Prétraitement des Données

Implémentez votre pipeline de prétraitement (voir README.md pour des suggestions).

[473]:
```
########################################################################
###############   À compléter   ########################################
########################################################################

# Encodage de la variable catégorielle 'beer_style'
le = LabelEncoder()
train_df['beer_style'] = le.fit_transform(train_df['beer_style'])

# La classification officiel est entre 4 et 8, on se concentre donc sur cette␣
 ↪plage compte tenu que les classes
# en dehors sont très peu représentées ou possiblement du bruit
rl_df = train_df[train_df['quality'].between(4,8)]

# ======================================== Nouvelles features␣
 ↪========================================
rl_df['gas_balance'] = rl_df['free_CO2'] / (rl_df['dissolved_oxygen'])
rl_df['mineral_strength'] = rl_df['gypsum_level'] * rl_df['sodium']
rl_df['fermentation_ratio'] = rl_df['fermentation_strength'] /␣
 ↪(rl_df['alcohol_ABV'] )
rl_df['acid_balance'] = rl_df['lactic_acid'] / (rl_df['pH']) # out
rl_df['acid_x_gas'] = rl_df['acid_balance'] * rl_df['gas_balance']
rl_df['gravity_drop'] = rl_df['original_gravity'] - rl_df['final_gravity'] #␣
 ↪out
rl_df['log_gravity_drop'] = np.log1p(rl_df['gravity_drop'].clip(lower=0))
#rl_df = rl_df.drop(columns=['bitterness_IBU','diacetyl_concentration'],␣
 ↪errors='ignore')

#======================================== Legacy features␣
 ↪========================================
```

```
# rl_df['log_final_gravity'] = np.log1p(rl_df['final_gravity']) # out
#rl_df['acid_balance'] = rl_df['lactic_acid'] / (rl_df['pH'] + 1e-5) # out
# rl_df['alcohol_efficiency'] = rl_df['alcohol_ABV'] / (rl_df['gravity_drop'] +␣
 ↪1e-5) # out
# rl_df['residual_sugar_index'] = rl_df['final_gravity'] /␣
 ↪(rl_df['original_gravity'] + 1e-5) # out
# rl_df['lactic_intensity'] = rl_df['lactic_acid'] *␣
 ↪rl_df['fermentation_strength'] # out
# rl_df['acid_x_gravity'] = rl_df['acid_balance'] * rl_df['gravity_drop'] # out
# rl_df['sqrt_alcohol_eff'] = np.sqrt(rl_df['alcohol_efficiency'].
 ↪clip(lower=0)) # out


## Visualisations
## Decommenter pour voir les corrélations entre les features et la qualité
"""
corr = train_df.corr(numeric_only=True)
sns.heatmap(corr, cmap='coolwarm', center=0)
sns.
 ↪pairplot(rl_df[['lactic_acid','pH','alcohol_ABV','final_gravity','quality']],␣
 ↪hue='quality')
plt.figure(figsize=(10,6))
sns.heatmap(rl_df[['gravity_drop','acid_balance','gas_balance','quality']].
 ↪corr(),
            annot=True, cmap='coolwarm', center=0)
plt.title("Corrélations des nouvelles features avec la qualité")
plt.show()

corr2 = rl_df[['acid_x_gas','log_gravity_drop','quality']].corr()
sns.heatmap(corr2, annot=True, cmap='coolwarm', center=0)
plt.title("Corrélations des features non linéaires avec la qualité")
plt.show()
"""

# Suppression des features à faible corrélation avec la cible et des features␣
 ↪redondantes
# Suppression des features à faible corrélation avec la cible
corr_target = rl_df.corr(numeric_only=True)['quality'].abs().
 ↪sort_values(ascending=False)
low_corr_features = corr_target[corr_target < 0.05].index
rl_df = rl_df.drop(columns=low_corr_features, errors='ignore')

# Suppression des features redondantes (corrélation > 0.9)
corr_matrix = rl_df.corr(numeric_only=True).abs()
upper_triangle = corr_matrix.where(np.triu(np.ones(corr_matrix.shape), k=1).
 ↪astype(bool))
```

```
high_corr_features = [column for column in upper_triangle.columns if␣
 ↪any(upper_triangle[column] > 0.9)]

features_to_drop = list(set(list(low_corr_features) + list(high_corr_features)))
rl_df = rl_df.drop(columns=high_corr_features, errors='ignore')
print("Features supprimées :", features_to_drop)

# Gestion des valeurs manquantes et infinies
rl_df = rl_df.replace([np.inf, -np.inf], np.nan)
rl_df = rl_df.dropna(subset=['quality'])
rl_df = rl_df.fillna(rl_df.mean())

# Préparation des données pour le modèle
if 'id' in rl_df.columns:
    rl_df =rl_df.drop(columns=['id'])

X = rl_df.drop(columns=['quality'])
y = rl_df['quality']
print('les colonnes de train_df sont :', X.columns)

# Normalisation des features



print(X.shape, y.shape)
print(f"shape finale de X : {X.shape}")
print('Distribution des classes de qualité :')
print(y.value_counts())
```

```
Features supprimées : ['gravity_drop', 'fermentation_strength', 'pH', 'id',
'final_gravity', 'beer_style', 'acid_balance', 'dissolved_oxygen']
les colonnes de train_df sont : Index(['bitterness_IBU',
'diacetyl_concentration', 'lactic_acid', 'sodium',
       'free_CO2', 'original_gravity', 'gypsum_level', 'alcohol_ABV',
       'gas_balance', 'mineral_strength', 'fermentation_ratio', 'acid_x_gas',
       'log_gravity_drop'],
      dtype='object')
(4445, 13) (4445,)
shape finale de X : (4445, 13)
Distribution des classes de qualité :
quality
6    1985
5    1496
7     755
4     116
8      93
Name: count, dtype: int64
```

```
/var/folders/y5/5rmdtyp17yz4dz_hjr0z9d600000gn/T/ipykernel_58184/851366543.py:14
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  rl_df['gas_balance'] = rl_df['free_CO2'] / (rl_df['dissolved_oxygen'])
/var/folders/y5/5rmdtyp17yz4dz_hjr0z9d600000gn/T/ipykernel_58184/851366543.py:15
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  rl_df['mineral_strength'] = rl_df['gypsum_level'] * rl_df['sodium']
/var/folders/y5/5rmdtyp17yz4dz_hjr0z9d600000gn/T/ipykernel_58184/851366543.py:16
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  rl_df['fermentation_ratio'] = rl_df['fermentation_strength'] /
(rl_df['alcohol_ABV'] )
/var/folders/y5/5rmdtyp17yz4dz_hjr0z9d600000gn/T/ipykernel_58184/851366543.py:17
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  rl_df['acid_balance'] = rl_df['lactic_acid'] / (rl_df['pH']) # out
/var/folders/y5/5rmdtyp17yz4dz_hjr0z9d600000gn/T/ipykernel_58184/851366543.py:18
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  rl_df['acid_x_gas'] = rl_df['acid_balance'] * rl_df['gas_balance']
/var/folders/y5/5rmdtyp17yz4dz_hjr0z9d600000gn/T/ipykernel_58184/851366543.py:19
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
```

```
  rl_df['gravity_drop'] = rl_df['original_gravity'] - rl_df['final_gravity'] #
out
/var/folders/y5/5rmdtyp17yz4dz_hjr0z9d600000gn/T/ipykernel_58184/851366543.py:20
: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame.
Try using .loc[row_indexer,col_indexer] = value instead

See the caveats in the documentation: https://pandas.pydata.org/pandas-
docs/stable/user_guide/indexing.html#returning-a-view-versus-a-copy
  rl_df['log_gravity_drop'] = np.log1p(rl_df['gravity_drop'].clip(lower=0))
```

### 1.4 Préparer les Données d'Entraînement et de Validation

Divisez vos données en ensembles d'entraînement et de validation.

[474]:
```
######################################################################
###############   À compléter   ####################################
######################################################################
print(y.value_counts())

scaler = StandardScaler()

X_scaled = scaler.fit_transform(X)

X_train, X_val, y_train, y_val = train_test_split(X_scaled, y, test_size = 0.2,␣
 ↪stratify=y,random_state=42)
```

```
quality
6    1985
5    1496
7     755
4     116
8      93
Name: count, dtype: int64
```

### 1.5 Entraîner les Modèles

Entraînez et comparez plusieurs modèles d'apprentissage automatique.

[475]:
```
"""
def knnModel():
    for k in range(1, 100):
        model = KNeighborsClassifier(n_neighbors=k)
        model.fit(X_train, y_train)
        y_pred = model.predict(X_val)
        print(f"k={k}, accuracy={accuracy_score(y_val, y_pred):.4f}")

    knn = KNeighborsClassifier(
        n_neighbors=27,
```

```
        weights='distance',
        metric='euclidean'
    )

    knn.fit(X_train, y_train)
    {'class_weight': 'balanced', 'max_depth': 10, 'min_samples_split': 2,␣
 ↪'n_estimators': 50}

"""
```

[475]:
```
'\ndef knnModel():\n    for k in range(1, 100):\n        model =
KNeighborsClassifier(n_neighbors=k)\n        model.fit(X_train, y_train)\n
y_pred = model.predict(X_val)\n        print(f"k={k},
accuracy={accuracy_score(y_val, y_pred):.4f}")\n\n    knn =
KNeighborsClassifier(\n        n_neighbors=27,\n        weights=\'distance\',\n
metric=\'euclidean\'\n    )\n\n    knn.fit(X_train, y_train)\n
{\'class_weight\': \'balanced\', \'max_depth\': 10, \'min_samples_split\': 2,
\'n_estimators\': 50}\n\n'
```

[476]:
```
rf = RandomForestClassifier(
    n_estimators=50,
    max_depth=10,
    class_weight='balanced',
    min_samples_split=2,
    random_state=42)
rf.fit(X_train, y_train)
```

[476]:
```
RandomForestClassifier(class_weight='balanced', max_depth=10, n_estimators=50,
                       random_state=42)
```

[477]:
```
Class_weight_manual = {4: 22.0, 5: 0.1, 6: 0.1, 7: 3.0, 8: 25.0}

svm = SVC(C=50.0,
        kernel='rbf',
        gamma=0.1,
        class_weight=Class_weight_manual,
        random_state=42
        )

svm.fit(X_train, y_train)
```

[477]:
```
SVC(C=50.0, class_weight={4: 22.0, 5: 0.1, 6: 0.1, 7: 3.0, 8: 25.0}, gamma=0.1,
    random_state=42)
```

[478]:
```
#######################################################################
###############   À compléter   ######################################
#######################################################################
```

```
# Logistic Regression Model

log_reg = LogisticRegression(
    multi_class='multinomial',
    solver='lbfgs',
    C=1.0,
    max_iter=100000,
    class_weight='balanced'
)

log_reg.fit(X_train, y_train)
```

```
/Users/yamira.poldosilva/Documents/UDEM/A25/IFT3395/kaggle_beer_comp/.venv/lib/p
ython3.13/site-packages/sklearn/linear_model/_logistic.py:1272: FutureWarning:
'multi_class' was deprecated in version 1.5 and will be removed in 1.8. From
then on, it will always use 'multinomial'. Leave it to its default value to
avoid this warning.
  warnings.warn(
```

[478]:
```
LogisticRegression(class_weight='balanced', max_iter=100000,
                   multi_class='multinomial')
```

### 1.6 Évaluer les Modèles

Analysez la performance de votre meilleur modèle (voir README.md pour les directives d'évaluation).

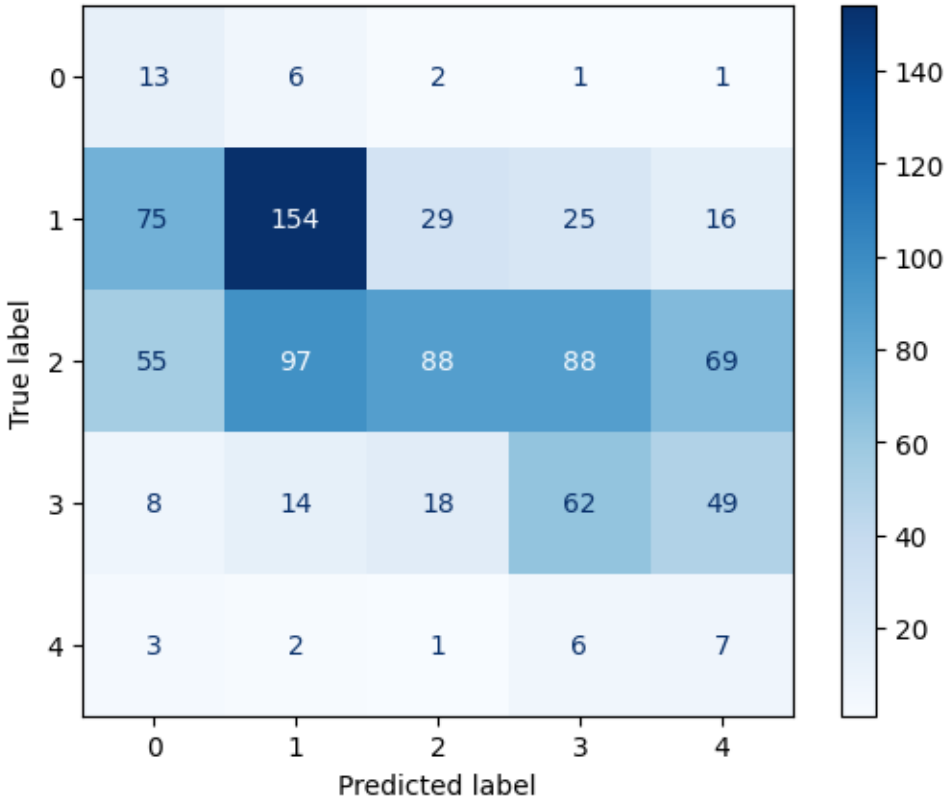
[479]:
```
########################################################################
###############   À compléter   ########################################
########################################################################
from sklearn.metrics import ConfusionMatrixDisplay
y_pred = log_reg.predict(X_val)
print("Exactitude:", accuracy_score(y_val,y_pred))
print(classification_report(y_val, y_pred))

cm = confusion_matrix(y_val, y_pred)
disp = ConfusionMatrixDisplay(confusion_matrix=cm)
disp.plot(cmap='Blues')
plt.show()
```

```
Exactitude: 0.3644544431946007
              precision    recall  f1-score   support

           4       0.08      0.57      0.15        23
           5       0.56      0.52      0.54       299
           6       0.64      0.22      0.33       397
           7       0.34      0.41      0.37       151
           8       0.05      0.37      0.09        19
```

```
              accuracy                           0.36       889
             macro avg       0.34      0.42      0.29       889
          weighted avg       0.54      0.36      0.40       889
```




### 1.7 Générer les Prédictions pour la Soumission Kaggle

Créez un fichier CSV avec les colonnes : `id` et `quality` (voir README.md pour les détails du format).

[480]:
```
##########################################################################
###############   À compléter   ##########################################
##########################################################################

# Charger les données de test
test_df = pd.read_csv("data/test.csv", sep=";")

# Encodage du style avec le même LabelEncoder
test_df['beer_style'] = le.transform(test_df['beer_style'])
```

```
# Créer les mêmes features dérivées
test_df['gravity_drop'] = test_df['original_gravity'] - test_df['final_gravity']
# test_df['log_final_gravity'] = np.log1p(test_df['final_gravity'])
test_df['acid_balance'] = test_df['lactic_acid'] / (test_df['pH'] + 1e-5)
test_df['gas_balance'] = test_df['free_CO2'] / (test_df['dissolved_oxygen'] +␣
 ↪1e-5)
test_df['mineral_strength'] = test_df['gypsum_level'] * test_df['sodium']
# test_df['alcohol_efficiency'] = test_df['alcohol_ABV'] /␣
 ↪(test_df['gravity_drop'] + 1e-5)
# test_df['residual_sugar_index'] = test_df['final_gravity'] /␣
 ↪(test_df['original_gravity'] + 1e-5)
test_df['fermentation_ratio'] = test_df['fermentation_strength'] /␣
 ↪(test_df['alcohol_ABV'] + 1e-5)
# test_df['lactic_intensity'] = test_df['lactic_acid'] *␣
 ↪test_df['fermentation_strength']
test_df['acid_x_gas'] = test_df['acid_balance'] * test_df['gas_balance']
# test_df['acid_x_gravity'] = test_df['acid_balance'] * test_df['gravity_drop']
test_df['log_gravity_drop'] = np.log1p(test_df['gravity_drop'].clip(lower=0))
# test_df['sqrt_alcohol_eff'] = np.sqrt(test_df['alcohol_efficiency'].
 ↪clip(lower=0))

test_df = test_df.replace([np.inf, -np.inf], np.nan)
test_df = test_df.fillna(test_df.mean())

# Sauvegarde de l'id pour la soumission
ids = test_df['id']
X_test = test_df.drop(columns=['id'])

# Assurer que les colonnes du test correspondent à celles du train
for col in X.columns:
    if col not in X_test.columns:
        test_df[col] = 0
X_test = test_df[X.columns]
print('les colonnes:', X_test.columns)
X_test_scaled = scaler.transform(X_test)


# Prédiction sur le test set
y_pred = log_reg.predict(X_test_scaled)

print("Test shape:", X_test_scaled.shape)

submission = pd.DataFrame({
    'id': ids,
    'quality': y_pred.astype(int)
})
```

```python
# Sauvegarde
submission.to_csv("ift3395_YamirPoldoSilvaV6.csv", index=False)

print(submission.head())

df1 = pd.read_csv("ift3395_YamirPoldoSilvaV6.csv")
df2 = pd.read_csv("ift3395_YamirPoldoSilvaV4.csv")

comparison = df1.compare(df2)
print(comparison)
```

```
les colonnes: Index(['bitterness_IBU', 'diacetyl_concentration', 'lactic_acid',
'sodium',
       'free_CO2', 'original_gravity', 'gypsum_level', 'alcohol_ABV',
       'gas_balance', 'mineral_strength', 'fermentation_ratio', 'acid_x_gas',
       'log_gravity_drop'],
      dtype='object')
Test shape: (511, 13)
   id  quality
0   0        5
1   1        5
2   2        7
3   3        7
4   4        8
Empty DataFrame
Columns: []
Index: []
```

---

Bonne chance pour la compétition !