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April 12, 2025

1 Final Project: Regression Analysis

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1.2 Date: 12 Apr 2025

1.3 Overview

In this report we have reviewed the UC Irvide data set covering Automobile MPG. We create a new feature from the car name, and use it alongside vehicle weight and model year to feed a linear regression model and predict mpg.

1.4 Dataset

Auto MPG Dataset (Predict fuel efficiency based on engine specs and weight) - UCI Auto MPG Dataset

1.5 Section 1. Import and Inspect the Data

1.5.1 1.0 Import necessary libraries

```
[]: import pandas as pd
     import numpy as np
     import matplotlib.pyplot as plt
     import seaborn as sns
     from sklearn.model_selection import train_test_split
     from sklearn.linear_model import LinearRegression
     from sklearn.preprocessing import StandardScaler, PolynomialFeatures
     from sklearn.impute import SimpleImputer
     from sklearn.pipeline import Pipeline
     from sklearn.metrics import mean squared error, mean absolute error, r2 score
     from scipy.stats import ks_2samp, wasserstein_distance, energy_distance
     import math
     import time
     # using this variable allows us to change all of the random state variables,
      → throughout the document at once
     # this can help us compare behavior of our methodology across seeds
     state_setter=747
```

We use pandas and numpy for data frame manipulation and calculations, matplotlib and seaborn are used to generate graphs, numpy and scipy were used for statistical calculations, and sklearn was used for model training and evaluation.

1.5.2 1.1 Load the dataset and display the first 10 rows.

I used utils/convert_to_csv.py to convert our original auto-mpg.data file to a csv for easy consumption by Pandas. Pandas also had trouble with the data set due to some corrupted values, so convert_to_csv converts any mismatched values in auto-mpg.data to blanks when generating auto-mpg.csv.

```
[]: # Load the dataset
df = pd.read_csv('data/auto-mpg.csv')

# Display the first 10 rows
print("First 10 rows of the dataset:")
display(df.head(10))
```

1.5.3 1.2 Check for missing values and display summary statistics.

```
[]: # Check for missing values
print("\nMissing values in each column:")
print(df.isnull().sum())
```

Horsepower is missing 6 values. We will address this in section 2.

```
[]: # Get summary statistics
pd.set_option('display.expand_frame_repr', False)

print("\nSummary statistics:")
print(df.describe(include='all').T)
```

Some summary statistics for the info. Note that unique, top, and freq are generated for categorical features whereas mean, std, and min are generated for numerical features.

```
[]: # Check data types
print("\nData types:")
print(df.dtypes)

# Check unique values in categorical columns
print("\nUnique values in 'origin' column:")
print(df['origin'].unique())
```

We have mostly numerical columns with a couple string columns.

1.5.4 Reflection 1: What do you notice about the dataset? Are there any data issues?

The 'origin' column contains only integers (1, 2, and 3), but they probably represent categorical information about manufacturing locations that should be properly encoded.

The dataset spans model years from the 1970s to early 1980s based on the 'model_year' column, making this a historical dataset that might not reflect current automotive technology. These issues will need to be resolved through appropriate data cleaning and transformation steps before proceeding with modeling. The engine is misfiring on this dataset, but with some fine-tuning, we'll have it purring in no time.

1.6 Section 2. Data Exploration and Preparation

1.6.1 2.1 Handle missing values and clean data

First, let's examine our missing values more closely and create a plan to handle them. We already identified that the 'horsepower' column has 6 missing values, and they appear to be represented as '?' characters. Let's double check that all got taken care of with our earlier work.

```
[]: # Function to check for mismatched data types in the dataframe
     def check_data_type_mismatches(df):
         print("Checking for data type mismatches in each column...")
         # Dictionary to store results
         mismatches = {}
         # Check each column
         for column in df.columns:
             # Get the data type of the column
             dtype = df[column].dtype
             # Check for mismatches based on the data type
             if dtype == 'int64' or dtype == 'float64':
                 # For numeric columns, check for non-numeric values
                 non_numeric_count = 0
                 non_numeric_indices = []
                 for i, value in enumerate(df[column]):
                     # Try to convert to float to see if it's numeric
                     try:
                         float(value)
                     except (ValueError, TypeError):
                         # If conversion fails, it's not numeric
                         non_numeric_count += 1
                         if non_numeric_count <= 5: # Limit to first 5 examples</pre>
                             non_numeric_indices.append(i)
                 if non_numeric_count > 0:
                     mismatches[column] = {
                          'expected_type': dtype,
                         'mismatch_count': non_numeric_count,
                          'example_indices': non_numeric_indices
                     }
```

```
# Print results
    if mismatches:
        print("\nMismatched data types found:")
        for column, info in mismatches.items():
            print(f"\nColumn: {column}")
            print(f"Expected type: {info['expected_type']}")
            print(f"Mismatches found: {info['mismatch_count']}")
            # Print examples
            print("Examples of mismatched values:")
            for idx in info['example_indices']:
                print(f" Row {idx}: '{df.loc[idx, column]}'")
    else:
        print("\nNo data type mismatches found!")
    return mismatches
# Run the function on our dataframe
mismatches = check_data_type_mismatches(df)
```

Looks good to go.

2.1.1 Impute or drop missing values Now that we've properly identified the missing values, we'll impute them using the median value of the horsepower column. This is a reasonable approach for this small number (6 out of \sim 400) of missing values in a numerical feature.

```
[]: # Create an imputer for the horsepower column
horsepower_imputer = SimpleImputer(strategy='median')

# Fit the imputer on the horsepower data and transform it
df['horsepower'] = horsepower_imputer.fit_transform(df[['horsepower']])

# Verify that missing values have been imputed
print("Missing values after imputation:")
print(df.isnull().sum())
```

Worked well!

2.1.2 Remove or transform outliers Let's identify potential outliers in our numerical columns using boxplots. This will help us determine if any data points are significantly outside the normal range and might need to be addressed.

```
[]: # Create boxplots for all numerical columns to identify outliers
plt.figure(figsize=(15, 10))

# Select only numerical columns
numerical_cols = df.select_dtypes(include=['int64', 'float64']).columns
```

```
# Create boxplots for each numerical column
for i, column in enumerate(numerical_cols):
    plt.subplot(3, 3, i+1)
    sns.boxplot(x=df[column])
    plt.title(f'Boxplot of {column}')
    plt.tight_layout()
plt.show()
# Calculate the IQR and identify outliers for each numerical column
for column in numerical_cols:
    Q1 = df[column].quantile(0.25)
    Q3 = df[column].quantile(0.75)
    IQR = Q3 - Q1
    lower_bound = Q1 - 1.5 * IQR
    upper_bound = Q3 + 1.5 * IQR
    outliers = ((df[column] < lower_bound) | (df[column] > upper_bound)).sum()
    if outliers > 0:
        print(f"Column '{column}' has {outliers} outliers")
```

The Boxplots show that some of the data has a wide range, but none of them are particularly plagued withoutliers. We shall proceed.

2.1.3 Convert categorical data to numerical format using encoding The 'origin' column is currently represented as integers (1, 2, 3) but it's actually a categorical feature representing the car's manufacturing region.

By examining a few example rows, we can see that 1 is america, 2 is Europe, and 3 is Asia. I pulled open the csv separately and confirmed this by comparing models to where I know the manufacturer is based, but here are some example rows evidencing that:

$\overline{\mathrm{mpg}}$	cylinders	displacement	horsepower	weight	acceleration	$model_$	year origin	car_name
18.0	8	307.0	130.0	3504.0	12.0	70	1	"chevrolet chevelle malibu"
15.0	8	350.0	165.0	3693.0	11.5	70	1	"buick skylark 320"
18.0	8	318.0	150.0	3436.0	11.0	70	1	"plymouth satel- lite"

mpg	cylinders	displacement	horsepower	weight	acceleration	model_yea	r origin	car_name
26.0	4	97.00	46.00	1835.0	20.5	70	2	"volkswager 1131 deluxe sedan"
25.0	4	110.0	87.00	2672.0	17.5	70	2	"peugeot 504"
24.0	4	107.0	90.00	2430.0	14.5	70	2	"audi 100 ls"
25.0	4	113.0	95.00	2228.0	14.0	71	3	"toyota corona"
27.0	4	97.00	88.00	2130.0	14.5	70	3	"datsun pl510"
35.0	4	72.00	69.00	1613.0	18.0	71	3	"datsun 1200"

Let's encode it properly using one-hot encoding.

```
[]: # First, let's understand what the origin values represent
print("Value counts for 'origin':")
print(df['origin'].value_counts())

# Convert 'origin' to a more meaningful categorical representation
origin_mapping = {1: 'america', 2: 'europe', 3: 'asia'}
df['origin_name'] = df['origin'].map(origin_mapping)

# Apply one-hot encoding to the 'origin' column
origin_encoded = pd.get_dummies(df['origin_name'], prefix='origin')

# Join the encoded columns to the original dataframe
df = pd.concat([df, origin_encoded], axis=1)

# Drop the original 'origin' and 'origin_name' columns
df = df.drop(['origin', 'origin_name'], axis=1)

# Display the first few rows to confirm the encoding
print("\nFirst 5 rows after encoding 'origin':")
display(df.head())
```

1.6.2 2.2 Explore data patterns and distributions

Now let's visualize our dataset's key features to better understand their distributions and relationships, starting with histograms of our numerical features.

2.2.1 Create histograms, boxplots, and count plots for categorical variables (as applicable). Let's create visualizations to understand the distributions of our features. These plots will help us identify patterns and relationships in the data that might influence our modeling approach.

Pretty reasonable distributions.

It's generally distributed evenly across model years.

Horsepower has an interesting spike around 250hp.

The Cylinder distribution is the most interesting - there are a plurality of 4 cylinder samples, some 6 and 8 cylinder samples, and just a few oddball 3-5 cylinder vehicles.

Given we've established the origin to continent mapping, let's look closer at how the dataset is distributed across regions.

```
[]: # Count plots for categorical variables (the encoded origin columns)
     plt.figure(figsize=(10, 6))
     origin_counts = df[['origin_america', 'origin_asia', 'origin_europe']].sum()
     # Calculate percentages
     total = origin_counts.sum()
     percentages = (origin_counts / total) * 100
     # Add percentage labels on top of each bar
     for i, v in enumerate(origin_counts.values):
         plt.text(i, v - 15, f"{percentages[i]:.1f}%",
                  ha='center', va='bottom', color='white', fontweight='bold')
     sns.barplot(x=origin_counts.index, y=origin_counts.values)
     plt.title('Distribution of Cars by Origin')
     plt.xlabel('Origin')
     plt.ylabel('Count')
     plt.xticks(rotation=45)
     plt.tight_layout()
     plt.show()
```

The dataset is a majority American, with a few dozen from the Asia and Europe regions as well.

2.2.2 Identify patterns, outliers, and anomalies in feature distributions. Now, let's examine relationships between features and identify potential outliers. Pulling up the correlation matrix and scatter plots will help us understand how features relate to our target variable (mpg) and to each other.

```
[]: # Correlation matrix to identify relationships between numerical features plt.figure(figsize=(12, 10)) correlation_matrix = df[numerical_features].corr() sns.heatmap(correlation_matrix, annot=True, cmap='coolwarm', linewidths=0.5) plt.title('Correlation Matrix of Numerical Features') plt.tight_layout() plt.show()
```

For numerical values, we are most focused on the left column. Given how weight, horsepower, displacement, and cylinder are both all closely associated with mpg with their high scores...but unfortunately they are all closely associated to one another. We will pick weight as our variable, given that it has the highest absolute correlation with mpg.

```
[]: # Scatter plots of important features vs. target variable (mpg)
plt.figure(figsize=(15, 10))
features_to_plot = ['displacement', 'horsepower', 'weight', 'acceleration']

for i, feature in enumerate(features_to_plot):
    plt.subplot(2, 2, i+1)
    sns.scatterplot(x=df[feature], y=df['mpg'], hue=df['model_year'])
    plt.title(f'{feature} vs. mpg')
    plt.xlabel(feature)
    plt.ylabel('mpg')

plt.tight_layout()
plt.show()
```

Reviewing displacement, weight, and horsepower, we can see the scatter plots are all quite similar.

```
[]: # Pair plots for key features to identify patterns and outliers
sns.pairplot(df[['mpg', 'displacement', 'horsepower', 'weight', 'model_year']])
plt.suptitle('Pair Plots of Key Features', y=1.02)
plt.show()
```

2.2.3 Check for class imbalance in the target variable (as applicable). While our target variable (mpg) is continuous for regression, we'll examine its distribution to ensure it's well-represented across its range and doesn't have concentrated values that could bias our model.

```
[]: # Examine the distribution of the target variable (mpg)
plt.figure(figsize=(10, 6))
sns.histplot(df['mpg'], bins=20, kde=True)
plt.title('Distribution of MPG (Target Variable)')
plt.xlabel('Miles Per Gallon (MPG)')
```

An interesting distribution. Leans left a bit, but has some strength on the far right which pulls the mean right.

Let's investigate whether there's a connection between mpg and the origin region we established previously.

```
[]: # Create mpg distribution by origin
     plt.figure(figsize=(15, 5))
     plt.subplot(1, 3, 1)
     sns.kdeplot(df[df['origin_america'] == True]['mpg'], fill=True, label='America')
     plt.title('MPG Distribution for American Cars')
     plt.xlabel('Miles Per Gallon (MPG)')
     plt.ylabel('Density')
     plt.subplot(1, 3, 2)
     sns.kdeplot(df[df['origin_europe'] == True]['mpg'], fill=True, label='Europe')
     plt.title('MPG Distribution for European Cars')
     plt.xlabel('Miles Per Gallon (MPG)')
     plt.ylabel('Density')
     plt.subplot(1, 3, 3)
     sns.kdeplot(df[df['origin_asia'] == True]['mpg'], fill=True, label='Asia')
     plt.title('MPG Distribution for Asian Cars')
     plt.xlabel('Miles Per Gallon (MPG)')
     plt.ylabel('Density')
     plt.tight_layout()
     plt.show()
```

Clearly MPG runs highest for Asian cars, then European ones, and then American ones.

```
[]: # Let's also look at MPG over the years to detect any trends
plt.figure(figsize=(12, 6))
sns.boxplot(x='model_year', y='mpg', data=df)
plt.title('MPG Distribution by Model Year')
plt.xlabel('Model Year')
plt.ylabel('Miles Per Gallon (MPG)')
plt.xticks(rotation=45)
plt.show()
```

We can see there is a correlation between model year and mpg as well - with mpg generally trending upward as the years went by. In addition to technology naturally making things more generally efficient over time, I suspect the 70s oil crisis and EPI requirements also had an influence on this...but that's for another study.

1.6.3 2.3 Feature selection and engineering

There was a clear association between the car's origin and its mpg. Interestingly, the car name column is not just the model - the first word of every entry appeared to be the vehicle's make. Let's see if we can extract the make of the car as a new column.

2.3.1 Create new features (as applicable).

```
[]: # Feature engineering: Extract car make from car_name

# Extract the car make (first word) from the car_name column

df['make'] = df['car_name'].str.split().str[0]

# Display the first 10 rows with the new 'make' column

print("First 10 rows with make column added:")

display(df.head(10))
```

Looks like it was created successfully! Let's look a little closer to see if we need to do any further work on it.

2.3.2 Transform or combine existing features to improve model performance

```
[]: # Show the make counts
make_counts = df['make'].value_counts()
print("Current make counts:")
print(make_counts)
```

We can see most of them are formatted with common names. A handful have strange names or typos - like vw and vokswagen. Let's manually edit them to put them in the bins they belong

2.3.3.1 Transform Makes

```
[]: # Define mapping dictionary for make standardization
make_mapping = {
    'chevy': 'chevrolet',
    'chevroelt': 'chevrolet',
    'vokswagen': 'volkswagen',
    'vw': 'volkswagen',
    'toyouta': 'toyota',
    'mercedes': 'mercedes-benz',
    'maxda': 'mazda',
    'hi': 'hindustan', # 'hi' appears to be Hindustan Motors
    'capri': 'ford' # Capri was a model made by Ford
}

# Apply the mapping to standardize makes
```

```
df['make'] = df['make'].replace(make_mapping)

# Show the updated make counts
make_counts = df['make'].value_counts()
print("Updated make counts after standardization:")
print(make_counts)

# Display the first 10 rows to verify changes
print("\nFirst 10 rows with standardized make column:")
display(df.head(10))
```

Looking much better! Lets check all of the unique makes again:

```
[]: print("All the unique makes") print(make_counts)
```

2.3.3.2 Confirm Make <-> **Origin connection** I hoped to use make as a feature. Part of my intent was that make may provide more information than origin, while also providing some of the information origin did since each make is only from one origin. To prove this I wanted to confirm each set with a specific make all had the same origin.

```
[]: # Create a function to check if each make has exactly one origin
     def check_make_origin_consistency(df):
         # Get unique makes
         makes = df['make'].unique()
         # Dictionary to store results
         make_origins = {}
         inconsistent_makes = {}
         # Check each make
         for make in makes:
             # Get data for this make
             make_data = df[df['make'] == make]
             # Check which origins this make has
             has america = make data['origin america'].any()
             has_asia = make_data['origin_asia'].any()
             has_europe = make_data['origin_europe'].any()
             # Count number of origins
             origin_count = sum([has_america, has_asia, has_europe])
             # Store the origin
             if has_america:
                 make_origins[make] = 'America'
             elif has_asia:
```

```
make_origins[make] = 'Asia'
        elif has_europe:
            make_origins[make] = 'Europe'
        # If more than one origin, this make is inconsistent
        if origin_count > 1:
            inconsistent makes[make] = {
                'America': has_america,
                'Asia': has asia,
                'Europe': has_europe
            }
    return make_origins, inconsistent_makes
# Run the check
make_origins, inconsistent_makes = check_make_origin_consistency(df)
# Show results
print("Number of unique makes:", len(make_origins))
print("\nOrigin countries by make:")
for make, origin in sorted(make_origins.items()):
    print(f"{make}: {origin}")
if inconsistent makes:
    print("\nWARNING: The following makes have inconsistent origins:")
    for make, origins in inconsistent makes.items():
        print(f"{make}: {origins}")
else:
    print("\nAll makes have consistent origins!")
```

Looks good! Let's visualize which one each is grouped to:

2.3.3.3 Remove Outlier Makes To avoid confusing the model with low sample count makes, and for the sake of minimizing dimensionality when testing our polynomial model, we removed makes with less than 10 instances in the sample.

While this meant losing 15% of our data set, I was eager enough to use this feature I created that I believed it to be a worthy sacrifice.

```
[]: # Get value counts of each make
     make_counts = df['make'].value_counts()
     # Identify makes with fewer than 10 instances
     rare makes = make counts[make counts < 10]</pre>
     print("Makes with fewer than 10 instances:")
     print(rare makes)
     # Calculate the total number of cars with these rare makes
     rare_makes_count = sum(rare_makes)
     total_cars = len(df)
     rare_percentage = (rare_makes_count / total_cars) * 100
     print(f"\nTotal cars in dataset: {total_cars}")
     print(f"Cars with rare makes (< 5 instances): {rare_makes_count}")</pre>
     print(f"Percentage of dataset with rare makes: {rare percentage:.2f}%")
[]: # Store the original dataframe size
     original_size = len(df)
     # Get the list of rare makes (makes with fewer than 5 instances)
     rare_makes_list = rare_makes.index.tolist()
     # Filter out rows with rare makes
     df filtered = df[~df['make'].isin(rare makes list)]
     # Calculate the new size
     new_size = len(df_filtered)
     removed_rows = original_size - new_size
     # Display results
     print(f"Original dataset size: {original_size} rows")
     print(f"After removing rare makes: {new_size} rows")
     print(f"Removed {removed_rows} rows ({(removed_rows/original_size)*100:.2f}% of_u

data)")
```

Looks good. This will help greatly in allowing us to use the categorial variable make in our polynomial regression.

Let's take a look at the mpg consumption by make just for the heck of it.

```
[]: # Get the most common makes (to avoid too many colors in the plot)
top_makes = df['make'].value_counts().head(10).index.tolist()
print(f"Top 10 makes: {top_makes}")
```

```
# Filter dataset to include only the top makes for better visualization
filtered_df = df[df['make'].isin(top_makes)]
# Create a figure with adequate size
plt.figure(figsize=(12, 8))
# Use a color palette that distinguishes between different makes
colors = sns.color_palette("husl", len(top_makes))
# Plot KDE curves for each make
for i, make in enumerate(top_makes):
    make_data = filtered_df[filtered_df['make'] == make]
    sns.kdeplot(make_data['mpg'], fill=True, color=colors[i], alpha=0.4,_
 ⇔label=make, common_norm=False)
# Add plot details
plt.title('MPG Distribution by Car Make', fontsize=16)
plt.xlabel('Miles Per Gallon (MPG)', fontsize=12)
plt.ylabel('Density', fontsize=12)
plt.grid(True, linestyle='--', alpha=0.7)
# Add a legend at the bottom
plt.legend(title='Car Make', bbox_to_anchor=(0.5, -0.15), loc='upper center', __
 ⇔ncol=5)
# Adjust layout to make room for the legend
plt.tight_layout()
plt.subplots_adjust(bottom=0.2)
# Display the plot
plt.show()
```

We can clearly see the American vehicles have lower humps than the Asian and European ones. Will be interesting to see how our model works with this.

- **2.3.3 Scale or normalize data (as applicable).** Given how minimal the outliers were in section 2.2.2, this step was skipped, particularly given the features we're using did not have outliers.
- 1.6.4 Reflection 2: What patterns or anomalies do you see? Do any features stand out? What preprocessing steps were necessary to clean and improve the data? Did you create or modify any features to improve performance?
- 1.7 Section 3. Feature Selection and Justification
- 1.7.1 3.1 Choose features and target
- 3.1.1 Select two or more input features We are going to use model year, weight, and make.

Since the data shows a fairly steady upward trend in mpg by model year (as seen in your boxplots), treating it as a numerical feature is likely sufficient and won't cause overfitting. The linear relationship appears reasonably strong.

- **3.1.2** Select a target variable (as applicable) The assignment indicated we ought to use MPG. I was hoping I could feed data and use it to predict the origin of the car or the make, and I might in the future as time allows.
- **3.1.3 Justify your selection with reasoning.** Weight had the strongest correlation with mpg, so that was a no brainer. While Horsepower and displacement had strong associations too, they also had very strong associations with weight, so they would not add new information.

My hope is make adds the same information origin would add, with an extra factor of association to the specific brand. I tested and confirmed it did generally result in higher R^2 values than origin. It is categorical, but by reducing it to the 14 makes with more than 10 samples, my hope is that the model will be able to split and calculate for it effectively.

Lastly, to add time as a factor, we will be using Model Year. Since the data shows a fairly steady upward trend in mpg by model year (as seen in the boxplots), treating it as a numerical feature is likely sufficient and won't cause overfitting. The linear relationship appears reasonably strong, and it helps us navigate the curse of dimensionality.

1.7.2 3.2 Define X and y

3.2.1 Assign input features to X

```
[]: # 3.2.1 Assign input features to X

# Select the features we want to use for our model
# Convert 'make' to a categorical variable using one-hot encoding
make_encoded = pd.get_dummies(df['make'], prefix='make', drop_first=True)

# Combine the encoded make columns with our other numerical features
X = pd.concat([
    df[['weight', 'model_year']],
    make_encoded
], axis=1)

# Display the first few rows of our feature set
print("First 5 rows of our features (X):")
display(X.head())

# Shape of the feature matrix
print(f"\nShape of X: {X.shape}")
print(f"Number of features: {X.shape[1]}")
```

3.2.2 Assign target variable to y (as applicable)

```
[]: # 3.2.2 Assign target variable to y
```

```
# Our target variable is 'mpg'
y = df['mpg']
# Display the first few values of our target
print("First 5 values of our target (y):")
display(y.head())
# Basic statistics of our target variable
print("\nBasic statistics of MPG (target variable):")
print(y.describe())
# Visualize the distribution of our target variable
plt.figure(figsize=(10, 6))
sns.histplot(y, kde=True)
plt.title('Distribution of MPG (Target Variable)')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Frequency')
plt.grid(True, alpha=0.3)
plt.show()
```

- 1.7.3 Reflection 3: Why did you choose these features? How might they impact predictions or accuracy?
- 1.8 Section 4. Train a Model (Linear Regression)
- 1.8.1 4.1 Split the data into training and test sets using train_test_split (or StratifiedShuffleSplit if class imbalance is an issue).

4.1.1 Initial Random Split

```
# Define common binning
bins = np.linspace(5, 50, 15) # 15 bins from 5 to 50 MPG
plt.subplot(1, 2, 1)
sns.histplot(y_train, bins=bins, kde=True, color='blue', stat='density')
plt.title('MPG Distribution - Training Set')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
plt.subplot(1, 2, 2)
sns.histplot(y_test, bins=bins, kde=True, color='green', stat='density')
plt.title('MPG Distribution - Testing Set')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
plt.tight_layout()
plt.show()
# Compare statistical measures
print("\nTraining set MPG statistics:")
print(y_train.describe())
print("\nTesting set MPG statistics:")
print(y_test.describe())
```

These distributions are concerningly different. Let's tackle it with a stratified test-train-split...but stratify it across what?

4.1.2 Stratified Test Train Split - Stratification Comparison Per our research earlier, there are too many small 'make' bins, so let's consider origin instead. Let's also look at separating MPG into Bins and stratifying according to the bins. We will them compare mpg distributions produced by these 2 methods against the random split we've done here and the original data set's mpg distribution

```
[]: # Function to evaluate similarity between distributions
def compare_distributions(original, sample, method_name):
    # Calculate statistical distances
    ks_stat, ks_pval = ks_2samp(original, sample)
    w_distance = wasserstein_distance(original, sample)
    e_distance = energy_distance(original, sample)

# Calculate basic statistics and their differences
orig_stats = original.describe()
sample_stats = sample.describe()
```

```
# Calculate absolute differences in key statistics
  mean_diff = abs(orig_stats['mean'] - sample_stats['mean'])
   std_diff = abs(orig_stats['std'] - sample_stats['std'])
   # Quartile differences
  q1_diff = abs(orig_stats['25%'] - sample_stats['25%'])
  median_diff = abs(orig_stats['50%'] - sample_stats['50%'])
  q3_diff = abs(orig_stats['75%'] - sample_stats['75%'])
   # Return a composite score
  # Weighted sum of distances
  composite_score = (ks_stat * 0.3) + (w_distance * 0.3) + (e_distance * 0.1)
→+ \
                       (mean\_diff * 0.1) + (std\_diff * 0.1) + 
                       (q1_diff * 0.03) + (median_diff * 0.04) + (q3_diff * 0.03)
   """The score is a weighted combination of several statistical distance\sqcup
\neg metrics:
  Kolmogorov-Smirnov statistic (30% weight): Measures the maximum difference \Box
_{\hookrightarrow}between two cumulative distribution functions. A value of 0 means identical_{\sqcup}
\ominus distributions.
   Wasserstein distance (30% weight): Also known as the "Earth Mover's_{\sqcup}
{\scriptscriptstyle \hookrightarrow} 	extit{Distance,"} it measures how much "work" it would take to transform one {\scriptscriptstyle \sqcup}
\negdistribution into another. Lower values mean distributions are more similar.
  Energy distance (10% weight): Another statistical distance metric that s_{\sqcup}
sensitive to differences in both shape and location of distributions.
  Differences in key statistics (30% total weight):
  Mean difference (10%)
  Standard deviation difference (10%)
   Quartile differences (10% total: 3% for Q1, 4% for median, 3% for Q3)
   These components capture different aspects of distribution similarity:
   The statistical distance metrics (KS, Wasserstein, Energy) capture overall_{\sqcup}
⇒shape differences
   The mean and standard deviation differences capture central tendency and \sqcup
\hookrightarrowspread
   The quartile differences capture structural details of the distribution"""
  return {
       'method': method_name,
```

```
'ks_stat': ks_stat,
        'ks_pval': ks_pval,
        'w_distance': w_distance,
        'e_distance': e_distance,
        'mean_diff': mean_diff,
        'std_diff': std_diff,
        'q1_diff': q1_diff,
        'median_diff': median_diff,
        'q3_diff': q3_diff,
        'composite_score': composite_score
    }
# Original data
y_original = df['mpg']
# Prepare features (same as before)
make_encoded = pd.get_dummies(df['make'], prefix='make', drop_first=True)
X = pd.concat([df[['weight', 'model_year']], make_encoded], axis=1)
# Method 1: Stratify by origin
strat_var_origin = np.where(df['origin_america'], 'america',
                   np.where(df['origin_europe'], 'europe', 'asia'))
X_train_origin, X_test_origin, y_train_origin, y_test_origin = train_test_split(
    X, y_original,
    test_size=0.2,
    random_state=state_setter,
    stratify=strat_var_origin
)
# Method 2: Stratify by 5 binned MPG values
mpg_bins = pd.qcut(df['mpg'], q=5, labels=False, duplicates='drop')
X_train_mpg, X_test_mpg, y_train_mpg, y_test_mpg = train_test_split(
    X, y_original,
    test_size=0.2,
    random_state=state_setter,
    stratify=mpg_bins
)
# Method 3: Regular random split (as baseline)
X_train_rand, X_test_rand, y_train_rand, y_test_rand = train_test_split(
    X, y_original,
    test_size=0.2,
   random_state=state_setter
)
```

```
# Compare distributions
origin_results = compare_distributions(y_original, y_test_origin, "Origin")
mpg_results = compare_distributions(y_original, y_test_mpg, "MPG Bins")
random_results = compare_distributions(y_original, y_test_rand, "Random")
# Visualize all distributions
plt.figure(figsize=(15, 10))
# Define common binning
bins = np.linspace(5, 50, 15)
# Original distribution
plt.subplot(2, 2, 1)
sns.histplot(y_original, bins=bins, kde=True, color='purple', stat='density')
plt.title('Original MPG Distribution')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
# Origin stratification
plt.subplot(2, 2, 2)
sns.histplot(y_test_origin, bins=bins, kde=True, color='blue', stat='density')
plt.title(f'Test Set - Stratified by Origin\nScore: u
 →{origin_results["composite_score"]:.4f}')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
# MPG bins stratification
plt.subplot(2, 2, 3)
sns.histplot(y_test_mpg, bins=bins, kde=True, color='green', stat='density')
plt.title(f'Test Set - Stratified by MPG Bins\nScore:
 →{mpg_results["composite_score"]:.4f}')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
# Random split
plt.subplot(2, 2, 4)
sns.histplot(y_test_rand, bins=bins, kde=True, color='red', stat='density')
plt.title(f'Test Set - Random Split\nScore: {random_results["composite_score"]:.

4f}')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
```

This suggests mpg bins is the best, and visually it definitely appears closest too. Given the small set of the data however, let's cross-validate across 10 splits to confirm we achieve the same results.

Note - the score represents the dissimilarity between the test set distribution and the original distribution. Lower scores indicate test sets that more closely match the original MPG distribution, which is why lower is better, and 0 would mean the distributions are identical.

If curious for more detail, review the comments and calculations in the python code.

4.1.3 Cross Validated Stratification Factor Comparison

```
[]: | # Function to evaluate similarity between distributions
     def compare distributions(original, sample, method name):
         # Calculate statistical distances
         ks_stat, ks_pval = ks_2samp(original, sample)
         w_distance = wasserstein_distance(original, sample)
         e_distance = energy_distance(original, sample)
         # Calculate basic statistics and their differences
         orig_stats = original.describe()
         sample_stats = sample.describe()
         # Calculate absolute differences in key statistics
         mean_diff = abs(orig_stats['mean'] - sample_stats['mean'])
         std_diff = abs(orig_stats['std'] - sample_stats['std'])
         # Quartile differences
         q1_diff = abs(orig_stats['25%'] - sample_stats['25%'])
         median_diff = abs(orig_stats['50%'] - sample_stats['50%'])
         q3_diff = abs(orig_stats['75%'] - sample_stats['75%'])
         # Return a composite score
         # Weighted sum of distances
         composite_score = (ks_stat * 0.3) + (w_distance * 0.3) + (e_distance * 0.1)_{\sqcup}
      →+ \
                           (mean_diff * 0.1) + (std_diff * 0.1) + \
                           (q1 diff * 0.03) + (median diff * 0.04) + (q3 diff * 0.03)
         return {
             'method': method_name,
             'ks_stat': ks_stat,
             'ks_pval': ks_pval,
```

```
'w_distance': w_distance,
        'e_distance': e_distance,
        'mean_diff': mean_diff,
        'std_diff': std_diff,
        'q1_diff': q1_diff,
        'median_diff': median_diff,
        'q3_diff': q3_diff,
        'composite_score': composite_score
    }
# Original data
y_original = df['mpg']
# Prepare features (same as before)
make_encoded = pd.get_dummies(df['make'], prefix='make', drop_first=True)
X = pd.concat([df[['weight', 'model_year']], make_encoded], axis=1)
# Number of cross-validation iterations
n_{iterations} = 10
# Initialize dictionaries to store results and test set distributions
results_origin = []
results_mpg = []
results random = []
# Initialize arrays to accumulate histograms for averaging
all_y_test_origin = []
all_y_test_mpg = []
all_y_test_random = []
# Cross-validation loop
for i in range(n_iterations):
    # Set random state based on state_setter + iteration
    random_state = state_setter + i
    # Method 1: Stratify by origin
    strat_var_origin = np.where(df['origin_america'], 'america',
                    np.where(df['origin_europe'], 'europe', 'asia'))
    X_train_origin, X_test_origin, y_train_origin, y_test_origin =_
 →train_test_split(
        X, y_original,
        test_size=0.2,
        random_state=random_state,
       stratify=strat_var_origin
    )
```

```
mpg_bins = pd.qcut(df['mpg'], q=5, labels=False, duplicates='drop')
   X_train_mpg, X_test_mpg, y_train_mpg, y_test_mpg = train_test_split(
       X, y_original,
        test size=0.2,
       random_state=random_state,
        stratify=mpg bins
   )
    # Method 3: Regular random split (as baseline)
   X_train_rand, X_test_rand, y_train_rand, y_test_rand = train_test_split(
        X, y_original,
       test_size=0.2,
       random_state=random_state
   )
    # Evaluate distributions
   results_origin.append(compare_distributions(y_original, y_test_origin,_u

¬"Origin"))
   results_mpg.append(compare_distributions(y_original, y_test_mpg, "MPGL
 ⇔Bins"))
   results random append(compare_distributions(y_original, y_test_rand,_

¬"Random"))
    # Store test set distributions for later averaging
   all_y_test_origin.append(y_test_origin)
   all_y_test_mpg.append(y_test_mpg)
   all_y_test_random.append(y_test_rand)
# Calculate average scores for each method
def average_results(results_list):
   avg_results = {
        'ks_stat': np.mean([r['ks_stat'] for r in results_list]),
        'ks pval': np.mean([r['ks pval'] for r in results list]),
        'w_distance': np.mean([r['w_distance'] for r in results_list]),
        'e_distance': np.mean([r['e_distance'] for r in results_list]),
        'mean_diff': np.mean([r['mean_diff'] for r in results_list]),
        'std_diff': np.mean([r['std_diff'] for r in results_list]),
        'q1_diff': np.mean([r['q1_diff'] for r in results_list]),
        'median_diff': np.mean([r['median_diff'] for r in results_list]),
        'q3_diff': np.mean([r['q3_diff'] for r in results_list]),
        'composite score': np.mean([r['composite score'] for r in results list])
   }
```

```
return avg_results
avg_origin = average_results(results_origin)
avg_mpg = average_results(results_mpg)
avg_random = average_results(results_random)
# Function to create a combined histogram representation across all \mathit{CV}_{\sqcup}
 \rightarrow iterations
def create_averaged_histogram(all_samples, bins=15):
    # Concatenate all samples across CV iterations
    combined = pd.concat(all_samples)
    return combined
# Create averaged histograms
avg_hist_origin = create_averaged_histogram(all_y_test_origin)
avg_hist_mpg = create_averaged_histogram(all_y_test_mpg)
avg_hist_random = create_averaged_histogram(all_y_test_random)
# Visualize the average distributions
plt.figure(figsize=(15, 10))
# Define common binning
bins = np.linspace(5, 50, 15)
# Original distribution
plt.subplot(2, 2, 1)
sns.histplot(y_original, bins=bins, kde=True, color='purple', stat='density')
plt.title('Original MPG Distribution')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
# Origin stratification (average across CV)
plt.subplot(2, 2, 2)
sns.histplot(avg_hist_origin, bins=bins, kde=True, color='blue', stat='density')
plt.title(f'Stratified by Origin\nAvg Score: {avg_origin["composite_score"]:.
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
# MPG bins stratification (average across CV)
plt.subplot(2, 2, 3)
sns.histplot(avg_hist_mpg, bins=bins, kde=True, color='green', stat='density')
```

```
plt.title(f'Test Set - Stratified by MPG Bins\nAvg Score:
 ⇔{avg_mpg["composite_score"]:.4f}')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
# Random split (average across CV)
plt.subplot(2, 2, 4)
sns.histplot(avg_hist_random, bins=bins, kde=True, color='red', stat='density')
plt.title(f'Test Set - Random Split\nAvg Score: {avg_random["composite_score"]:.
 <4f}¹)
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
plt.tight_layout()
plt.suptitle('Comparison of Distribution Preservation Methods (10-fold ∪
 →CV)\n(Lower Score = Better Match)', fontsize=16, y=1.02)
plt.show()
# Create a summary table of average results
methods = \Gamma
    {'method': 'Origin', **avg_origin},
    {'method': 'MPG Bins', **avg_mpg},
   {'method': 'Random', **avg random}
comparison_df = pd.DataFrame(methods)
comparison_df = comparison_df.set_index('method')
# Sort by composite score (lower is better)
comparison_df = comparison_df.sort_values('composite_score')
print("\n--- Summary of Average Distribution Similarity Across 10 Splits ---")
print(comparison_df[['ks_stat', 'w_distance', 'mean_diff', 'std_diff', "
# Determine the winner
winner = comparison_df.index[0]
print(f"\nBest stratification method: {winner}")
# Show standard deviation of scores to see consistency
std_origin = np.std([r['composite_score'] for r in results_origin])
std_mpg = np.std([r['composite_score'] for r in results_mpg])
std_random = np.std([r['composite_score'] for r in results_random])
```

```
print("\n--- Standard Deviation of Scores Across 10 Splits ---")
print(f"Origin: {std_origin:.4f}")
print(f"MPG Bins: {std_mpg:.4f}")
print(f"Random: {std_random:.4f}")
```

This clearly confirms the mpg binning method gave the lowest score, and a distribution closest to the original. No surprise given the distribution of mpg itself is what we're interested in! But still wise to cross-validate.

Stratifying the split across a greater number of bins should obviously help it match the the original distribution, but let's double check that and also confirm there aren't major performance implications. With our smaller data set, it probably won't have performance implications, but let's double check and confirm a larger number of bins is ideal.

4.1.4 Bin Count Stratification Fine Tuning

```
[]: # Function to evaluate similarity between distributions (same as before)
     def compare_distributions(original, sample, method_name):
         # Calculate statistical distances
         ks stat, ks pval = ks 2samp(original, sample)
         w_distance = wasserstein_distance(original, sample)
         e_distance = energy_distance(original, sample)
         # Calculate basic statistics and their differences
         orig_stats = original.describe()
         sample_stats = sample.describe()
         # Calculate absolute differences in key statistics
         mean_diff = abs(orig_stats['mean'] - sample_stats['mean'])
         std_diff = abs(orig_stats['std'] - sample_stats['std'])
         # Quartile differences
         q1_diff = abs(orig_stats['25%'] - sample_stats['25%'])
         median_diff = abs(orig_stats['50%'] - sample_stats['50%'])
         q3_diff = abs(orig_stats['75%'] - sample_stats['75%'])
         # Return a composite score (lower is better)
         composite_score = (ks_stat * 0.3) + (w_distance * 0.3) + (e_distance * 0.1)
      + \
                           (\text{mean\_diff} * 0.1) + (\text{std\_diff} * 0.1) + 
                           (q1_diff * 0.03) + (median_diff * 0.04) + (q3_diff * 0.03)
         return {
             'method': method_name,
             'ks_stat': ks_stat,
             'ks_pval': ks_pval,
             'w_distance': w_distance,
             'e_distance': e_distance,
             'mean_diff': mean_diff,
```

```
'std_diff': std_diff,
        'q1_diff': q1_diff,
        'median_diff': median_diff,
        'q3_diff': q3_diff,
        'composite_score': composite_score
   }
# Original data
y_original = df['mpg']
# Prepare features
make_encoded = pd.get_dummies(df['make'], prefix='make', drop_first=True)
X = pd.concat([df[['weight', 'model_year']], make_encoded], axis=1)
# Number of cross-validation iterations
n_{iterations} = 10
# Different bin counts to test
bin_counts = [3, 5, 8, 15, 25]
# Dictionary to store results for different bin counts
bin results = {}
bin_times = {}
all_distributions = {}
# Baseline: Origin stratification for comparison
all_y_test_origin = []
results_origin = []
origin_times = []
# Run cross-validation for origin stratification as baseline
for i in range(n_iterations):
   random_state = state_setter + i
    # Measure time for origin stratification
   start_time = time.time()
   # Method: Stratify by origin
   strat_var_origin = np.where(df['origin_america'], 'america',
                     np.where(df['origin_europe'], 'europe', 'asia'))
   X_train_origin, X_test_origin, y_train_origin, y_test_origin =
 ⇔train_test_split(
       X, y_original,
       test_size=0.2,
       random_state=random_state,
       stratify=strat_var_origin
```

```
end_time = time.time()
    origin_times.append(end_time - start_time)
    # Evaluate distribution
    results_origin.append(compare_distributions(y_original, y_test_origin,_u

¬"Origin"))
    all_y_test_origin.append(y_test_origin)
# Average origin results
avg_origin = {
    'ks_stat': np.mean([r['ks_stat'] for r in results_origin]),
    'w_distance': np.mean([r['w_distance'] for r in results_origin]),
    'mean_diff': np.mean([r['mean_diff'] for r in results_origin]),
    'std_diff': np.mean([r['std_diff'] for r in results_origin]),
    'composite_score': np.mean([r['composite_score'] for r in results_origin])
avg_origin_time = np.mean(origin_times)
# Run cross-validation for each bin count
for bin count in bin counts:
    method_name = f"MPG-{bin_count}bins"
    bin_results[method_name] = []
    bin_times[method_name] = []
    all_distributions[method_name] = []
    for i in range(n_iterations):
        random_state = state_setter + i
        # Measure time
        start_time = time.time()
        # Create bins and stratify
        mpg_bins = pd.qcut(df['mpg'], q=bin_count, labels=False,__

duplicates='drop')
        X_train_bins, X_test_bins, y_train_bins, y_test_bins = train_test_split(
            X, y_original,
            test_size=0.2,
            random_state=random_state,
            stratify=mpg_bins
        end_time = time.time()
        bin_times[method_name].append(end_time - start_time)
```

```
# Evaluate distribution
       bin_results[method_name].append(compare_distributions(y_original,_
 →y_test_bins, method_name))
        all_distributions[method_name].append(y_test_bins)
# Calculate averages for each bin count
avg_results = {}
for method_name in bin_results:
   avg_results[method_name] = {
        'ks_stat': np.mean([r['ks_stat'] for r in bin_results[method_name]]),
        'w_distance': np.mean([r['w_distance'] for r in_
 ⇔bin_results[method_name]]),
        'mean_diff': np.mean([r['mean_diff'] for r in_
 ⇒bin_results[method_name]]),
        'std diff': np.mean([r['std_diff'] for r in bin results[method name]]),
        'composite_score': np.mean([r['composite_score'] for r in_
 ⇔bin_results[method_name]])
   }
# Average times
avg times = {method: np.mean(times) for method, times in bin times.items()}
# Function to create a combined histogram
def create_averaged_histogram(all_samples):
   return pd.concat(all_samples)
# Create averaged histograms
avg_hist_origin = create_averaged_histogram(all_y_test_origin)
avg_hist_bins = {method: create_averaged_histogram(dists)
                for method, dists in all_distributions.items()}
# Visualize the distributions
plt.figure(figsize=(15, 10))
bins = np.linspace(5, 50, 15)
# Visualize the distributions
plt.figure(figsize=(15, 10))
bins = np.linspace(5, 50, 15)
# Original distribution
plt.subplot(2, 3, 1)
sns.histplot(y_original, bins=bins, kde=True, color='purple', stat='density')
plt.title('Original MPG Distribution')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
```

```
plt.xlim(5, 50)
# Different bin counts
colors = ['green', 'orange', 'red', 'brown', 'blue'] # Added blue as the 5th
 ⇔color
subplot positions = [2, 3, 4, 5, 6] # Using all positions in the 2x3 grid
for i, ((method, dist), color, pos) in enumerate(zip(avg_hist_bins.items(),__
 →colors, subplot_positions)):
    plt.subplot(2, 3, pos)
    sns.histplot(dist, bins=bins, kde=True, color=color, stat='density')
    plt.title(f'{method}\nScore: {avg results[method]["composite score"]:.

→4f}\nTime: {avg_times[method]*1000:.2f} ms')
    plt.xlabel('Miles Per Gallon (MPG)')
    plt.ylabel('Density')
    plt.grid(True, alpha=0.3)
    plt.xlim(5, 50)
plt.tight_layout()
plt.suptitle('MPG Distribution Comparison with Different Bin Counts (10-fold ∪
 →CV)\n(Lower Score = Better Match)', fontsize=16, y=1.02)
plt.show()
# Create a summary table
summary_data = []
# Add origin as baseline
summary_data.append({
    'Method': 'Origin',
    'Score': avg_origin['composite_score'],
    'Time (ms)': avg_origin_time * 1000,
    'KS Stat': avg_origin['ks_stat'],
    'W-Distance': avg_origin['w_distance'],
    'Mean Diff': avg_origin['mean_diff'],
    'Std Diff': avg_origin['std_diff']
})
# Add bin methods
for method in avg_results:
    summary_data.append({
        'Method': method,
        'Score': avg_results[method]['composite_score'],
        'Time (ms)': avg_times[method] * 1000,
        'KS Stat': avg_results[method]['ks_stat'],
        'W-Distance': avg_results[method]['w_distance'],
        'Mean Diff': avg_results[method]['mean_diff'],
        'Std Diff': avg_results[method]['std_diff']
```

```
summary_df = pd.DataFrame(summary_data)
```

For our small data set, using a big bin count still worked out! We'll use 25 bins in our final stratification.

A couple notes: - The 15 bin and 25 bin distributions were mapped to 12 bin diagrams for easy comparison across splits. - Bin Counts over 25, some bins only had a single sample and thus couldn't be stratified. 25 turned out to be the max we could support, which conveniently does not have performance implications for our data set.

4.1.5 Stratified Test Train Split We are finally ready to split the data! We will split it across 25 bins for mpg to keep the distribution equal.

```
[]: # 4.1.5 Test Train Split using MPG stratification with 25 bins
     # Original data
     y = df['mpg']
     # Prepare features
     make encoded = pd.get dummies(df['make'], prefix='make', drop first=True)
     X = pd.concat([df[['weight', 'model_year']], make_encoded], axis=1)
     # Create 25 mpg bins for stratification (our optimal bin count from earlier
     ⇔analysis)
     mpg_bins = pd.qcut(df['mpg'], q=25, labels=False, duplicates='drop')
     # Split the data with stratification
     X_train, X_test, y_train, y_test = train_test_split(
         Х, у,
         test_size=0.2,
         random_state=state_setter,
         stratify=mpg_bins
     )
     # Display the shapes of our training and testing sets
     print(f"X_train shape: {X_train.shape}")
     print(f"X_test shape: {X_test.shape}")
     print(f"y_train shape: {y_train.shape}")
     print(f"y_test shape: {y_test.shape}")
     # Visualize our final train/test distributions with the same number of bins
     plt.figure(figsize=(12, 5))
     # Define a fixed set of bins for both plots - using exactly 12 bins
     fixed_bins = np.linspace(y.min(), y.max(), 13) # 13 edges = 12 bins
```

```
plt.subplot(1, 2, 1)
sns.histplot(y_train, bins=fixed_bins, kde=True, color='blue', stat='density')
plt.title('MPG Distribution - Training Set')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
plt.subplot(1, 2, 2)
sns.histplot(y_test, bins=fixed_bins, kde=True, color='green', stat='density')
plt.title('MPG Distribution - Testing Set')
plt.xlabel('Miles Per Gallon (MPG)')
plt.ylabel('Density')
plt.grid(True, alpha=0.3)
plt.xlim(5, 50)
plt.tight_layout()
plt.show()
# Compare statistical measures to verify balance
print("\nTraining set MPG statistics:")
print(y train.describe())
print("\nTesting set MPG statistics:")
print(y_test.describe())
# Calculate distribution similarity score between original and test set
similarity_score = compare_distributions(y, y_test, "Final Split")
print(f"\nFinal test set similarity score: {similarity_score['composite_score']:

  .4f}")
```

Looks good. Onward to training.

1.8.2 4.2 Train model using Scikit-Learn model.fit() method

```
[]: # 4.2 Train model using Scikit-Learn's Linear Regression

# Initialize the linear regression model
lr_model = LinearRegression()

# Train the model on the training data
start_time = time.time()
lr_model.fit(X_train, y_train)
training_time = time.time() - start_time

print(f"Model trained in {training_time:.4f} seconds")

# Get the coefficients and intercept
```

```
print("\nModel Parameters:")
print(f"Intercept: {lr_model.intercept_:.4f}")
# Display some of the most influential coefficients
coefficients = pd.DataFrame({
    'Feature': X_train.columns,
    'Coefficient': lr_model.coef_
})
# Sort coefficients by absolute value (to find most influential features)
coefficients['Abs Coefficient'] = np.abs(coefficients['Coefficient'])
sorted_coeffs = coefficients.sort_values('Abs_Coefficient', ascending=False)
print("\nTop 10 most influential features:")
display(sorted_coeffs.head(10))
# Make predictions on the training and test sets
y_train_pred = lr_model.predict(X_train)
y_test_pred = lr_model.predict(X_test)
# Create a dataframe to store actual vs predicted values for the test set
results_df = pd.DataFrame({
    'Actual': y_test,
    'Predicted': y test pred,
    'Residual': y_test - y_test_pred
})
# Display the first few rows of predictions vs. actual values
print("\nSample of Actual vs. Predicted values (Test Set):")
display(results_df.head(10))
# Plot actual vs predicted for test set
plt.figure(figsize=(10, 6))
plt.scatter(y_test, y_test_pred, alpha=0.7)
plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')
plt.xlabel('Actual MPG')
plt.ylabel('Predicted MPG')
plt.title('Actual vs. Predicted MPG (Test Set)')
plt.grid(True, alpha=0.3)
plt.tight_layout()
plt.show()
```

Trained and ready for evaluation. Clearly our makes had a big impact!

1.8.3 4.3 Evalulate performance

4.3.1 Regression: R², MAE, RMSE

```
[]: # 4.3.1 Evaluate performance with R^2, MAE, and RMSE
     # Function to calculate and display performance metrics
     def evaluate_model(y_true, y_pred, dataset_name):
        # Calculate metrics
        r2 = r2_score(y_true, y_pred)
        mae = mean_absolute_error(y_true, y_pred)
        rmse = np.sqrt(mean_squared_error(y_true, y_pred))
         # Calculate additional metrics
        # Mean Absolute Percentage Error (MAPE)
        mape = np.mean(np.abs((y_true - y_pred) / y_true)) * 100
        # Median Absolute Error
        med_ae = np.median(np.abs(y_true - y_pred))
         # Print metrics
        print(f"\n--- {dataset_name} Metrics ---")
        print(f"R2 Score: {r2:.4f}")
        print(f"Mean Absolute Error (MAE): {mae:.4f}")
        print(f"Root Mean Squared Error (RMSE): {rmse:.4f}")
        print(f"Mean Absolute Percentage Error (MAPE): {mape:.2f}%")
        print(f"Median Absolute Error: {med_ae:.4f}")
        return {
             'R2': r2,
             'MAE': mae,
             'RMSE': rmse,
             'MAPE': mape,
             'MedianAE': med_ae
        }
     # Evaluate on training set
     train_metrics = evaluate_model(y_train, y_train_pred, "Training Set")
     # Evaluate on test set
     test_metrics = evaluate_model(y_test, y_test_pred, "Test Set")
     # Compare training vs test metrics to check for overfitting
     metrics_comparison = pd.DataFrame({
         'Training': [train_metrics['R2'], train_metrics['MAE'], __

¬train_metrics['RMSE']],
         'Testing': [test_metrics['R2'], test_metrics['MAE'], test_metrics['RMSE']]
     }, index=['R² Score', 'Mean Absolute Error (MAE)', 'Root Mean Squared Error⊔
      print("\n--- Training vs Testing Performance ---")
```

```
display(metrics_comparison)
```

- 1.8.4 Reflection 4: How well did the model perform? Any surprises in the results?
- 1.9 Section 5. Improve the Model or Try Alternates (Implement Pipelines)
- 1.9.1 5.1 Implement Pipeline 1: Imputer \rightarrow StandardScaler \rightarrow Linear Regression.

```
[]: # 5.1 Implement Pipeline 1: Imputer → StandardScaler → Linear Regression
     print("### 5.1 Pipeline 1: Imputer → StandardScaler → Linear Regression ###")
     # Create a pipeline with imputer, scaler, and linear regression
     pipeline1 = Pipeline([
         ('imputer', SimpleImputer(strategy='median')),
         ('scaler', StandardScaler()),
         ('regressor', LinearRegression())
     ])
     # Train the pipeline on the training data
     start_time = time.time()
     pipeline1.fit(X_train, y_train)
     pipeline1_training_time = time.time() - start_time
     print(f"Pipeline 1 trained in {pipeline1_training_time:.4f} seconds")
     # Make predictions on training and test sets
     y_train_pred_pipeline1 = pipeline1.predict(X_train)
     y_test_pred_pipeline1 = pipeline1.predict(X_test)
     # Evaluate pipeline1 performance
     train_metrics_pipeline1 = evaluate_model(y_train, y_train_pred_pipeline1,_

¬"Pipeline 1 (Training Set)")
     test_metrics_pipeline1 = evaluate_model(y_test, y_test_pred_pipeline1,_

¬"Pipeline 1 (Test Set)")
     # Get the linear regression model from the pipeline
     linear_model = pipeline1.named_steps['regressor']
     # Display some information about the model
     print("\nPipeline 1 Model Parameters:")
     print(f"Intercept: {linear_model.intercept_:.4f}")
     # Display top coefficients (note: these are scaled coefficients now)
     coefficients_pipeline1 = pd.DataFrame({
         'Feature': X_train.columns,
         'Coefficient': linear_model.coef_
     })
```

```
# Sort coefficients by absolute value
coefficients_pipeline1['Abs_Coefficient'] = np.
 →abs(coefficients_pipeline1['Coefficient'])
sorted_coeffs_pipeline1 = coefficients_pipeline1.sort_values('Abs_Coefficient',_
 ⇔ascending=False)
print("\nTop 10 most influential features (after scaling):")
display(sorted_coeffs_pipeline1.head(10))
# Visualize actual vs predicted for test set
plt.figure(figsize=(10, 6))
plt.scatter(y_test, y_test_pred_pipeline1, alpha=0.7)
plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')
plt.xlabel('Actual MPG')
plt.ylabel('Predicted MPG')
plt.title('Pipeline 1: Actual vs. Predicted MPG (Test Set)')
plt.grid(True, alpha=0.3)
plt.tight_layout()
plt.show()
# Create a dataframe to store actual vs predicted values for the test set
results_df_pipeline1 = pd.DataFrame({
    'Actual': y_test,
    'Predicted': y_test_pred_pipeline1,
    'Residual': y_test - y_test_pred_pipeline1
})
```

1.9.2 5.2 Implement Pipeline 2: Imputer \rightarrow Polynomial Features (degree=3) \rightarrow StandardScaler \rightarrow Linear Regression.

```
[]: # 5.2 Implement Pipeline 2: Imputer → Polynomial Features (degree=3) →

StandardScaler → Linear Regression

print("\n### 5.2 Pipeline 2: Imputer → Polynomial Features (degree=3) →

StandardScaler → Linear Regression ###")

# Create a pipeline with imputer, polynomial features, scaler, and linear

→regression

pipeline2 = Pipeline([
    ('imputer', SimpleImputer(strategy='median')),
    ('poly', PolynomialFeatures(degree=3, include_bias=False)),
    ('scaler', StandardScaler()),
    ('regressor', LinearRegression())

])

# Use all features including make dummies
```

```
# No need to restrict to only numerical features since you mentioned your
 ⇔processor can handle it
X_train_full = X_train.copy() # Use all features
X test full = X test.copy() # Use all features
# Print feature count to understand the scale
print(f"Number of input features: {X train full.shape[1]}")
print(f"Expected polynomial features (degree=3): {int((X_train_full.shape[1] +__
 # Train the pipeline on the training data with all features
start time = time.time()
pipeline2.fit(X_train_full, y_train)
pipeline2_training_time = time.time() - start_time
print(f"Pipeline 2 trained in {pipeline2_training_time:.4f} seconds")
# Make predictions on training and test sets
y_train_pred_pipeline2 = pipeline2.predict(X_train_full)
y_test_pred_pipeline2 = pipeline2.predict(X_test_full)
# Evaluate pipeline2 performance
train_metrics_pipeline2 = evaluate_model(y_train, y_train_pred_pipeline2,__

¬"Pipeline 2 (Training Set)")
test metrics pipeline2 = evaluate model(y test, y test pred pipeline2,

¬"Pipeline 2 (Test Set)")
# Get all feature names for reference
# Since we're using all features, we need to get all column names
feature_names = X_train_full.columns.tolist()
# Get the polynomial feature names
poly features = pipeline2.named steps['poly'].
 →get_feature_names_out(feature_names)
# Get the linear regression model from the pipeline
linear_model2 = pipeline2.named_steps['regressor']
# Display model information
print("\nPipeline 2 Model Parameters:")
print(f"Intercept: {linear_model2.intercept_:.4f}")
print(f"Number of features after polynomial transformation:
 →{len(poly_features)}")
# Display top coefficients
coefficients_pipeline2 = pd.DataFrame({
```

```
'Feature': poly_features,
    'Coefficient': linear_model2.coef_
})
# Sort coefficients by absolute value
coefficients_pipeline2['Abs_Coefficient'] = np.
 ⇔abs(coefficients_pipeline2['Coefficient'])
sorted_coeffs_pipeline2 = coefficients_pipeline2.sort_values('Abs_Coefficient',__
 ⇔ascending=False)
print("\nTop 10 most influential polynomial features (after scaling):")
display(sorted coeffs pipeline2.head(10))
# Visualize actual vs predicted for test set
plt.figure(figsize=(10, 6))
plt.scatter(y_test, y_test_pred_pipeline2, alpha=0.7)
plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')
plt.xlabel('Actual MPG')
plt.ylabel('Predicted MPG')
plt.title('Pipeline 2: Actual vs. Predicted MPG (Test Set)')
plt.grid(True, alpha=0.3)
plt.tight_layout()
plt.show()
# Create a dataframe to store actual vs predicted values for the test set
results_df_pipeline2 = pd.DataFrame({
    'Actual': y test,
    'Predicted': y_test_pred_pipeline2,
    'Residual': y_test - y_test_pred_pipeline2
})
```

1.9.3 5.3 Compare performance of all models across the same performance metrics

```
}, index=['R2 Score', 'Mean Absolute Error (MAE)', 'Root Mean Squared Error⊔
 → (RMSE)', 'Mean Absolute Percentage Error (MAPE)'])
print("\n--- Test Set Performance Comparison ---")
display(models_comparison)
# Training time comparison
training_times = pd.DataFrame({
    'Model': ['Baseline Linear Regression', 'Pipeline 1 (Scaling)', 'Pipeline 2_{\sqcup}
 ⇔(Polynomial)'],
    'Training Time (seconds)': [training_time, pipeline1_training_time, u
 →pipeline2_training_time]
})
print("\n--- Training Time Comparison ---")
display(training_times)
# Visualize performance comparison - fixed version
metrics_to_plot = ['R2 Score', 'Mean Absolute Error (MAE)', 'Root Mean Squared_

→Error (RMSE)']
fig, axes = plt.subplots(1, 3, figsize=(15, 5))
# Plot each metric
for i, metric in enumerate(metrics_to_plot):
    values = models_comparison.loc[metric].values
    model_names = models_comparison.columns
    # For R2, higher is better
    if metric == 'R2 Score':
        axes[i].bar(range(len(model_names)), values)
        axes[i].set_title(f'Comparison of {metric}\n(higher is better)')
    # For error metrics, lower is better
    else:
        axes[i].bar(range(len(model_names)), values)
        axes[i].set_title(f'Comparison of {metric}\n(lower is better)')
    axes[i].set_xticks(range(len(model_names)))
    axes[i].set_xticklabels(model_names, rotation=45, ha='right')
    axes[i].grid(True, alpha=0.3)
    # Add value labels on top of bars
    for j, v in enumerate(values):
        axes[i].text(j, v + (0.01 \text{ if metric} == \frac{R^2}{R^2} \text{ Score'} \text{ else } 0.05),
                    f'{v:.3f}', ha='center', va='bottom')
plt.tight_layout()
plt.show()
```

Looks like the simple linear regression beat both Pipeline 1 and Pipeline 2 on R²! We will review further in our Reflection and Section 6.

```
[]: # Create a scatter plot of all models predictions vs actual values
    plt.figure(figsize=(15, 5))
    # Base model
    plt.subplot(1, 3, 1)
    plt.scatter(y_test, y_test_pred, alpha=0.7)
    plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')
    plt.xlabel('Actual MPG')
    plt.ylabel('Predicted MPG')
    plt.title(f'Baseline Linear Regression\nR2 = {test metrics["R2"]:.3f}, RMSE = [1]
      plt.grid(True, alpha=0.3)
    # Pipeline 1
    plt.subplot(1, 3, 2)
    plt.scatter(y_test, y_test_pred_pipeline1, alpha=0.7)
    plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')
    plt.xlabel('Actual MPG')
    plt.ylabel('Predicted MPG')
    plt.title(f'Pipeline 1 (Scaling)\nR2 = {test_metrics_pipeline1["R2"]:.3f}, RMSE_
      ←= {test_metrics_pipeline1["RMSE"]:.3f}')
    plt.grid(True, alpha=0.3)
    # Pipeline 2
    plt.subplot(1, 3, 3)
    plt.scatter(y_test, y_test_pred_pipeline2, alpha=0.7)
    plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')
    plt.xlabel('Actual MPG')
    plt.ylabel('Predicted MPG')
    plt.title(f'Pipeline 2 (Polynomial)\nR2 = {test_metrics_pipeline2["R2"]:.3f},__
      →RMSE = {test_metrics_pipeline2["RMSE"]:.3f}')
    plt.grid(True, alpha=0.3)
    plt.tight_layout()
    plt.show()
```

Here are the distributions themselves. I am curious as to why Pipeline 1 and the Baseline LR got identical results. We will review further below. In the meantime, I want to give the Polynomial a fighting chance and try a few different degrees...

5.3.1 Polynomial optimization Despite our categorical variables, I wanted to see how well the models would calculate when we try higher degrees, and if we could achieve better results.

```
[]: # 5.3.1 Optimizing Polynomial Degree (Testing degrees 3, 4, 6, and 9)
     print("\n### 5.3.1 Optimizing Polynomial Degree ###")
     # Degrees to test
     poly_degrees = [3, 4, 5, 7]
     # Dictionary to store results for each degree
     poly results = {}
     poly_train_metrics = {}
     poly test metrics = {}
     poly_training_times = {}
     poly_predictions = {}
     # Only use numerical features to avoid feature explosion
     X_train_numeric = X_train[['weight', 'model_year']]
     X_test_numeric = X_test[['weight', 'model_year']]
     # Test each polynomial degree
     for degree in poly_degrees:
         print(f"\nTesting Polynomial Degree {degree}")
         # Create pipeline with the current degree
         poly pipeline = Pipeline([
             ('imputer', SimpleImputer(strategy='median')),
             ('poly', PolynomialFeatures(degree=degree, include_bias=False)),
             ('scaler', StandardScaler()), # Important to scale after polynomial
      \hookrightarrow transformation
             ('regressor', LinearRegression())
         ])
         # Train the pipeline
         start_time = time.time()
         poly_pipeline.fit(X_train_numeric, y_train)
         train_time = time.time() - start_time
         poly_training_times[degree] = train_time
         print(f"Training time: {train_time:.4f} seconds")
         # Get the polynomial feature names
         poly_features = poly_pipeline.named_steps['poly'].

¬get_feature_names_out(['weight', 'model_year'])
         print(f"Number of features after polynomial transformation:
      →{len(poly_features)}")
         # Make predictions
         y_train_pred = poly_pipeline.predict(X_train_numeric)
```

```
y_test_pred = poly_pipeline.predict(X_test_numeric)

# Store predictions for later visualization
poly_predictions[degree] = {
    'train': y_train_pred,
    'test': y_test_pred
}

# Evaluate performance
train_metrics = evaluate_model(y_train, y_train_pred, f"Degree {degree}_\_
(Training Set)")
test_metrics = evaluate_model(y_test, y_test_pred, f"Degree {degree} (Test_\_
Set)")

# Store results
poly_results[degree] = poly_pipeline
poly_train_metrics[degree] = train_metrics
poly_test_metrics[degree] = test_metrics
```

R² increases slightly with degree 4, but then clearly drops off quickly from overfitting.

```
if metric == 'R2 Score':
        axes[i].bar(x_pos, values, color='green')
        axes[i].set_title(f'Comparison of {metric}\n(higher is better)')
    # For error metrics, lower is better
    else:
        axes[i].bar(x_pos, values, color='blue')
        axes[i].set_title(f'Comparison of {metric}\n(lower is better)')
    axes[i].set xticks(x pos)
    axes[i].set_xticklabels([f'Degree {d}' for d in poly_degrees])
    axes[i].grid(True, alpha=0.3)
    # Add value labels on top of bars
    for j, v in enumerate(values):
        axes[i].text(j, v + (0.01 \text{ if metric} == \frac{R^2}{N^2} \frac{\text{Score}}{\text{else } 0.05}),
                    f'{v:.3f}', ha='center', va='bottom')
plt.tight_layout()
plt.show()
\# Check for signs of overfitting by comparing R^2 on training vs test sets
plt.figure(figsize=(10, 6))
train_r2 = [poly_train_metrics[d]['R2'] for d in poly_degrees]
test_r2 = [poly_test_metrics[d]['R2'] for d in poly_degrees]
x = range(len(poly_degrees))
width = 0.35
plt.bar([i - width/2 for i in x], train r2, width, label='Training R2', u

color='green', alpha=0.7)

plt.bar([i + width/2 for i in x], test_r2, width, label='Test R2',u

color='blue', alpha=0.7)
plt.xlabel('Polynomial Degree')
plt.ylabel('R2 Score')
plt.title('Training vs Test R² Score (Higher gap indicates potential⊔
 ⇔overfitting)')
plt.xticks(x, [f'{d}' for d in poly_degrees])
plt.legend()
plt.grid(True, alpha=0.3)
# Add value labels
for i, v in enumerate(train r2):
    plt.text(i - width/2, v + 0.01, f'{v:.3f}', ha='center', va='bottom')
for i, v in enumerate(test_r2):
    plt.text(i + width/2, v + 0.01, f'{v:.3f}', ha='center', va='bottom')
```

```
plt.tight_layout()
plt.show()
```

Interesiting to see test vs training improvements on 3, 4, and 5, but on degree 4, both test and training R^2 capped out. The degree 7 training R^2 was the highest of any training R^2 , but had by far the least test R^2 - a classic sign of extreme overfitting.

- 1.9.4 Reflection 5: Which models performed better? How does scaling impact results?
- 1.10 Section 6. Final Thoughts & Insights
- 1.10.1 6.1 Summarize findings.
- 1.10.2 6.2 Discuss challenges faced.
- 1.10.3 6.3 If you had more time, what would you try next?
- 1.10.4 Reflection 6: What did you learn from this project?