AI-CA3

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1 AI - CA3 - Machine Learning

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1.1.1 Data preprocessing and feature engineering

[1]:
```
import pandas as pd
import numpy as np
from sklearn.impute import KNNImputer
from sklearn.preprocessing import LabelEncoder
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.naive_bayes import GaussianNB
from sklearn.metrics import classification_report, confusion_matrix,␣
 ↪accuracy_score
from sklearn.tree import DecisionTreeClassifier, plot_tree
import matplotlib.pyplot as plt
from sklearn.ensemble import RandomForestClassifier
from sklearn.model_selection import RandomizedSearchCV
from xgboost import XGBClassifier
from sklearn.model_selection import GridSearchCV
import warnings
from collections import Counter
```

Column deletion We will remove columns with: - Too many missing values. - Irrelevant information (e.g., IDs, duplicate columns, or columns with the same value for all rows).

[2]:
```
df = pd.read_csv('Grades.csv')
missing = df.isnull().sum()
print("Missing values per column:\n", missing)
```

```
Missing values per column:
 university          0
sex                 0
age                 0
address             0
motherEducation     0
fatherEducation     0
```

```
motherJob           0
fatherJob           0
reason              0
travelTime          0
studyTime           0
failures            0
universitySupport   0
paid                0
higher              0
internet            0
romantic            0
freeTime            0
goOut               0
Dalc                0
Walc                0
absences            0
EPSGrade            0
DSGrade             0
finalGrade          0
dtype: int64
```

As we can see, we don't have missing values in any of the columns and we don't have any columns with irrelevant information. So there's no need to delete any columns.

Filling missing data

Numerical columns:

- Mean Imputation: Replacing missing values with the mean.
- Median Imputation: Replacing missing values with the median.
- KNN Imputation: Using KNN to estimate missing values.

Categorical columns:

- Mode Imputation: Replacing missing values with the most frequent value.
- Constant Imputation: Replacing missing values with a constant (e.g., 'Unknown').
- KNN Imputation: Using KNN for categorical data as well.

Again, as we can see, we have no missing values and there is no need to make any changes in this section.

Extract Numeric Data from Text Columns Since the numeric data is only in the form of numbers in the dataset, there is no need to do this.

Convert Categorical Data to Numeric

- Using Label Encoding for ordinal data.
- Using One-Hot Encoding for nominal data.

We will use Label Encoding.

[3]:
```python
cat_cols = df.select_dtypes(include=['object']).columns
df_updated = df.copy()

label_encoders = {}
for col in cat_cols:
    le = LabelEncoder()
    df_updated[col] = le.fit_transform(df_updated[col].astype(str))
    label_encoders[col] = le

print("Categorical columns after encoding:\n", df_updated[cat_cols])
```

```
Categorical columns after encoding:
      university  sex  address  motherJob  fatherJob  reason  \
0             1    0        1          0          4       0
1             1    0        1          0          2       0
2             1    0        1          0          2       2
3             1    0        1          1          3       1
4             1    0        1          2          2       1
..          …   …       …         …          …      …
392           0    1        0          2          2       0
393           0    1        0          3          2       0
394           0    1        1          2          0       0
395           1    0        1          0          4       0
396           0    1        0          2          3       2

     universitySupport  paid  higher  internet  romantic
0                    1     0       1         0         0
1                    0     0       1         1         0
2                    1     1       1         1         0
3                    0     1       1         1         1
4                    0     1       1         0         0
..                 …    …      …         …         …
392                  0     0       1         0         0
393                  0     0       1         1         0
394                  0     0       1         1         0
395                  1     0       1         0         0
396                  0     0       1         0         0

[397 rows x 11 columns]
```

Create classes for grades

- A: Above 17
- B: Between 14 and 17
- C: Between 10 and 14
- D: Under 10

[4]:
```python
def grade_to_class(grade):
    if grade > 17:
        return 'A'
    elif grade >= 14:
        return 'B'
    elif grade >= 10:
        return 'C'
    else:
        return 'D'

df_updated['finalGradeClass'] = df_updated['finalGrade'].apply(grade_to_class)
print(df_updated[['finalGrade', 'finalGradeClass']].head())
```

```
   finalGrade finalGradeClass
0           6               D
1           6               D
2          10               C
3          15               B
4          10               C
```

1.1.2 Development, training and evaluation of models

Train-Test split

[5]:
```python
X = df_updated.drop(['finalGrade', 'finalGradeClass'], axis=1)
y = df_updated['finalGradeClass']

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

print("Train shape:", X_train.shape)
print("Test shape:", X_test.shape)
print("Train class distribution:\n", y_train.value_counts())
print("Test class distribution:\n", y_test.value_counts())
```

```
Train shape: (317, 24)
Test shape: (80, 24)
Train class distribution:
 finalGradeClass
C    132
D    105
B     66
A     14
Name: count, dtype: int64
Test class distribution:
 finalGradeClass
C    33
D    27
```

```
B     16
A      4
Name: count, dtype: int64
```

Normalization / Standardization `StandardScaler()` from scikit-learn standardizes features by removing the mean and scaling to unit variance.

`z = (x - mean) / std`

[6]:
```
num_cols = X_train.select_dtypes(include=[np.number]).columns
scaler = StandardScaler()
X_train[num_cols] = scaler.fit_transform(X_train[num_cols])
X_test[num_cols] = scaler.transform(X_test[num_cols])
```

Sklearn Models

Naive Bayes

[7]:
```
nb_model = GaussianNB()
nb_model.fit(X_train, y_train)

y_pred = nb_model.predict(X_test)

print("Naive Bayes Accuracy:", accuracy_score(y_test, y_pred))
print("\nClassification Report:\n", classification_report(y_test, y_pred))
print("\nConfusion Matrix:\n", confusion_matrix(y_test, y_pred))
```

```
Naive Bayes Accuracy: 0.575

Classification Report:
               precision    recall  f1-score   support

           A       0.23      0.75      0.35         4
           B       0.27      0.38      0.32        16
           C       0.87      0.39      0.54        33
           D       0.80      0.89      0.84        27

    accuracy                           0.57        80
   macro avg       0.54      0.60      0.51        80
weighted avg       0.69      0.57      0.59        80


Confusion Matrix:
 [[ 3  1  0  0]
 [10  6  0  0]
 [ 0 14 13  6]
 [ 0  1  2 24]]
```

Decision Tree

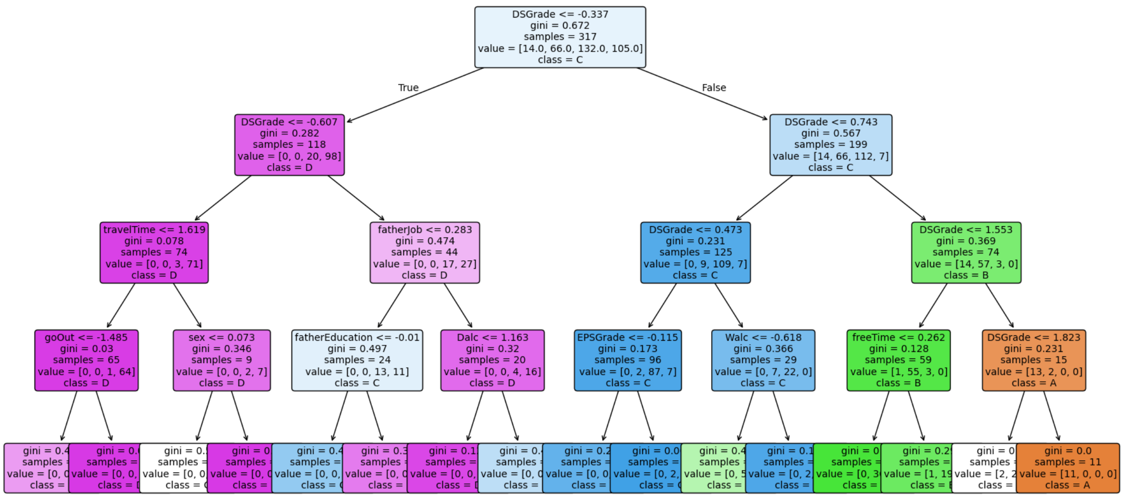
[8]:
```
dt_model = DecisionTreeClassifier(
    max_depth=4,
    min_samples_leaf=3,
    random_state=42
)
dt_model.fit(X_train, y_train)

y_pred_dt = dt_model.predict(X_test)

print("Decision Tree Accuracy:", accuracy_score(y_test, y_pred_dt))
print("\nClassification Report:\n", classification_report(y_test, y_pred_dt))
print("\nConfusion Matrix:\n", confusion_matrix(y_test, y_pred_dt))

plt.figure(figsize=(20,10))
plot_tree(
    dt_model,
    feature_names=X_train.columns,
    class_names=dt_model.classes_,
    filled=True,
    rounded=True,
    fontsize=10
)
plt.title("Decision Tree visualization")
plt.show()

importances = dt_model.feature_importances_
feature_importance_df = pd.DataFrame({
    'feature': X_train.columns,
    'importance': importances
}).sort_values(by='importance', ascending=False)

print("\nFeature importances:")
print(feature_importance_df)
```

```
Decision Tree Accuracy: 0.8875

Classification Report:
               precision    recall  f1-score   support

           A       0.80      1.00      0.89         4
           B       0.93      0.88      0.90        16
           C       0.86      0.91      0.88        33
           D       0.92      0.85      0.88        27

    accuracy                           0.89        80
   macro avg       0.88      0.91      0.89        80
```

```
weighted avg       0.89      0.89      0.89        80
```

```
Confusion Matrix:
 [[ 4  0  0  0]
 [ 1 14  1  0]
 [ 0  1 30  2]
 [ 0  0  4 23]]
```

Decision Tree visualization




```
Feature importances:
              feature  importance
23            DSGrade    0.912784
20               Walc    0.019854
7           fatherJob    0.015552
19               Dalc    0.013026
5     fatherEducation    0.012466
22           EPSGrade    0.007309
1                 sex    0.006784
17           freeTime    0.004212
9          travelTime    0.004130
18              goOut    0.003883
14             higher    0.000000
21           absences    0.000000
16           romantic    0.000000
15           internet    0.000000
0          university    0.000000
13               paid    0.000000
11           failures    0.000000
```

```
10          studyTime    0.000000
8              reason    0.000000
6           motherJob    0.000000
4     motherEducation    0.000000
3             address    0.000000
2                 age    0.000000
12  universitySupport    0.000000
```

As we can see, DSGrade is the most important feature and has a huge impact by far.

Random Forest

[9]:
```
param_dist = {
    'n_estimators': [50, 100, 200],
    'max_depth': [None, 4, 6, 8, 10],
    'min_samples_split': [2, 3, 4, 5],
    'min_samples_leaf': [1, 2, 3, 4],
    'max_features': ['sqrt', 'log2']
}

rf = RandomForestClassifier(random_state=42)

rf_search = RandomizedSearchCV(
    rf, param_distributions=param_dist,
    n_iter=20, cv=3, scoring='accuracy', random_state=42, n_jobs=-1
)
rf_search.fit(X_train, y_train)

best_rf = rf_search.best_estimator_

y_pred_rf = best_rf.predict(X_test)

print("Random Forest Accuracy:", accuracy_score(y_test, y_pred_rf))
print("\nClassification Report:\n", classification_report(y_test, y_pred_rf))
print("\nConfusion Matrix:\n", confusion_matrix(y_test, y_pred_rf))
print("\nBest Hyperparameters:", rf_search.best_params_)

rf_importances = best_rf.feature_importances_
rf_feature_importance_df = pd.DataFrame({
    'feature': X_train.columns,
    'importance': rf_importances
}).sort_values(by='importance', ascending=False)

print("\nFeature importances:")
print(rf_feature_importance_df)
```

```
Random Forest Accuracy: 0.8625

Classification Report:
```

```
              precision    recall  f1-score   support

           A       1.00      1.00      1.00         4
           B       0.87      0.81      0.84        16
           C       0.84      0.82      0.83        33
           D       0.86      0.93      0.89        27

    accuracy                           0.86        80
   macro avg       0.89      0.89      0.89        80
weighted avg       0.86      0.86      0.86        80


Confusion Matrix:
 [[ 4  0  0  0]
 [ 0 13  3  0]
 [ 0  2 27  4]
 [ 0  0  2 25]]

Best Hyperparameters: {'n_estimators': 100, 'min_samples_split': 2,
'min_samples_leaf': 1, 'max_features': 'log2', 'max_depth': 10}

Feature importances:
              feature  importance
23            DSGrade    0.338656
22           EPSGrade    0.191099
21           absences    0.050771
20               Walc    0.035382
4     motherEducation    0.032891
2                 age    0.030135
11           failures    0.029782
18              goOut    0.028095
7           fatherJob    0.027049
17           freeTime    0.026691
10          studyTime    0.025091
6           motherJob    0.024596
5     fatherEducation    0.024263
8              reason    0.023090
19               Dalc    0.017858
9          travelTime    0.017351
12  universitySupport    0.014427
13               paid    0.012761
1                 sex    0.012402
16           romantic    0.010860
3             address    0.010839
15           internet    0.006589
0          university    0.004702
14             higher    0.004620
```

As we can see, DSGrade is still the most important feature, but this time its difference from other features is less.

XGBoost

[10]:
```
warnings.filterwarnings('ignore', category=UserWarning, module='xgboost')

param_grid = {
    'learning_rate': [0.01, 0.05, 0.1],
    'n_estimators': [50, 100, 200],
    'max_depth': [3, 4, 6, 8],
    'min_child_weight': [1, 2, 3],  # min_child_weight instead of␣
 ↪min_samples_leaf
    'min_split_loss': [0, 1, 2],    # min_split_loss instead of␣
 ↪min_samples_split
    'max_leaves': [0, 5, 10],
    'colsample_bytree': [0.8, 1.0], # colsample_bytree instead of max_features
}

le_y = LabelEncoder()
y_train_xgb = le_y.fit_transform(y_train)
y_test_xgb = le_y.transform(y_test)

xgb = XGBClassifier(
    objective='multi:softmax',
    num_class=len(le_y.classes_),
    use_label_encoder=False,
    eval_metric='mlogloss',
    random_state=42
)

xgb_search = GridSearchCV(
    xgb, param_grid=param_grid,
    cv=3, scoring='accuracy', n_jobs=-1
)
xgb_search.fit(X_train, y_train_xgb)

best_xgb = xgb_search.best_estimator_
y_pred_xgb = best_xgb.predict(X_test)

y_pred_xgb_labels = le_y.inverse_transform(y_pred_xgb)

print("XGBoost Accuracy:", accuracy_score(y_test, y_pred_xgb_labels))
print("\nClassification Report:\n", classification_report(y_test,␣
 ↪y_pred_xgb_labels))
print("\nConfusion Matrix:\n", confusion_matrix(y_test, y_pred_xgb_labels))
print("\nBest Hyperparameters:", xgb_search.best_params_)
```

```
XGBoost Accuracy: 0.8875

Classification Report:
               precision    recall  f1-score   support

           A       0.80      1.00      0.89         4
           B       1.00      0.75      0.86        16
           C       0.86      0.91      0.88        33
           D       0.89      0.93      0.91        27

    accuracy                           0.89        80
   macro avg       0.89      0.90      0.88        80
weighted avg       0.89      0.89      0.89        80


Confusion Matrix:
 [[ 4  0  0  0]
 [ 1 12  3  0]
 [ 0  0 30  3]
 [ 0  0  2 25]]

Best Hyperparameters: {'colsample_bytree': 0.8, 'learning_rate': 0.05,
'max_depth': 6, 'max_leaves': 0, 'min_child_weight': 2, 'min_split_loss': 1,
'n_estimators': 100}
```

Decision Tree from Scratch

[11]:
```
class DecisionTreeScratch:
    def __init__(self, max_depth=4, min_samples_split=2):
        self.max_depth = max_depth
        self.min_samples_split = min_samples_split
        self.tree = None

    def _entropy(self, y):
        counts = np.bincount(y)
        probabilities = counts / len(y)
        return -np.sum([p * np.log2(p) for p in probabilities if p > 0])

    def _best_split(self, X, y):
        best_gain = 0
        best_feature = None
        best_threshold = None
        n_features = X.shape[1]
        current_entropy = self._entropy(y)
        for feature in range(n_features):
            thresholds = np.unique(X[:, feature])
            for threshold in thresholds:
                left_mask = X[:, feature] <= threshold
```

```
                right_mask = X[:, feature] > threshold
                if np.sum(left_mask) == 0 or np.sum(right_mask) == 0:
                    continue
                left_entropy = self._entropy(y[left_mask])
                right_entropy = self._entropy(y[right_mask])
                n = len(y)
                n_left = np.sum(left_mask)
                n_right = np.sum(right_mask)
                weighted_entropy = (n_left / n) * left_entropy + (n_right / n)␣
↪* right_entropy
                info_gain = current_entropy - weighted_entropy
                if info_gain > best_gain:
                    best_gain = info_gain
                    best_feature = feature
                    best_threshold = threshold
        return best_feature, best_threshold

    def _build_tree(self, X, y, depth):
        num_samples, num_features = X.shape
        num_labels = len(np.unique(y))

        if (depth >= self.max_depth or num_labels == 1 or num_samples < self.
↪min_samples_split):
            leaf_value = Counter(y).most_common(1)[0][0]
            return {'type': 'leaf', 'class': leaf_value}

        feature, threshold = self._best_split(X, y)
        if feature is None:
            leaf_value = Counter(y).most_common(1)[0][0]
            return {'type': 'leaf', 'class': leaf_value}

        left_mask = X[:, feature] <= threshold
        right_mask = X[:, feature] > threshold

        left_subtree = self._build_tree(X[left_mask], y[left_mask], depth + 1)
        right_subtree = self._build_tree(X[right_mask], y[right_mask], depth +␣
↪1)

        return {
            'type': 'node',
            'feature': feature,
            'threshold': threshold,
            'left': left_subtree,
            'right': right_subtree
        }

    def fit(self, X, y):
```

```
        if not np.issubdtype(y.dtype, np.integer):
            classes, y = np.unique(y, return_inverse=True)
            self.classes_ = classes
        else:
            self.classes_ = np.unique(y)
        self.tree = self._build_tree(np.array(X), np.array(y), 0)

    def _predict_one(self, x, node):
        if node['type'] == 'leaf':
            return node['class']
        if x[node['feature']] <= node['threshold']:
            return self._predict_one(x, node['left'])
        else:
            return self._predict_one(x, node['right'])

    def predict(self, X):
        X = np.array(X)
        preds = [self._predict_one(x, self.tree) for x in X]
        if hasattr(self, 'classes_') and not np.issubdtype(self.classes_.dtype,␣
 ↪np.integer):
            preds = [self.classes_[i] for i in preds]
        return np.array(preds)

dt_scratch = DecisionTreeScratch(max_depth=4)
dt_scratch.fit(X_train, y_train)
y_pred = dt_scratch.predict(X_test)

print("DTFS Accuracy:", accuracy_score(y_test, y_pred))
print("\nClassification Report:\n", classification_report(y_test, y_pred))
print("\nConfusion Matrix:\n", confusion_matrix(y_test, y_pred))
```

```
DTFS Accuracy: 0.8625

Classification Report:
               precision    recall  f1-score   support

           A       0.80      1.00      0.89         4
           B       1.00      0.69      0.81        16
           C       0.85      0.85      0.85        33
           D       0.84      0.96      0.90        27

    accuracy                           0.86        80
   macro avg       0.87      0.87      0.86        80
weighted avg       0.87      0.86      0.86        80


Confusion Matrix:
```

```
[[ 4  0  0  0]
 [ 1 11  4  0]
 [ 0  0 28  5]
 [ 0  0  1 26]]
```

Decision Tree from Scratch (Library implementation)

[12]:
```python
sk_dt = DecisionTreeClassifier(max_depth=4, min_samples_leaf=2, random_state=42)
sk_dt.fit(X_train, y_train)
y_pred_sk = sk_dt.predict(X_test)

print("Scikit-learn Decision Tree Accuracy:", accuracy_score(y_test, y_pred_sk))
print("\nClassification Report:\n", classification_report(y_test, y_pred_sk))
print("\nConfusion Matrix:\n", confusion_matrix(y_test, y_pred_sk))
```

```
Scikit-learn Decision Tree Accuracy: 0.8875

Classification Report:
               precision    recall  f1-score   support

           A       0.80      1.00      0.89         4
           B       0.93      0.88      0.90        16
           C       0.86      0.91      0.88        33
           D       0.92      0.85      0.88        27

    accuracy                           0.89        80
   macro avg       0.88      0.91      0.89        80
weighted avg       0.89      0.89      0.89        80


Confusion Matrix:
 [[ 4  0  0  0]
 [ 1 14  1  0]
 [ 0  1 30  2]
 [ 0  0  4 23]]
```

As we can see, the version implemented by the library is more accurate.

We can use manual implementation to learn and demonstrate the algorithm, and use scikit-learn for real data analysis, better performance, and more features.