Preprocessing data

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scikit-learn requirements

- Numeric data
- No missing values

- With real-world data:
  - This is rarely the case
  - We will often need to preprocess our data first

Dealing with categorical features

- scikit-learn will not accept categorical features by default
- Need to convert categorical features into numeric values
- Convert to binary features called dummy variables
  - 0: Observation was NOT that category
  - 1: Observation was that category

Dummy variables

genre
Alternative
Anime
Blues
Classical
Country
Electronic
Hip-Hop
Jazz
Rap
Rock

Dummy variables

genre
Alternative
Anime
Blues
Classical
Country
Electronic
Hip-Hop
Jazz
Rap
Rock

Alternative	Anime	Blues	Classical	Country	Electronic	Hip-Hop	Jazz	Rap	Rock
1	0	0	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0	0
0	0	0	1	0	0	0	0	0	0
0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0
0	0	0	0	0	0	1	0	0	0
0	0	0	0	0	0	0	1	0	0
0	0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	0	0	1

Dummy variables

genre
Alternative
Anime
Blues
Classical
Country
Electronic
Hip-Hop
Jazz
Rap
Rock

Alternative	Anime	Blues	Classical	Country	Electronic	Hip-Hop	Jazz	Rap
1	0	0	0	0	0	0	0	0
0	1	0	0	0	0	0	0	0
0	0	1	0	0	0	0	0	0
0	0	0	1	0	0	0	0	0
0	0	0	0	1	0	0	0	0
0	0	0	0	0	1	0	0	0
0	0	0	0	0	0	1	0	0
0	0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	0	1
0	0	0	0	0	0	0	0	0

Dealing with categorical features in Python

- scikit-learn: `OneHotEncoder()`
- pandas: `get_dummies()`

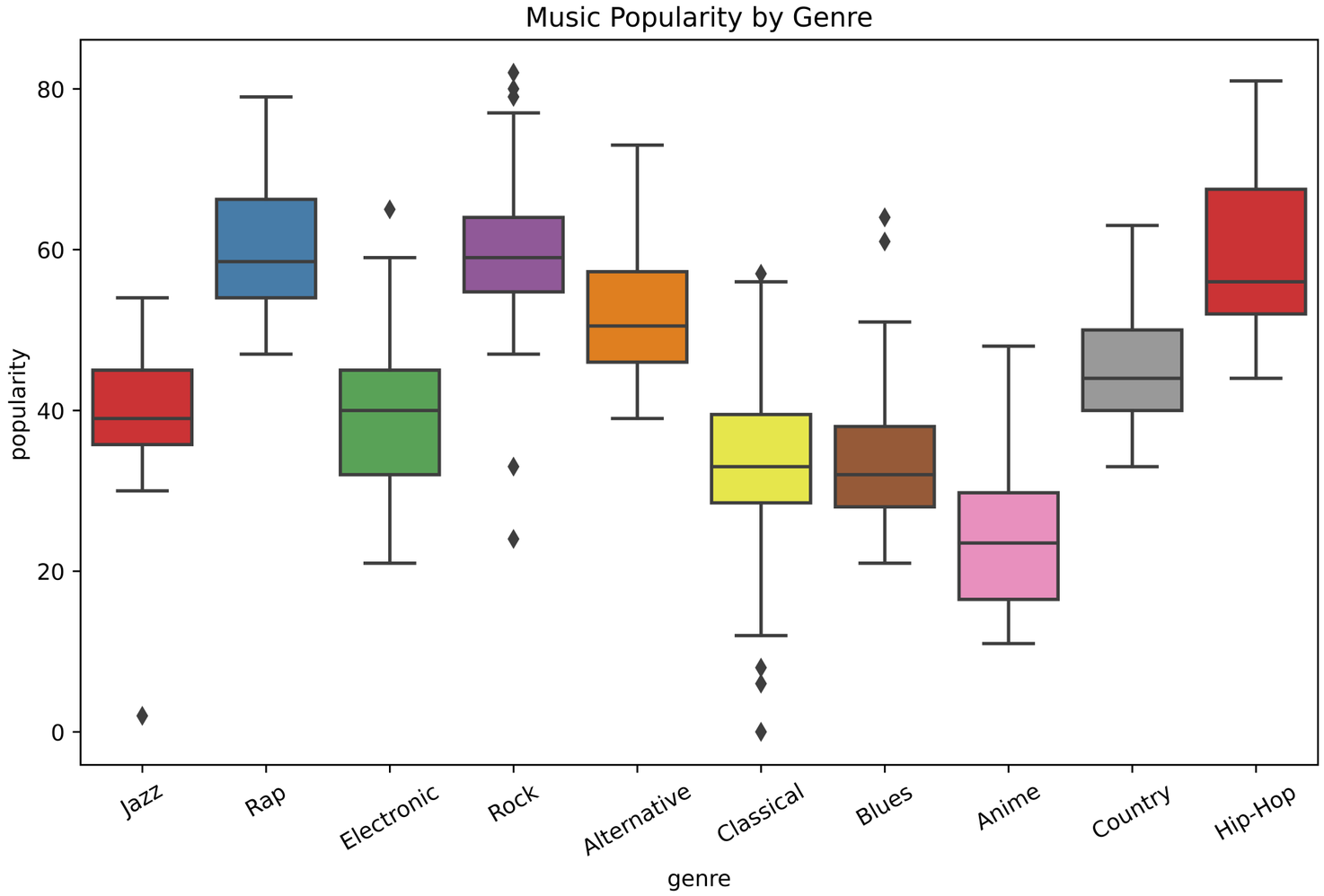
Music dataset

- `popularity` : Target variable
- `genre` : Categorical feature

```
print(music.info())
```

```
    popularity    acousticness    danceability    ...    tempo         valence    genre
0   41.0          0.6440          0.823           ...    102.619000    0.649      Jazz
1   62.0          0.0855          0.686           ...    173.915000    0.636      Rap
2   42.0          0.2390          0.669           ...    145.061000    0.494      Electronic
3   64.0          0.0125          0.522           ...    120.406497    0.595      Rock
4   60.0          0.1210          0.780           ...    96.056000     0.312      Rap
```

EDA w/ categorical feature



Encoding dummy variables

```
import pandas as pd
music_df = pd.read_csv('music.csv')
music_dummies = pd.get_dummies(music_df["genre"], drop_first=True)
print(music_dummies.head())
```

```
   Anime  Blues  Classical  Country  Electronic  Hip-Hop  Jazz  Rap  Rock
0      0      0          0        0           0        0     1    0     0
1      0      0          0        0           0        0     0    1     0
2      0      0          0        0           1        0     0    0     0
3      0      0          0        0           0        0     0    0     1
4      0      0          0        0           0        0     0    1     0
```

```
music_dummies = pd.concat([music_df, music_dummies], axis=1)
music_dummies = music_dummies.drop("genre", axis=1)
```

Encoding dummy variables

```
music_dummies = pd.get_dummies(music_df, drop_first=True)
print(music_dummies.columns)
```

```
Index(['popularity', 'acousticness', 'danceability', 'duration_ms', 'energy',
       'instrumentalness', 'liveness', 'loudness', 'speechiness', 'tempo',
       'valence', 'genre_Anime', 'genre_Blues', 'genre_Classical',
       'genre_Country', 'genre_Electronic', 'genre_Hip-Hop', 'genre_Jazz',
       'genre_Rap', 'genre_Rock'],
      dtype='object')
```

Linear regression with dummy variables

```
from sklearn.model_selection import cross_val_score, KFold
from sklearn.linear_model import LinearRegression
X = music_dummies.drop("popularity", axis=1).values
y = music_dummies["popularity"].values
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
                                                    random_state=42)
kf = KFold(n_splits=5, shuffle=True, random_state=42)
linreg = LinearRegression()
linreg_cv = cross_val_score(linreg, X_train, y_train, cv=kf,
                            scoring="neg_mean_squared_error")
print(np.sqrt(-linreg_cv))
```

```
[8.15792932, 8.63117538, 7.52275279, 8.6205778, 7.91329988]
```

Let's practice!

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Handling missing data

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Missing data

- No value for a feature in a particular row
- This can occur because:
  - There may have been no observation
  - The data might be corrupt
- We need to deal with missing data

Music dataset

```
print(music_df.isna().sum().sort_values())
```

```
genre                8
popularity          31
loudness            44
liveness            46
tempo               46
speechiness         59
duration_ms         91
instrumentalness    91
danceability       143
valence            143
acousticness       200
energy             200
dtype: int64
```

Dropping missing data

```
music_df = music_df.dropna(subset=["genre", "popularity", "loudness", "liveness", "tempo"])
print(music_df.isna().sum().sort_values())
```

```
popularity           0
liveness             0
loudness             0
tempo                0
genre                0
duration_ms         29
instrumentalness    29
speechiness         53
danceability       127
valence            127
acousticness       178
energy             178
dtype: int64
```

Imputing values

- Imputation - use subject-matter expertise to replace missing data with educated guesses
- Common to use the mean
- Can also use the median, or another value
- For categorical values, we typically use the most frequent value - the mode
- Must split our data first, to avoid *data leakage*

Imputation with scikit-learn

```
from sklearn.impute import SimpleImputer
X_cat = music_df["genre"].values.reshape(-1, 1)
X_num = music_df.drop(["genre", "popularity"], axis=1).values
y = music_df["popularity"].values
X_train_cat, X_test_cat, y_train, y_test = train_test_split(X_cat, y, test_size=0.2,
                                                            random_state=12)
X_train_num, X_test_num, y_train, y_test = train_test_split(X_num, y, test_size=0.2,
                                                            random_state=12)
imp_cat = SimpleImputer(strategy="most_frequent")
X_train_cat = imp_cat.fit_transform(X_train_cat)
X_test_cat = imp_cat.transform(X_test_cat)
```

Imputation with scikit-learn

```
imp_num = SimpleImputer()
X_train_num = imp_num.fit_transform(X_train_num)
X_test_num = imp_num.transform(X_test_num)
X_train = np.append(X_train_num, X_train_cat, axis=1)
X_test = np.append(X_test_num, X_test_cat, axis=1)
```

- Imputers are known as transformers

Imputing within a pipeline

```
from sklearn.pipeline import Pipeline
music_df = music_df.dropna(subset=["genre", "popularity", "loudness", "liveness", "tempo"])
music_df["genre"] = np.where(music_df["genre"] == "Rock", 1, 0)
X = music_df.drop("genre", axis=1).values
y = music_df["genre"].values
```

Imputing within a pipeline

```
steps = [("imputation", SimpleImputer()),
         ("logistic_regression", LogisticRegression())]
pipeline = Pipeline(steps)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
                                                    random_state=42)
pipeline.fit(X_train, y_train)
pipeline.score(X_test, y_test)
```

```
0.7593582887700535
```

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Centering and scaling

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Why scale our data?

```
print(music_df[["duration_ms", "loudness", "speechiness"]].describe())
```

```
       duration_ms     loudness      speechiness
count    1.000000e+03  1000.000000  1000.000000
mean     2.176493e+05    -8.284354     0.078642
std      1.137703e+05     5.065447     0.088291
min     -1.000000e+00   -38.718000     0.023400
25%      1.831070e+05    -9.658500     0.033700
50%      2.176493e+05    -7.033500     0.045000
75%      2.564468e+05    -5.034000     0.078642
max      1.617333e+06    -0.883000     0.710000
```

Why scale our data?

- Many models use some form of distance to inform them
- Features on larger scales can disproportionately influence the model
- Example: KNN uses distance explicitly when making predictions
- We want features to be on a similar scale
- Normalizing or standardizing (scaling and centering)

How to scale our data

- Subtract the mean and divide by variance
  - All features are centered around zero and have a variance of one
  - This is called **standardization**
- Can also subtract the minimum and divide by the range
  - Minimum zero and maximum one
- Can also *normalize* so the data ranges from -1 to +1
- See scikit-learn docs for further details

Scaling in scikit-learn

```
from sklearn.preprocessing import StandardScaler
X = music_df.drop("genre", axis=1).values
y = music_df["genre"].values
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
                                                    random_state=42)
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
print(np.mean(X), np.std(X))
print(np.mean(X_train_scaled), np.std(X_train_scaled))
```

```
19801.42536120538, 71343.52910125865
2.260817795600319e-17, 1.0
```

Scaling in a pipeline

```
steps = [('scaler', StandardScaler()),
         ('knn', KNeighborsClassifier(n_neighbors=6))]
pipeline = Pipeline(steps)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
                                                    random_state=21)
knn_scaled = pipeline.fit(X_train, y_train)
y_pred = knn_scaled.predict(X_test)
print(knn_scaled.score(X_test, y_test))
```

```
0.81
```

Comparing performance using unscaled data

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
                                                    random_state=21)
knn_unscaled = KNeighborsClassifier(n_neighbors=6).fit(X_train, y_train)
print(knn_unscaled.score(X_test, y_test))
```

```
0.53
```

CV and scaling in a pipeline

```
from sklearn.model_selection import GridSearchCV
steps = [('scaler', StandardScaler()),
         ('knn', KNeighborsClassifier())]
pipeline = Pipeline(steps)
parameters = {"knn__n_neighbors": np.arange(1, 50)}
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
                                                    random_state=21)
cv = GridSearchCV(pipeline, param_grid=parameters)
cv.fit(X_train, y_train)
y_pred = cv.predict(X_test)
```

Checking model parameters

```
print(cv.best_score_)
```

```
0.8199999999999999
```

```
print(cv.best_params_)
```

```
{'knn__n_neighbors': 12}
```

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Evaluating multiple models

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Different models for different problems

Some guiding principles

- Size of the dataset
  - Fewer features = simpler model, faster training time
  - Some models require large amounts of data to perform well
- Interpretability
  - Some models are easier to explain, which can be important for stakeholders
  - Linear regression has high interpretability, as we can understand the coefficients
- Flexibility
  - May improve accuracy, by making fewer assumptions about data
  - KNN is a more flexible model, doesn't assume any linear relationships

It's all in the metrics

- Regression model performance:
  - RMSE
  - R-squared
- Classification model performance:
  - Accuracy
  - Confusion matrix
  - Precision, recall, F1-score
  - ROC AUC
- Train several models and evaluate performance out of the box

A note on scaling

- Models affected by scaling:
  - KNN
  - Linear Regression (plus Ridge, Lasso)
  - Logistic Regression
  - Artificial Neural Network

- Best to scale our data before evaluating models

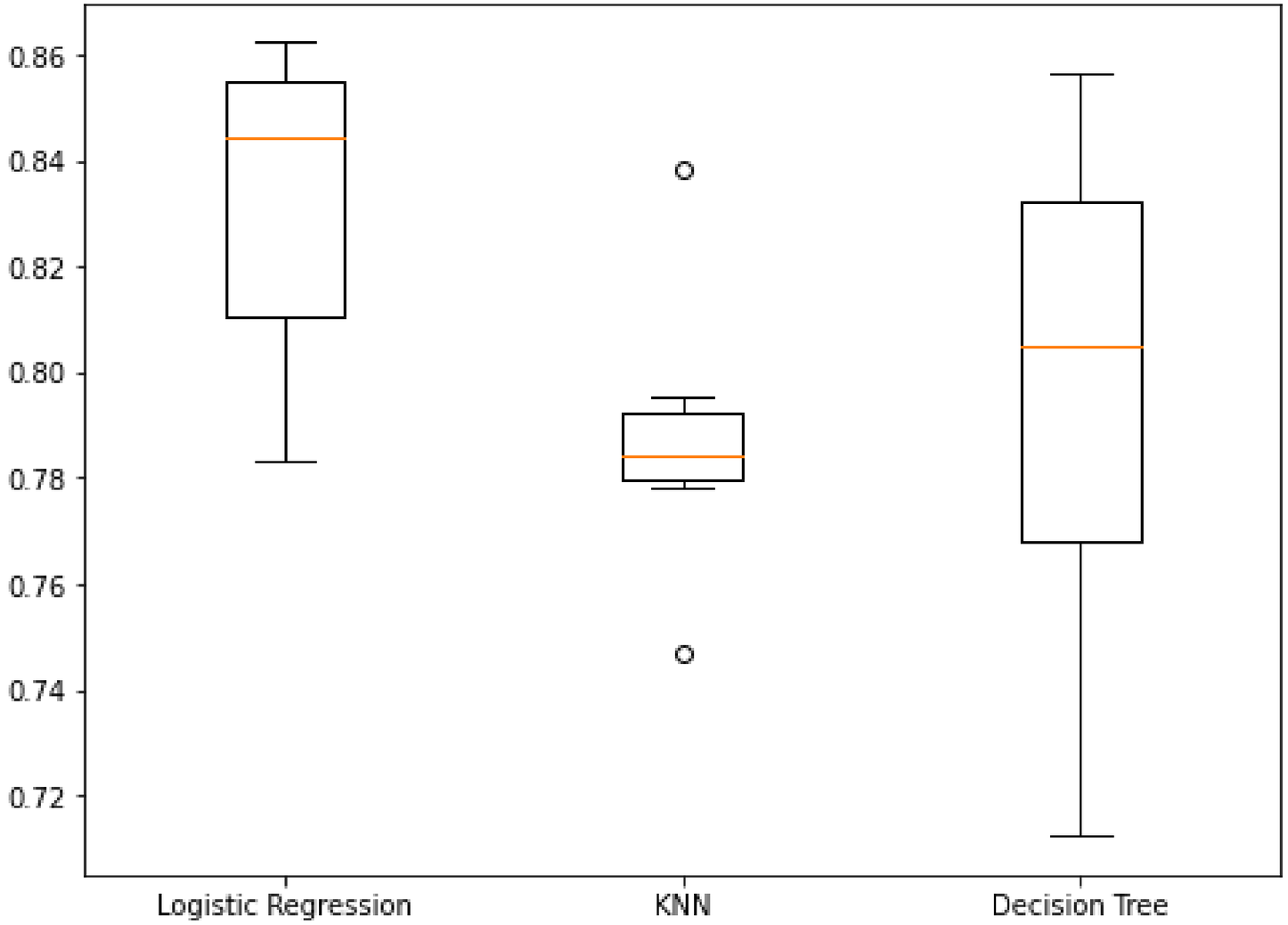
Evaluating classification models

```
import matplotlib.pyplot as plt
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import cross_val_score, KFold, train_test_split
from sklearn.neighbors import KNeighborsClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier
X = music.drop("genre", axis=1).values
y = music["genre"].values
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

Evaluating classification models

```
models = {"Logistic Regression": LogisticRegression(), "KNN": KNeighborsClassifier(),
          "Decision Tree": DecisionTreeClassifier()}
results = []
for model in models.values():
     kf = KFold(n_splits=6, random_state=42, shuffle=True)
     cv_results = cross_val_score(model, X_train_scaled, y_train, cv=kf)
     results.append(cv_results)
plt.boxplot(results, labels=models.keys())
plt.show()
```

Visualizing results



Test set performance

```
for name, model in models.items():
  model.fit(X_train_scaled, y_train)
  test_score = model.score(X_test_scaled, y_test)
  print("{} Test Set Accuracy: {}".format(name, test_score))
```

```
Logistic Regression Test Set Accuracy: 0.844
KNN Test Set Accuracy: 0.82
Decision Tree Test Set Accuracy: 0.832
```

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Congratulations

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What you've covered

- Using supervised learning techniques to build predictive models
- For both regression and classification problems
- Underfitting and overfitting
- How to split data
- Cross-validation

What you've covered

- Data preprocessing techniques
- Model selection
- Hyperparameter tuning
- Model performance evaluation
- Using pipelines

Where to go from here?

- Machine Learning with Tree-Based Models in Python
- Preprocessing for Machine Learning in Python
- Model Validation in Python
- Feature Engineering for Machine Learning in Python
- Unsupervised Learning in Python
- Machine Learning Projects

Thank you!

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