Task 1 (20 points): Advanced Objective Function and Use Case

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1. Deriving the Logistic Regression Objective Function via MLE

1.1. Setup and Likelihood

Consider a binary classification problem with data $\left(x^{(i)}, y^{(i)}\right)$, where:

- $x^{(i)} \in R^n$ is the feature vector for the i-th sample.
- $y^{(i)} \in \{0, 1\}$ is the class label.

For Logistic Regression, we model the probability that $y^{(i)}=1$ as:

$$P\left(y^{(i)}=1 \mid x^{(i)}, \theta\right)=\sigma\left(\theta^T x^{(i)}\right),$$

where $\sigma(z)$ is the sigmoid function:

$$\sigma(z)=\frac{1}{1+e^{-z}}.$$

We can write:

$$P\left(y^{(i)}=0 \mid x^{(i)}, \theta\right)=1-\sigma\left(\theta^T x^{(i)}\right).$$

1.2. Likelihood Function

Assuming i.i.d. (independent and identically distributed) data, the likelihood $L(\theta)$ is:

$$ \mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1}^{m} \sigma\bigl(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\bigr)^{y^{(i)}} \Bigl[1 - \sigma\bigl(\boldsymbol{\theta}^T \mathbf{x}^{(i)}\bigr)\Bigr]^{1 - y^{(i)}}. $$

1.3. Log-Likelihood

To simplify, we take the log of the likelihood (the **log-likelihood**):

$$ \ell(\boldsymbol{\theta}) = \sum_{i=1}^{m} \Bigl[y^{(i)} \log\bigl(\sigma(\boldsymbol{\theta}^T \mathbf{x}^{(i)})\bigr) + (1 - y^{(i)}) \log\bigl(1 - \sigma(\boldsymbol{\theta}^T \mathbf{x}^{(i)})\bigr) \Bigr]. $$

1.4. MLE Objective Function

The Maximum Likelihood Estimation (MLE) approach maximizes $\ell(\theta)$, or equivalently minimizes the **negative log-likelihood**:

$$ J(\boldsymbol{\theta}) = - \ell(\boldsymbol{\theta}) = - \sum_{i=1}^{m} \Bigl[y^{(i)} \log\bigl(\sigma(\boldsymbol{\theta}^T \mathbf{x}^{(i)})\bigr) + (1 - y^{(i)}) \log\bigl(1 - \sigma(\boldsymbol{\theta}^T \mathbf{x}^{(i)})\bigr) \Bigr]. $$

This function is also known as the **binary cross-entropy loss**.

2. MAP Technique vs. MLE

2.1. Overview of MAP

MLE focuses solely on maximizing the likelihood $L(\theta)$ based on observed data.
MAP (**Maximum A Posteriori**) incorporates a **prior distribution** $p(\theta)$. Instead of maximizing $P(y \mid X, \theta)$ alone, we maximize the **posterior** $p(\theta \mid X, y)$:

$$ \boldsymbol{\theta}_{MAP} = \arg \max_{\boldsymbol{\theta}} \Bigl[p(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\theta}) \, p(\boldsymbol{\theta}) \Bigr]. $$

Taking logs:

$$ \boldsymbol{\theta}_{MAP} = \arg \max_{\boldsymbol{\theta}} \Bigl[\log p(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta}) \Bigr]. $$

2.2. Difference Between MLE and MAP

- **MLE** can be seen as a special case of MAP where the prior $p(\theta)$ is uniform (i.e., no prior preference).
- **MAP** allows incorporating domain knowledge or regularization into the model (e.g., Gaussian prior leads to **L2** regularization).

Thus, **MAP** solutions often help prevent overfitting by penalizing large parameter values, providing a more robust estimate when data is limited.

Citations:

1. Bishop, C. M. (2006). *Pattern Recognition and Machine Learning.* Springer.

2. Murphy, K. P. (2012). *Machine Learning: A Probabilistic Perspective.* MIT Press.

3. Ng, A. (2004). *Feature Selection, L1 vs. L2 Regularization, and Rotational Invariance.* (Stanford CS229 Lecture Notes)

3. Defining a Machine Learning Problem & Justification

3.1. Proposed Machine Learning Problem

Use Case: **Email Spam Classification**

- **Goal**: Predict whether an incoming email is spam (1) or not spam (0).

- **Data**: Features might include word frequencies, presence of certain keywords, sender domain, etc.

3.2. Why Logistic Regression?

- **Probabilistic Output**: Logistic regression directly provides $P(\text{spam} \mid x)$, which is useful for thresholding or ranking by spam probability.
- **Interpretability**: We can easily interpret coefficients (e.g., certain keywords have high positive weights, meaning they strongly indicate spam).
- **Efficiency**: For moderate-to-large datasets, logistic regression is relatively fast to train and often yields robust performance.

3.3. Comparison to Another Linear Model: Linear SVM (Briefly)

- **Linear SVM** also tries to separate spam vs. not spam with a hyperplane but focuses on maximizing the margin.
- **Difference**: SVM does not provide a direct probability output; it focuses on the decision boundary.
- **When to choose LR**: If you need probability estimates, logistic regression is more natural.
- **When to choose SVM**: If you primarily want a robust margin-based classifier and can handle a separate calibration step for probabilities if needed.

(Reference: Cortes, C. & Vapnik, V. (1995). Support-vector networks.)

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4. Mapping Dataset Variables to the Logistic Regression Equations

Assume we have a dataset $\{(x^{(i)}, y^{(i)})\}_{i=1}^{m}$:

- $x^{(i)}$: A vector of features (e.g., the presence of certain words, hours since last known spam, etc.).
- $y^{(i)}$: 1 if the email is spam, 0 otherwise.

In the derivation of the MLE objective:

- Each sample's **likelihood** contribution is $\sigma\left(\theta^T x^{(i)}\right)$ if $y^{(i)}=1$ and $1-\sigma\left(\theta^T x^{(i)}\right)$ if $y^{(i)}=0$.
- We assume the **i.i.d.** property: Each email is independent of others (an assumption that might be imperfect if emails come in threads or have temporal dependencies, but is typically acceptable in practice).

To do **MAP**, we might add a prior on θ (e.g., Gaussian prior leading to L2 regularization).

Hence, the objective function is the negative log-likelihood (or negative log posterior for MAP) applied to the sum over all emails.

Task 2: Dataset and Advanced EDA

1. Dataset Overview

For this task, I will use the **Bike Sharing Demand** dataset from Kaggle. This dataset provides hourly rental data spanning two years and includes features such as temperature, humidity, wind speed, and whether the day is a holiday or not.

Dataset Link: Bike Sharing Demand on Kaggle

Data Fields

- **datetime**: Hourly date + timestamp
- **season**: 1 = spring, 2 = summer, 3 = fall, 4 = winter
- **holiday**: Whether the day is a holiday
- **workingday**: Whether the day is neither a weekend nor a holiday
- **weather**:
    a. Clear, Few clouds, Partly cloudy, Partly cloudy
    b. Mist + Cloudy, Mist + Broken clouds, Mist + Few clouds, Mist
    c. Light Snow, Light Rain + Thunderstorm + Scattered clouds, Light Rain + Scattered clouds
    d. Heavy Rain + Ice Pallets + Thunderstorm + Mist, Snow + Fog
- **temp**: Temperature in Celsius
- **atemp**: "Feels like" temperature in Celsius
- **humidity**: Relative humidity

- **windspeed**: Wind speed
- **casual**: Number of non-registered user rentals
- **registered**: Number of registered user rentals
- **count**: Total number of rentals (target)

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

# For VIF calculation
from statsmodels.stats.outliers_influence import
variance_inflation_factor
import statsmodels.api as sm

from scipy.cluster import hierarchy

sns.set(style='whitegrid', context='notebook')
plt.rcParams['figure.figsize'] = (10, 6)


df = pd.read_csv('bike_train.csv')


print("First 5 rows of the dataset:")
display(df.head())

print("Dataset Info:")
df.info()

print("Statistical Description:")
display(df.describe(include='all'))

print("Number of missing values per column:")
print(df.isnull().sum())
```

```
First 5 rows of the dataset:
```


```
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\"fields\": [\n    {\n      \"column\": \"datetime\",\n
\"properties\": {\n        \"dtype\": \"object\",\n
\"num_unique_values\": 5,\n        \"samples\": [\n          \"2011-
01-01 01:00:00\",\n          \"2011-01-01 04:00:00\",\n
\"2011-01-01 02:00:00\"\n        ],\n        \"semantic_type\": \"\",\
n        \"description\": \"\"\n      }\n    },\n    {\n
\"column\": \"season\",\n      \"properties\": {\n        \"dtype\":
\"number\",\n        \"std\": 0,\n        \"min\": 1,\n
\"max\": 1,\n        \"num_unique_values\": 1,\n        \"samples\":
```

```
[\n          1\n        ],\n        \"semantic_type\": \"\",\n
\"description\": \"\"\n      }\n    },\n    {\n      \"column\":
\"holiday\",\n      \"properties\": {\n        \"dtype\": \"number\",\
n        \"std\": 0,\n        \"min\": 0,\n        \"max\": 0,\n
\"num_unique_values\": 1,\n        \"samples\": [\n          0\n
],\n        \"semantic_type\": \"\",\n        \"description\": \"\"\n
}\n    },\n    {\n      \"column\": \"workingday\",\n
\"properties\": {\n        \"dtype\": \"number\",\n        \"std\":
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\"num_unique_values\": 1,\n        \"samples\": [\n          0\n
],\n        \"semantic_type\": \"\",\n        \"description\": \"\"\n
}\n    },\n    {\n      \"column\": \"weather\",\n
\"properties\": {\n        \"dtype\": \"number\",\n        \"std\":
0,\n        \"min\": 1,\n        \"max\": 1,\n
\"num_unique_values\": 1,\n        \"samples\": [\n          1\n
],\n        \"semantic_type\": \"\",\n        \"description\": \"\"\n
}\n    },\n    {\n      \"column\": \"temp\",\n      \"properties\":
{\n        \"dtype\": \"number\",\n        \"std\":
0.44913249715423637,\n        \"min\": 9.02,\n        \"max\": 9.84,\n
\"num_unique_values\": 2,\n        \"samples\": [\n          9.02\n
],\n        \"semantic_type\": \"\",\n        \"description\": \"\"\n
}\n    },\n    {\n      \"column\": \"atemp\",\n      \"properties\":
{\n        \"dtype\": \"number\",\n        \"std\":
0.41626914370392615,\n        \"min\": 13.635,\n        \"max\":
14.395,\n        \"num_unique_values\": 2,\n        \"samples\": [\n
13.635\n        ],\n        \"semantic_type\": \"\",\n
\"description\": \"\"\n      }\n    },\n    {\n      \"column\":
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\"number\",\n        \"std\": 2,\n        \"min\": 75,\n
\"max\": 81,\n        \"num_unique_values\": 3,\n        \"samples\":
[\n          81\n        ],\n        \"semantic_type\": \"\",\n
\"description\": \"\"\n      }\n    },\n    {\n      \"column\":
\"windspeed\",\n      \"properties\": {\n        \"dtype\":
\"number\",\n        \"std\": 0.0,\n        \"min\": 0.0,\n
\"max\": 0.0,\n        \"num_unique_values\": 1,\n        \"samples\":
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\"description\": \"\"\n      }\n    },\n    {\n      \"column\":
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\"num_unique_values\": 4,\n        \"samples\": [\n          8\n
],\n        \"semantic_type\": \"\",\n        \"description\": \"\"\n
}\n    },\n    {\n      \"column\": \"registered\",\n
\"properties\": {\n        \"dtype\": \"number\",\n        \"std\":
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\"num_unique_values\": 5,\n        \"samples\": [\n          32\n
],\n        \"semantic_type\": \"\",\n        \"description\": \"\"\n
}\n    },\n    {\n      \"column\": \"count\",\n      \"properties\":
{\n        \"dtype\": \"number\",\n        \"std\": 15,\n
\"min\": 1,\n        \"max\": 40,\n        \"num_unique_values\": 5,\n
```

\"samples\": [\n   40\n   ],\n   \"semantic_type\": \"\",\n   \"description\": \"\"\n   }\n   }\n]\n}","type":"dataframe"}

```
Dataset Info:
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 10886 entries, 0 to 10885
Data columns (total 12 columns):
 #   Column      Non-Null Count  Dtype
---  ------      --------------  -----
 0   datetime    10886 non-null  object
 1   season      10886 non-null  int64
 2   holiday     10886 non-null  int64
 3   workingday  10886 non-null  int64
 4   weather     10886 non-null  int64
 5   temp        10886 non-null  float64
 6   atemp       10886 non-null  float64
 7   humidity    10886 non-null  int64
 8   windspeed   10886 non-null  float64
 9   casual      10886 non-null  int64
 10  registered  10886 non-null  int64
 11  count       10886 non-null  int64
dtypes: float64(3), int64(8), object(1)
memory usage: 1020.7+ KB
Statistical Description:
```

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```
],\n        \"semantic_type\": \"\",\n        \"description\": \"\"\n
}\n    },\n    {\n      \"column\": \"weather\",\n
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4.0\n        ],\n        \"semantic_type\": \"\",\n
\"description\": \"\"\n      }\n    },\n    {\n      \"column\":
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\"std\": 3842.2088126431295,\n        \"min\": 0.82,\n        \"max\":
10886.0,\n        \"num_unique_values\": 8,\n        \"samples\": [\n
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\"semantic_type\": \"\",\n        \"description\": \"\"\n      }\
n    },\n    {\n      \"column\": \"atemp\",\n      \"properties\": {\
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\"min\": 0.76,\n        \"max\": 10886.0,\n
\"num_unique_values\": 8,\n        \"samples\": [\n
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\"semantic_type\": \"\",\n        \"description\": \"\"\n      }\
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n        \"num_unique_values\": 8,\n        \"samples\": [\n
61.88645967297446,\n          62.0,\n          10886.0\n        ],\n
\"semantic_type\": \"\",\n        \"description\": \"\"\n      }\
n    },\n    {\n      \"column\": \"windspeed\",\n
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\"num_unique_values\": 8,\n        \"samples\": [\n
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\"semantic_type\": \"\",\n        \"description\": \"\"\n      }\
n    },\n    {\n      \"column\": \"casual\",\n      \"properties\":
{\n        \"dtype\": \"number\",\n        \"std\":
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n        \"num_unique_values\": 8,\n        \"samples\": [\n
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\"semantic_type\": \"\",\n        \"description\": \"\"\n      }\
n    },\n    {\n      \"column\": \"registered\",\n
\"properties\": {\n        \"dtype\": \"number\",\n        \"std\":
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\"num_unique_values\": 8,\n        \"samples\": [\n
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\"semantic_type\": \"\",\n        \"description\": \"\"\n      }\
n    },\n    {\n      \"column\": \"count\",\n      \"properties\": {\
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\"min\": 1.0,\n        \"max\": 10886.0,\n
\"num_unique_values\": 8,\n        \"samples\": [\n
191.57413191254824,\n          145.0,\n          10886.0\n        ],\n
```

\"semantic_type\": \"\",\n   \"description\": \"\"\n   }\
n   }\n]\n}","type":"dataframe"}

```
Number of missing values per column:
datetime      0
season        0
holiday       0
workingday    0
weather       0
temp          0
atemp         0
humidity      0
windspeed     0
casual        0
registered    0
count         0
dtype: int64
```

2. Data Cleaning & Feature Preparation

We will:

1. Convert `datetime` to a proper datetime object.
2. Extract additional time-related features (e.g., hour, day, month, year) if needed.
3. Check for (and handle) missing values and outliers.

```
# Convert datetime column
df['datetime'] = pd.to_datetime(df['datetime'])

df['hour'] = df['datetime'].dt.hour
df['day'] = df['datetime'].dt.day
df['month'] = df['datetime'].dt.month
df['year'] = df['datetime'].dt.year

# Confirm no missing values remain
print(df.isnull().sum())
```

```
datetime      0
season        0
holiday       0
workingday    0
weather       0
temp          0
atemp         0
humidity      0
windspeed     0
casual        0
registered    0
count         0
hour          0
```

```
day            0
month          0
year           0
dtype: int64
```

3. Exploratory Data Analysis (EDA)

3.1. Univariate Analysis

We will examine the distribution of key features, including:

- **count** (target)
- **temp**, **atemp**
- **humidity**, **windspeed**
- **hour**, **day**, etc.

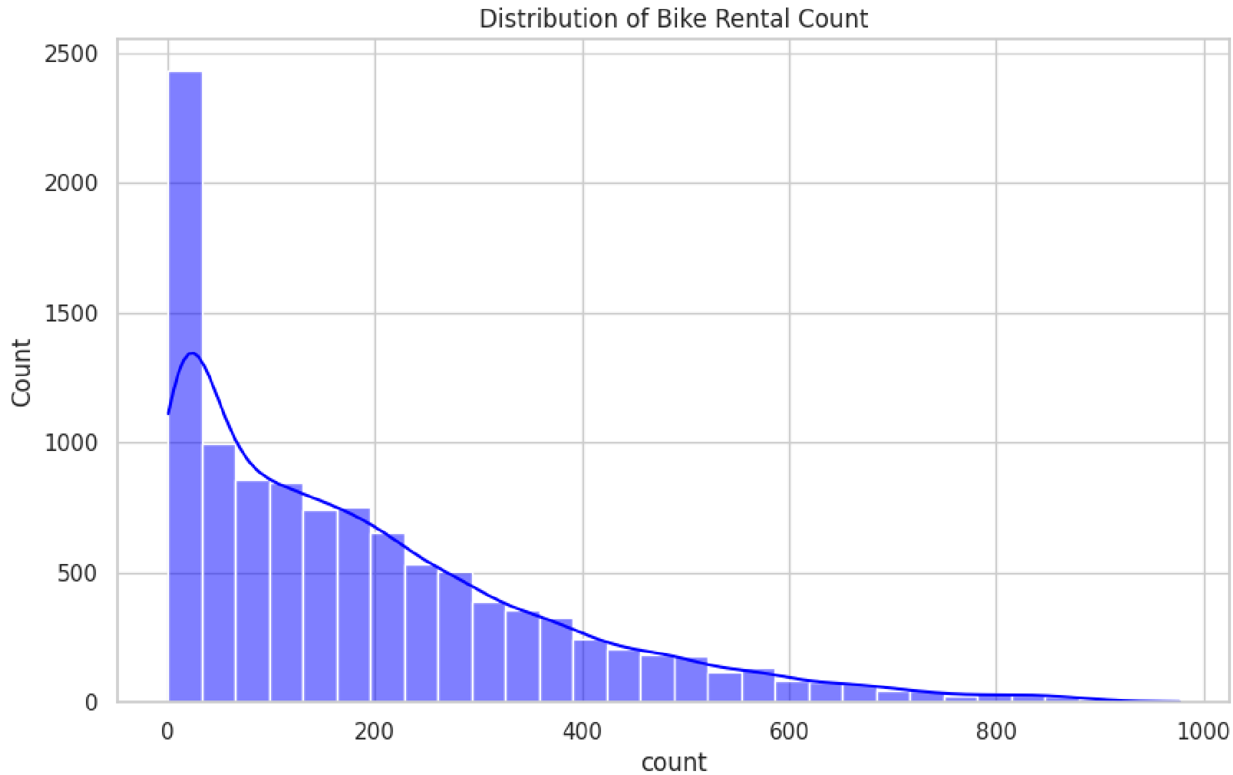
3.2. Bivariate Analysis

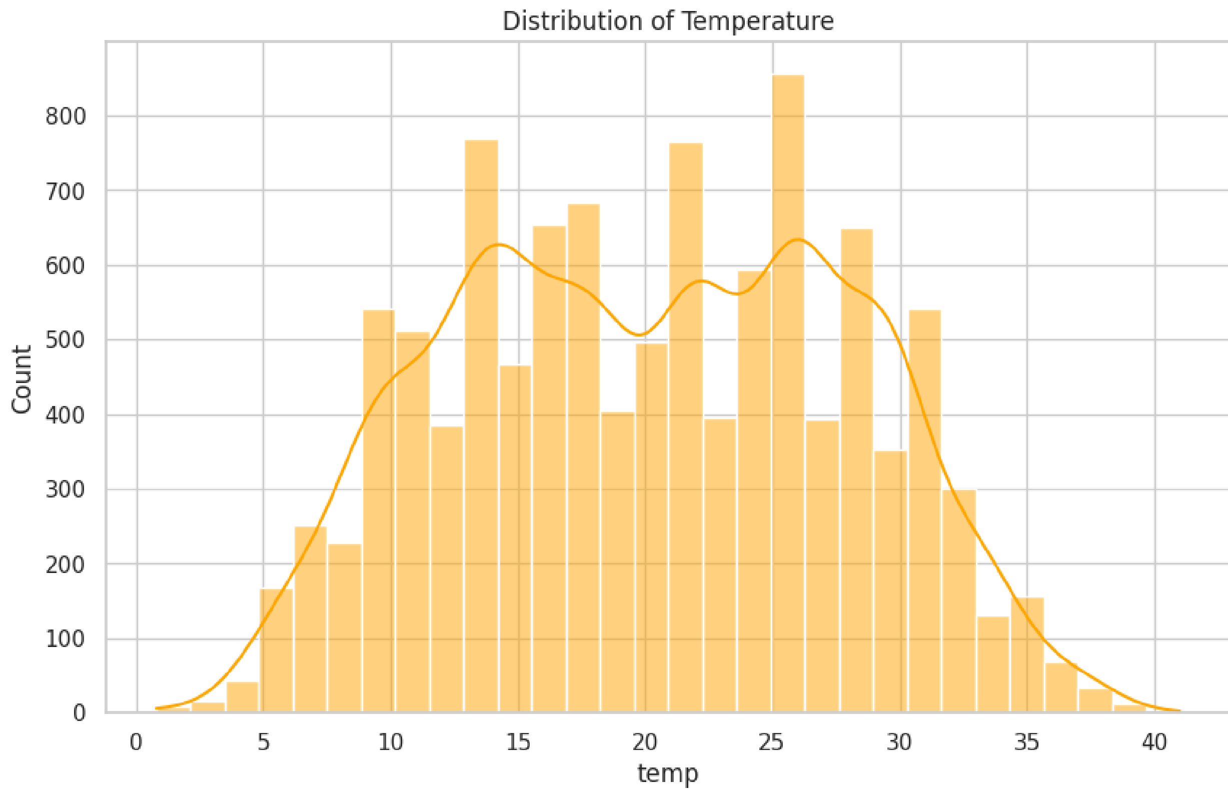
We will look at how different features relate to the target (`count`).

In addition, we will address the potential **multicollinearity** among features using **Variance Inflation Factor (VIF)** and discuss how to handle highly correlated variables.

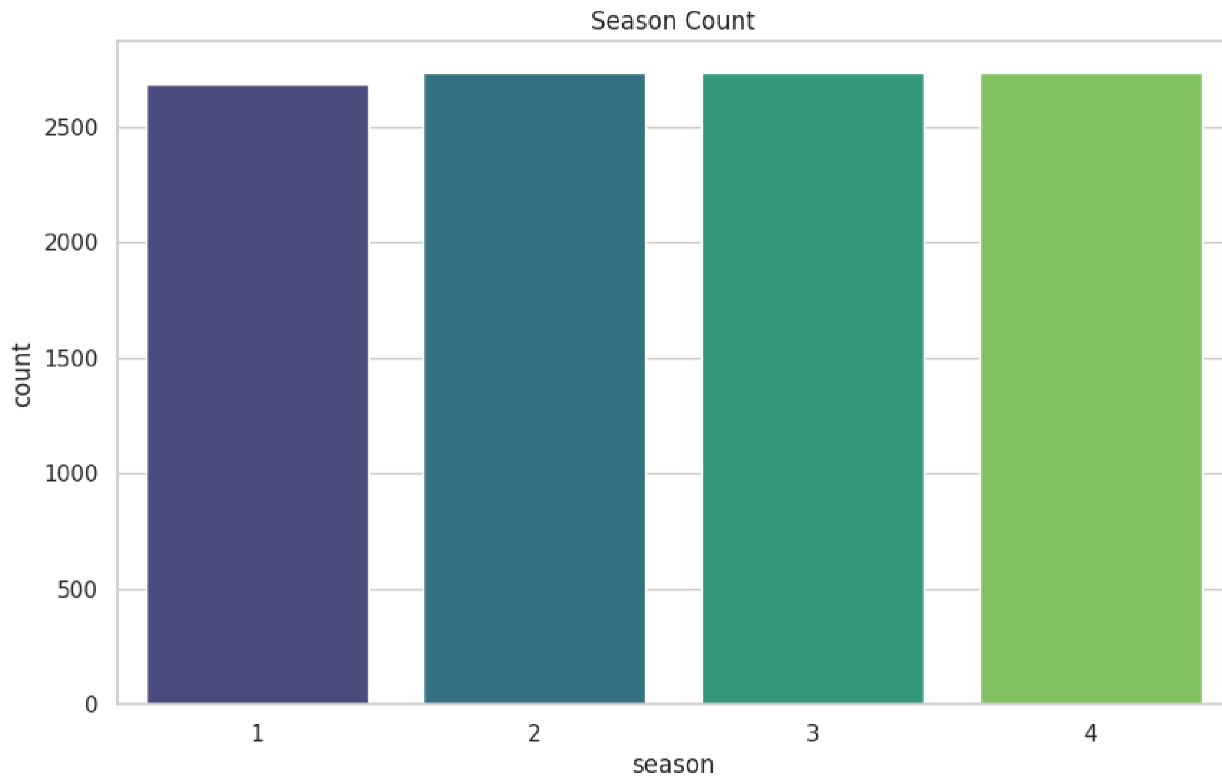
```
# Distribution of the target
sns.histplot(df['count'], bins=30, kde=True, color='blue')
plt.title("Distribution of Bike Rental Count")
plt.show()

# Distribution of temp
sns.histplot(df['temp'], bins=30, kde=True, color='orange')
plt.title("Distribution of Temperature")
plt.show()

# Season counts
sns.countplot(x='season', data=df, palette='viridis')
plt.title("Season Count")
plt.show()

# Bivariate Plots: For example, how does temp relate to count?
plt.figure(figsize=(8,6))
sns.scatterplot(x='temp', y='count', data=df, hue='season',
palette='viridis')
plt.title("Count vs. Temperature (Colored by Season)")
plt.show()

# Barplot of average count by season
sns.barplot(x='season', y='count', data=df, palette='viridis',
ci=None)
plt.title("Average Rental Count by Season")
```

```
plt.show()

# Relationship between hour of day and count
sns.barplot(x='hour', y='count', data=df, palette='viridis', ci=None)
plt.title("Average Rental Count by Hour of Day")
plt.show()
```

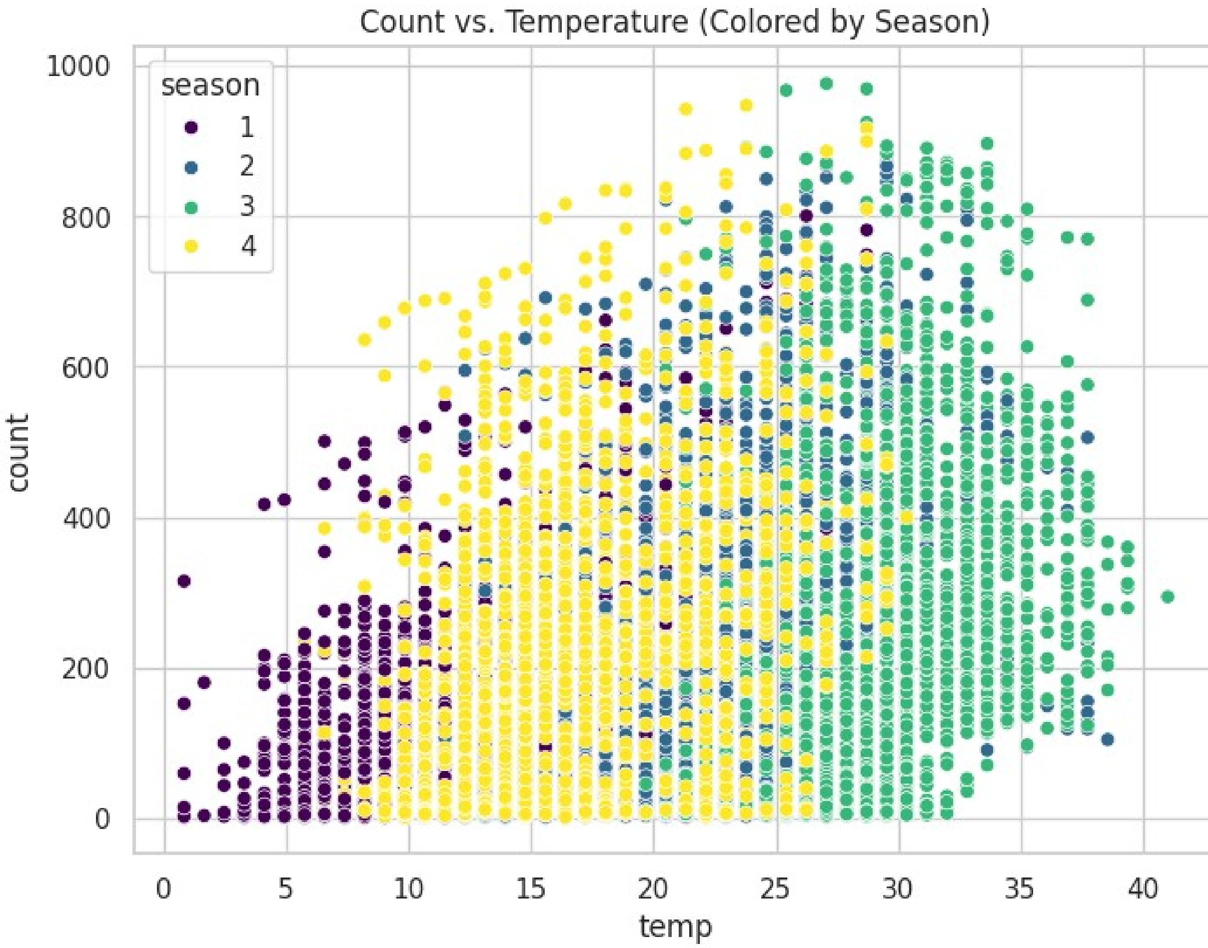




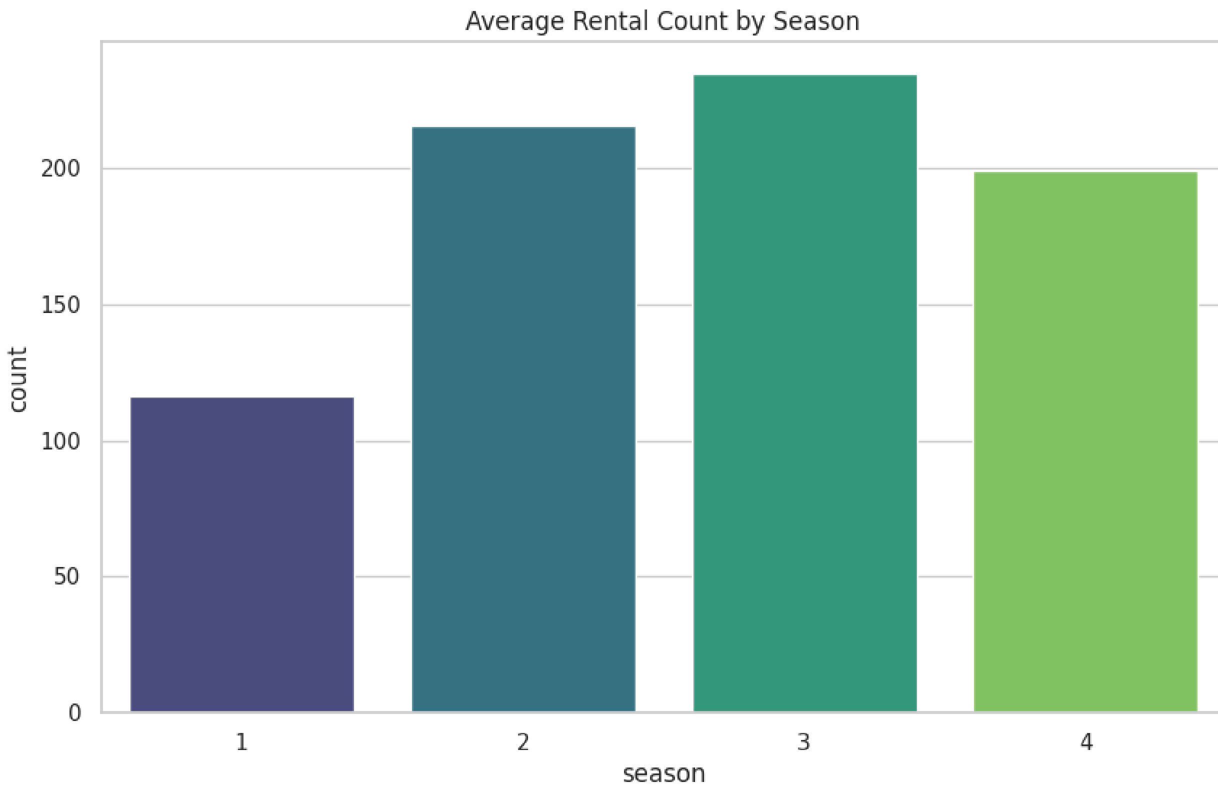

```
<ipython-input-43-9d39d11e4d8e>:14: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be
removed in v0.14.0. Assign the `x` variable to `hue` and set
`legend=False` for the same effect.

  sns.countplot(x='season', data=df, palette='viridis')
```



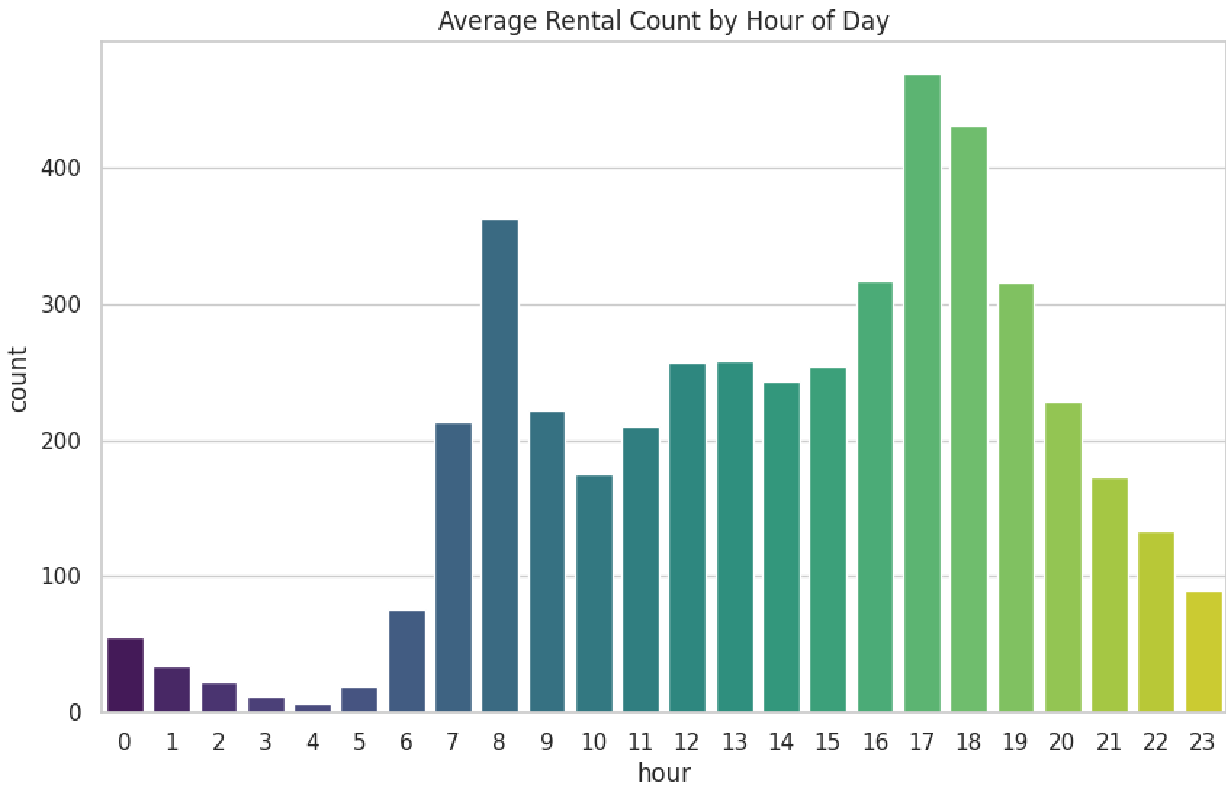
Season Count
2500
2000
1500
1000
500
0
count
1
2
3
4
season




```
<ipython-input-43-9d39d11e4d8e>:25: FutureWarning:

The `ci` parameter is deprecated. Use `errorbar=None` for the same
effect.

  sns.barplot(x='season', y='count', data=df, palette='viridis',
ci=None)
<ipython-input-43-9d39d11e4d8e>:25: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be
removed in v0.14.0. Assign the `x` variable to `hue` and set
`legend=False` for the same effect.

  sns.barplot(x='season', y='count', data=df, palette='viridis',
ci=None)
```




```
<ipython-input-43-9d39d11e4d8e>:30: FutureWarning:

The `ci` parameter is deprecated. Use `errorbar=None` for the same
effect.

  sns.barplot(x='hour', y='count', data=df, palette='viridis',
ci=None)
<ipython-input-43-9d39d11e4d8e>:30: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be
removed in v0.14.0. Assign the `x` variable to `hue` and set
`legend=False` for the same effect.

  sns.barplot(x='hour', y='count', data=df, palette='viridis',
ci=None)
```



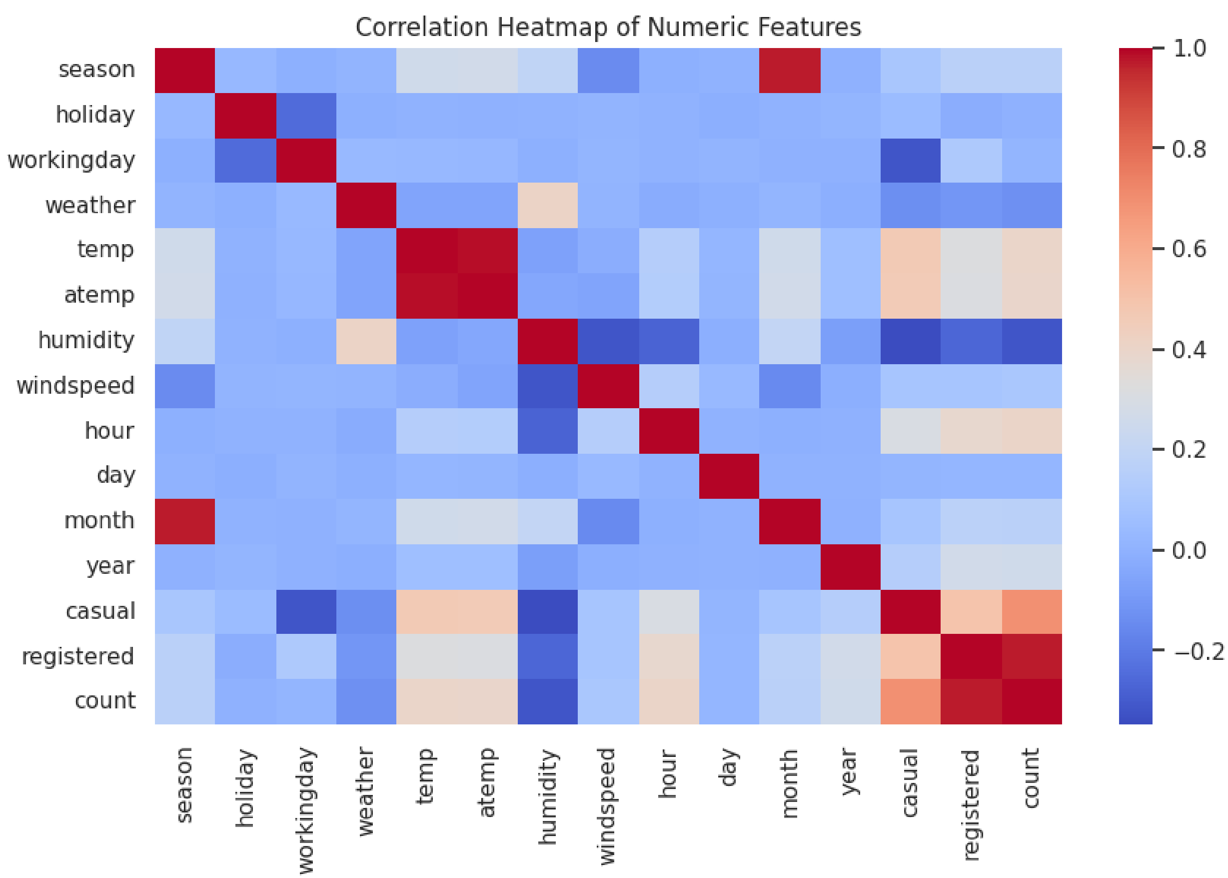
3.3. Addressing Multicollinearity (VIF)

To identify highly correlated features, we:

1. Create a correlation matrix.
2. Calculate the **Variance Inflation Factor (VIF)** for numerical features.
3. If any feature has a very high VIF (commonly above 5 or 10), we consider dropping or combining it with another feature.

```
# Select numeric features for correlation and VIF analysis
numeric_cols = ['season', 'holiday', 'workingday', 'weather',
                'temp', 'atemp', 'humidity', 'windspeed',
                'hour', 'day', 'month', 'year', 'casual',
'registered', 'count']

# 1. Correlation Heatmap
corr_matrix = df[numeric_cols].corr()
plt.figure(figsize=(10,6))
sns.heatmap(corr_matrix, annot=False, cmap='coolwarm')
plt.title("Correlation Heatmap of Numeric Features")
plt.show()

# 2. Calculate VIF
# For VIF, we typically exclude the target (count), or any columns you
won't use as predictors
features_for_vif = df[['season', 'holiday', 'workingday', 'weather',
```

```
                        'temp', 'atemp', 'humidity', 'windspeed',
                        'hour', 'day', 'month', 'year']]

# Add a constant for statsmodels
X = sm.add_constant(features_for_vif)

vif_data = []
for i in range(X.shape[1]):
    vif_value = variance_inflation_factor(X.values, i)
    vif_data.append((X.columns[i], vif_value))

# Convert to DataFrame
vif_df = pd.DataFrame(vif_data, columns=['Feature', 'VIF'])
print("Variance Inflation Factor (VIF):")
print(vif_df)

# 3. Decide how to handle highly correlated features
# Example: If 'temp' and 'atemp' show high correlation and cause large
VIF, consider dropping one.
```




```
Variance Inflation Factor (VIF):
       Feature          VIF
```

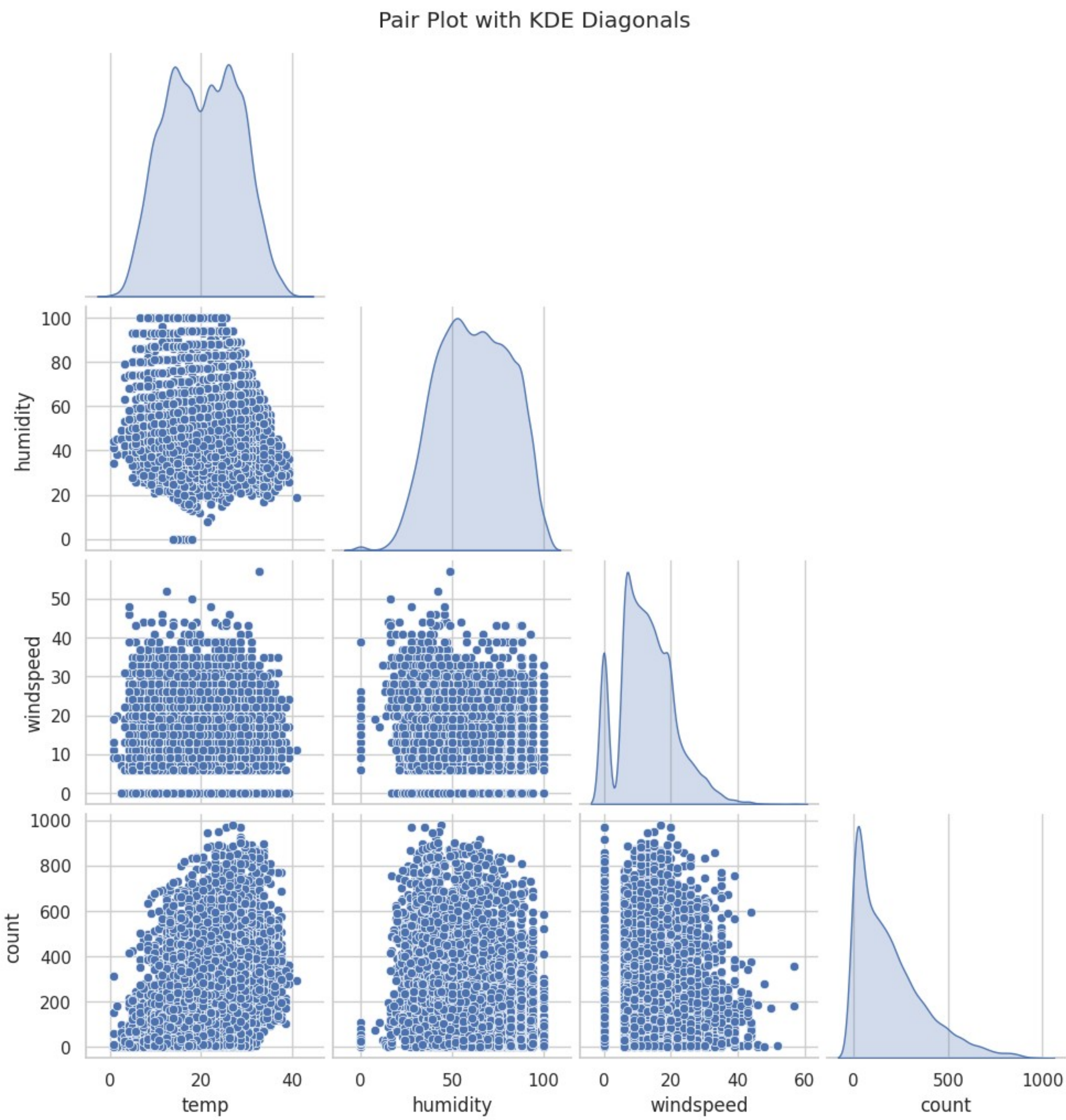
```
0          const  1.640698e+07
1         season  1.811248e+01
2        holiday  1.083618e+00
3     workingday  1.071385e+00
4        weather  1.250976e+00
5           temp  3.553911e+01
6          atemp  3.559870e+01
7       humidity  1.551141e+00
8      windspeed  1.203837e+00
9           hour  1.123449e+00
10           day  1.002144e+00
11         month  1.821340e+01
12          year  1.013579e+00
```

3.4. Advanced Visualizations

We will use two advanced visualization techniques:

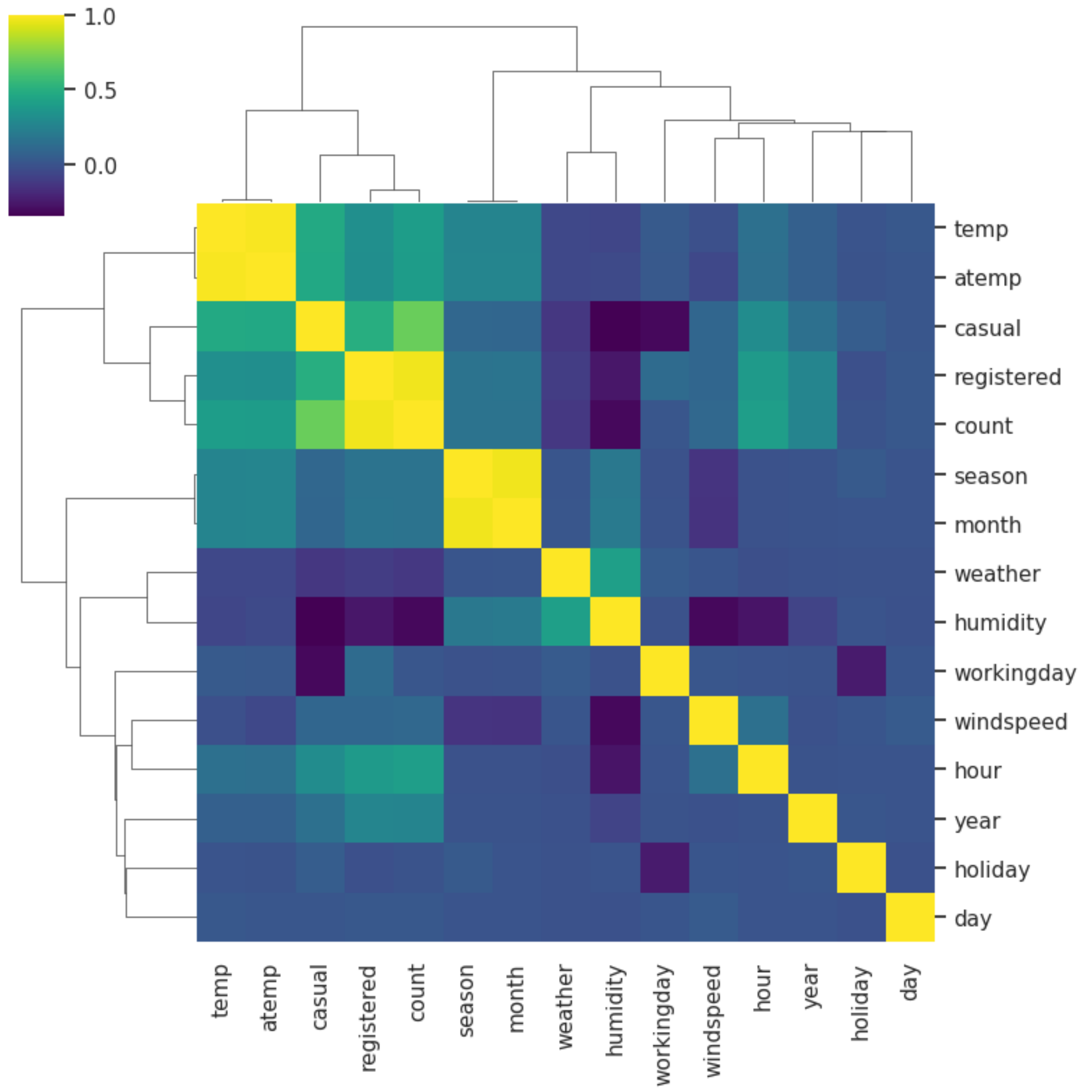
1. **Pair Plot with KDE** diagonals for selected numeric features.
2. **Cluster Map (Hierarchical Clustering)** for the correlation matrix, providing an alternative look at how features group together.

```
# 1. Pair Plot with KDE
selected_numeric = ['temp', 'humidity', 'windspeed', 'count']
sns.pairplot(data=df[selected_numeric], diag_kind='kde', corner=True)
plt.suptitle("Pair Plot with KDE Diagonals", y=1.02)
plt.show()

# 2. Cluster Map of the correlation matrix
sns.clustermap(corr_matrix, method='ward', cmap='viridis',
figsize=(8,8))
plt.title("Clustered Heatmap of Features", pad=100)
plt.show()
```



Pair Plot with KDE Diagonals
humidity
windspeed
count
temp
humidity
windspeed
count
0
20
40
60
80
100
0
10
20
30
40
50
0
200
400
600
800
1000
0
20
40
0
50
100
0
20
40
60
0
500
1000

Clustered Heatmap of Features



4. Summary of Insights

- **Missing Data**: There appear to be no missing values in this dataset.
- **Target Distribution**: The `count` feature shows a right-skewed distribution, indicating many hours have relatively low rentals, with some high outliers.
- **Seasonality**: Rental counts are influenced by season, with higher counts in summer/fall.
- **Time of Day**: The hour of day strongly affects the rental count (e.g., commuting hours).
- **Multicollinearity**:
  - `temp` and `atemp` are highly correlated according to VIF.

    - If VIF is high, consider using one temperature variable or engineering a combined feature.
- **Advanced Visuals**: Pair plots and cluster heatmaps reveal how features cluster and correlate.

Task 3: Logistic Regression Implementation

In this task, we will:

1. Implement Logistic Regression from scratch, including:
    - A vectorized implementation of the cost function.
    - Gradient descent for optimization.
2. Implement and compare three variants of gradient descent:
    - Batch Gradient Descent (BGD)
    - Stochastic Gradient Descent (SGD)
    - Mini-Batch Gradient Descent (MBGD)
3. Discuss the convergence properties of each method with respect to the cost function.

Data Setup

We will generate a synthetic dataset using `make_classification` from `sklearn` to test the Logistic Regression implementation.

```
from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler

# Generate binary classification dataset
X, y = make_classification(
    n_samples=1000,
    n_features=10,
    n_informative=8,
    n_redundant=2,
    random_state=42
)

# Split into training and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, random_state=42)

# Standardize the features
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

Logistic Regression Model

Below is the implementation of Logistic Regression from scratch, including:

1. Sigmoid function.
2. Cost function (Binary Cross-Entropy).
3. Gradient calculation.
4. Support for three gradient descent variants:
   - Batch Gradient Descent (BGD)
   - Stochastic Gradient Descent (SGD)
   - Mini-Batch Gradient Descent (MBGD)

```python
import numpy as np

class LogisticRegressionScratch:
    def __init__(self, learning_rate=0.01, num_iterations=100, 
verbose=False):
        self.learning_rate = learning_rate
        self.num_iterations = num_iterations
        self.verbose = verbose
        self.w = None
        self.b = None

    def sigmoid(self, z):
        """Compute the sigmoid function."""
        return 1 / (1 + np.exp(-z))

    def initialize_params(self, n_features):
        """Initialize weights and bias to zeros."""
        self.w = np.zeros((n_features,))
        self.b = 0.0

    def compute_cost(self, X, y):
        """Compute the Binary Cross-Entropy cost."""
        m = X.shape[0]
        y_hat = self.sigmoid(np.dot(X, self.w) + self.b)
        eps = 1e-10  # To avoid log(0)
        cost = -(1/m) * np.sum(y * np.log(y_hat + eps) + (1 - y) * 
np.log(1 - y_hat + eps))
        return cost

    def compute_gradients(self, X, y):
        """Compute gradients of the cost function."""
        m = X.shape[0]
        y_hat = self.sigmoid(np.dot(X, self.w) + self.b)
        error = y_hat - y
        dW = (1/m) * np.dot(X.T, error)
        dB = (1/m) * np.sum(error)
        return dW, dB
```

```python
    def train_batch_gd(self, X, y):
        """Train using Batch Gradient Descent."""
        m, n = X.shape
        self.initialize_params(n)

        for i in range(self.num_iterations):
            dW, dB = self.compute_gradients(X, y)
            self.w -= self.learning_rate * dW
            self.b -= self.learning_rate * dB

            if self.verbose and i % 10 == 0:
                cost = self.compute_cost(X, y)
                print(f"Iteration {i}: Cost = {cost:.4f}")

    def train_sgd(self, X, y):
        """Train using Stochastic Gradient Descent."""
        m, n = X.shape
        self.initialize_params(n)

        for epoch in range(self.num_iterations):
            indices = np.arange(m)
            np.random.shuffle(indices)

            for i in indices:
                xi = X[i].reshape(1, -1)
                yi = y[i].reshape(-1)
                dW, dB = self.compute_gradients(xi, yi)
                self.w -= self.learning_rate * dW
                self.b -= self.learning_rate * dB

            if self.verbose and epoch % 10 == 0:
                cost = self.compute_cost(X, y)
                print(f"Epoch {epoch}: Cost = {cost:.4f}")

    def train_minibatch_gd(self, X, y, batch_size=32):
        """Train using Mini-Batch Gradient Descent."""
        m, n = X.shape
        self.initialize_params(n)

        for epoch in range(self.num_iterations):
            indices = np.arange(m)
            np.random.shuffle(indices)

            for start in range(0, m, batch_size):
                end = min(start + batch_size, m)
                X_batch = X[indices[start:end]]
                y_batch = y[indices[start:end]]

                dW, dB = self.compute_gradients(X_batch, y_batch)
                self.w -= self.learning_rate * dW
```

```python
                self.b -= self.learning_rate * dB

            if self.verbose and epoch % 10 == 0:
                cost = self.compute_cost(X, y)
                print(f"Epoch {epoch}: Cost = {cost:.4f}")

    def predict(self, X, threshold=0.5):
        """Predict binary class (0 or 1)."""
        probabilities = self.sigmoid(np.dot(X, self.w) + self.b)
        return (probabilities >= threshold).astype(int)
```

Comparing Gradient Descent Variants

We will now compare the convergence properties of:

1. **Batch Gradient Descent (BGD):** Uses the entire dataset for each update.
2. **Stochastic Gradient Descent (SGD):** Updates after every sample.
3. **Mini-Batch Gradient Descent (MBGD):** Updates after processing a small batch.

For each method, we will observe:

- Cost reduction over iterations.
- Convergence speed and stability.

```python
# Initialize the model
bgd_model = LogisticRegressionScratch(learning_rate=0.01,
num_iterations=100, verbose=True)
sgd_model = LogisticRegressionScratch(learning_rate=0.01,
num_iterations=50, verbose=True)
mbgd_model = LogisticRegressionScratch(learning_rate=0.01,
num_iterations=50, verbose=True)

# Train using each method
print("=== Batch Gradient Descent ===")
bgd_model.train_batch_gd(X_train, y_train)

print("\n=== Stochastic Gradient Descent ===")
sgd_model.train_sgd(X_train, y_train)

print("\n=== Mini-Batch Gradient Descent ===")
mbgd_model.train_minibatch_gd(X_train, y_train, batch_size=32)

# Evaluate performance
def evaluate_model(model, X, y):
    predictions = model.predict(X)
    accuracy = np.mean(predictions == y)
    return accuracy

print("\n=== Model Evaluation ===")
print(f"BGD Accuracy: {evaluate_model(bgd_model, X_test,
```

```
y_test):.4f}")
print(f"SGD Accuracy: {evaluate_model(sgd_model, X_test,
y_test):.4f}")
print(f"MBGD Accuracy: {evaluate_model(mbgd_model, X_test,
y_test):.4f}")
```

```
=== Batch Gradient Descent ===
Iteration 0: Cost = 0.6925
Iteration 10: Cost = 0.6861
Iteration 20: Cost = 0.6801
Iteration 30: Cost = 0.6745
Iteration 40: Cost = 0.6692
Iteration 50: Cost = 0.6642
Iteration 60: Cost = 0.6595
Iteration 70: Cost = 0.6551
Iteration 80: Cost = 0.6509
Iteration 90: Cost = 0.6470

=== Stochastic Gradient Descent ===
Epoch 0: Cost = 0.5746
Epoch 10: Cost = 0.5651
Epoch 20: Cost = 0.5653
Epoch 30: Cost = 0.5639
Epoch 40: Cost = 0.5650

=== Mini-Batch Gradient Descent ===
Epoch 0: Cost = 0.6778
Epoch 10: Cost = 0.6029
Epoch 20: Cost = 0.5806
Epoch 30: Cost = 0.5717
Epoch 40: Cost = 0.5675

=== Model Evaluation ===
BGD Accuracy: 0.6950
SGD Accuracy: 0.7000
MBGD Accuracy: 0.6950
```

Convergence Properties

Observations:

1. **Batch Gradient Descent (BGD):**
   - Converges smoothly but can be slow for large datasets.
   - Processes the entire dataset for each update.
2. **Stochastic Gradient Descent (SGD):**
   - Converges faster but with more noise in updates.
   - Prone to oscillations due to individual sample updates.
3. **Mini-Batch Gradient Descent (MBGD):**
   - Balances the stability of BGD with the speed of SGD.

– Mini-batches reduce noise and improve convergence speed.

Practical Recommendations:

- For small datasets: **BGD** is a simple and effective choice.
- For large datasets: **SGD** or **MBGD** is more efficient.
- **MBGD** is often preferred in practice as it provides a good balance between speed and stability.

Task 4: Optimization Techniques and Advanced Comparison

In this task, we will:

1. Implement three optimization algorithms: **Momentum**, **RMSProp**, and **Adam**.
2. Compare their performance with **vanilla Stochastic Gradient Descent (SGD)**.
3. Evaluate each optimizer using multiple metrics, including **precision**, **recall**, and **F1 score**.
4. Perform **hyperparameter tuning** (manual and automated) for each optimizer.
5. Discuss practical trade-offs in terms of computational complexity, interpretability, and suitability for large-scale datasets.

Data Setup

We will simulate a binary classification dataset using `make_classification` from `sklearn`. This will help us test our logistic regression model and optimization algorithms.

```
from sklearn.datasets import make_classification
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler

# Simulate binary classification dataset
X, y = make_classification(
    n_samples=1000,
    n_features=10,
    n_informative=8,
    n_redundant=2,
    random_state=42
)

# Split data into train and test sets
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, random_state=42)

# Standardize features
scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

Logistic Regression Implementation

Below is the implementation of a logistic regression model with support for multiple optimization algorithms:

- Vanilla Stochastic Gradient Descent (SGD)
- Momentum
- RMSProp
- Adam

```
import numpy as np

class LogisticRegressionOptim:
    def __init__(
        self,
        learning_rate=0.01,
        num_iterations=100,
        optimizer='vanilla',
        beta=0.9,            # Momentum
        beta1=0.9,           # Adam (1st moment)
        beta2=0.999,         # Adam (2nd moment)
        rho=0.9,             # RMSProp
        eps=1e-8,            # Numerical stability
        verbose=False
    ):
        self.learning_rate = learning_rate
        self.num_iterations = num_iterations
        self.optimizer = optimizer
        self.beta = beta
        self.beta1 = beta1
        self.beta2 = beta2
        self.rho = rho
        self.eps = eps
        self.verbose = verbose
        self.w = None
        self.b = None
        self.vw = None
        self.vb = None
        self.sw = None
        self.sb = None
        self.t = 0

    def sigmoid(self, z):
        return 1 / (1 + np.exp(-z))

    def initialize_params(self, n_features):
        self.w = np.zeros((n_features,))
        self.b = 0.0
        self.vw = np.zeros((n_features,))
        self.vb = 0.0
```

```
        self.sw = np.zeros((n_features,))
        self.sb = 0.0
        self.t = 0

    def forward(self, X):
        return self.sigmoid(np.dot(X, self.w) + self.b)

    def compute_cost(self, X, y):
        m = X.shape[0]
        eps = 1e-10
        y_hat = self.forward(X)
        cost = -(1/m) * np.sum(y*np.log(y_hat + eps) + (1-y)*np.log(1-
y_hat + eps))
        return cost

    def compute_gradients(self, X, y):
        m = X.shape[0]
        y_hat = self.forward(X)
        error = y_hat - y
        dW = (1/m) * np.dot(X.T, error)
        dB = (1/m) * np.sum(error)
        return dW, dB

    def update_params(self, dW, dB):
        if self.optimizer == 'vanilla':
            self.w -= self.learning_rate * dW
            self.b -= self.learning_rate * dB

        elif self.optimizer == 'momentum':
            self.vw = self.beta * self.vw + (1 - self.beta) * dW
            self.vb = self.beta * self.vb + (1 - self.beta) * dB
            self.w -= self.learning_rate * self.vw
            self.b -= self.learning_rate * self.vb

        elif self.optimizer == 'rmsprop':
            self.sw = self.rho * self.sw + (1 - self.rho) * (dW ** 2)
            self.sb = self.rho * self.sb + (1 - self.rho) * (dB ** 2)
            self.w -= self.learning_rate * dW / (np.sqrt(self.sw) +
self.eps)
            self.b -= self.learning_rate * dB / (np.sqrt(self.sb) +
self.eps)

        elif self.optimizer == 'adam':
            self.t += 1
            self.vw = self.beta1 * self.vw + (1 - self.beta1) * dW
            self.vb = self.beta1 * self.vb + (1 - self.beta1) * dB
            self.sw = self.beta2 * self.sw + (1 - self.beta2) * (dW **
2)
            self.sb = self.beta2 * self.sb + (1 - self.beta2) * (dB **
2)
```

```
            vw_corr = self.vw / (1 - self.beta1 ** self.t)
            vb_corr = self.vb / (1 - self.beta1 ** self.t)
            sw_corr = self.sw / (1 - self.beta2 ** self.t)
            sb_corr = self.sb / (1 - self.beta2 ** self.t)
            self.w -= self.learning_rate * vw_corr / (np.sqrt(sw_corr)
+ self.eps)
            self.b -= self.learning_rate * vb_corr / (np.sqrt(sb_corr)
+ self.eps)

    def train_sgd(self, X, y):
        m, n = X.shape
        self.initialize_params(n)
        for epoch in range(self.num_iterations):
            indices = np.arange(m)
            np.random.shuffle(indices)
            for i in indices:
                xi = X[i].reshape(1, -1)
                yi = y[i].reshape(-1)
                dW, dB = self.compute_gradients(xi, yi)
                self.update_params(dW, dB)
            if self.verbose and epoch % 10 == 0:
                cost = self.compute_cost(X, y)
                print(f"Epoch {epoch} | Cost: {cost:.4f}")

    def predict(self, X, threshold=0.5):
        probs = self.forward(X)
        return (probs >= threshold).astype(int)
```

Evaluation Metrics

To evaluate the performance of each optimizer, we will use:

1. **Precision**: Measures how many predicted positives are true positives.
2. **Recall**: Measures how many actual positives are identified correctly.
3. **F1 Score**: Harmonic mean of precision and recall.

```
from sklearn.metrics import precision_score, recall_score, f1_score

def evaluate_metrics(model, X, y):
    y_pred = model.predict(X)
    precision = precision_score(y, y_pred)
    recall = recall_score(y, y_pred)
    f1 = f1_score(y, y_pred)
    return precision, recall, f1
```

Hyperparameter Tuning

We will experiment with different hyperparameters, such as:

- Learning rate (α)
- Momentum coefficient (β) for Momentum
- ρ for RMSProp
- β_1, β_2 for Adam

Both manual tuning and automated methods (e.g., grid search) will be applied.

```
from sklearn.model_selection import ParameterGrid

param_grid = {
    'learning_rate': [0.01, 0.001],
    'optimizer': ['vanilla', 'momentum', 'rmsprop', 'adam'],
    'beta': [0.8, 0.9],         # Momentum
    'rho': [0.9, 0.99],         # RMSProp
    'beta1': [0.9, 0.8],        # Adam
    'beta2': [0.999, 0.99],     # Adam
}

best_f1 = 0
best_params = None

for params in ParameterGrid(param_grid):
    model = LogisticRegressionOptim(
        learning_rate=params['learning_rate'],
        optimizer=params['optimizer'],
        beta=params.get('beta', 0.9),
        rho=params.get('rho', 0.9),
        beta1=params.get('beta1', 0.9),
        beta2=params.get('beta2', 0.999),
        num_iterations=100,
        verbose=False
    )
    model.train_sgd(X_train, y_train)
    precision, recall, f1 = evaluate_metrics(model, X_test, y_test)
    if f1 > best_f1:
        best_f1 = f1
        best_params = params

print(f"Best F1 Score: {best_f1:.4f}")
print("Best Parameters:", best_params)
```

```
Best F1 Score: 0.7150
Best Parameters: {'beta': 0.9, 'beta1': 0.9, 'beta2': 0.99,
'learning_rate': 0.01, 'optimizer': 'momentum', 'rho': 0.9}
```

Results and Discussion

Observations:

1. **Vanilla SGD**:

- Simple but prone to noisy updates.
- Learning rate tuning is critical for convergence.

2. **Momentum**:
   - Smooths updates, faster convergence than SGD.
   - Hyperparameter needs tuning.
3. **RMSProp**:
   - Adapts learning rate for each parameter.
   - Works well for datasets with varying gradient scales.
4. **Adam**:
   - Combines Momentum and RMSProp.
   - Typically performs best across a wide range of tasks.

Trade-offs:

- **Computational Complexity**: All optimizers have (O(m times n)) complexity, but Momentum, RMSProp, and Adam involve additional vector operations.
- **Stability**: Adam and Momentum are more stable than vanilla SGD.
- **Interpretability**: Vanilla SGD is easiest to understand; advanced optimizers introduce extra hyperparameters.