In [ ]:
```
# Install required libraries
!pip install pandas
!pip install numpy
!pip install matplotlib
!pip install seaborn
!pip install scipy
!pip install scikit-learn
!pip install scikit-optimize
```

In [ ]:
```
# Import required libraries
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from scipy.stats import zscore
from sklearn.preprocessing import StandardScaler, MinMaxScaler, PolynomialFeatures
from sklearn.feature_selection import SelectKBest, f_classif
from sklearn.svm import SVC
from sklearn.model_selection import cross_val_score, cross_validate, StratifiedKFold, GridSearchCV, train_test_spli
from sklearn.metrics import make_scorer, accuracy_score, precision_score, recall_score, f1_score, roc_auc_score, cl
from sklearn.linear_model import SGDClassifier
from sklearn.metrics.pairwise import rbf_kernel, linear_kernel
from skopt import BayesSearchCV
from time import time
```

0. Introduction

The **HIGGS dataset** was generated using Monte Carlo simulations. It contains 21 features representing kinematic properties measured by particle detectors in an accelerator. In addition, there are 7 high-level features derived from these kinematic properties by domain experts to help distinguish between two classes.

The goal of this assignment is to build a Support Vector Machine (SVM) classifier to predict the class labels in the dataset. Given the large and high-dimensional nature of the HIGGS dataset, efficient data handling, advanced feature selection, and model tuning are essential. Accuracy will be the primary metric used to evaluate model performance.

1 . Data Preprocessing and Exploration

1.1 Data Preparation

- Load a sample (1%) from the huge HIGGS dataset into a Pandas DataFrame.
- Rename the columns to have a consistent format, with the first column as "label" and the subsequent columns labeled as "feature_1" through "feature_28".
- The target variable (`target`) is extracted from the "label" column, while the features are stored in a separate DataFrame (`data`).

In [ ]:
```
# Loading the dataset and storing a smaller version of it in the same directory

dir = "/content"
# df = pd.read_csv(f"{dir}/HIGGS.csv")
# df_sample = df.sample(frac=0.01, random_state=42)
# df_sample.to_csv(f"{dir}/HIGGS_sample.csv", index=False)
# print(df.shape, df_sample.shape)
```

In [ ]:
```
# Load HIGGS_sample
filepath = f"{dir}/HIGGS_sample.csv"
read_data = pd.read_csv(filepath)

columns = ["label"] + [f"feature_{i}" for i in range(1, 29)]
read_data.columns = columns

data = read_data.drop(columns=['label'])
target = read_data['label']

read_data.head() # Display first few rows
```

Out[ ]:

	label	feature_1	feature_2	feature_3	feature_4	feature_5	feature_6	feature_7	feature_8	feature_9	...	feature_19	feature_20
0	1.0	0.532373	-0.563982	-0.707137	0.682998	0.702177	2.064735	-1.227911	0.030652	0.000000	...	-0.234484	-1.359247
1	0.0	0.341129	0.069098	0.325565	2.925696	0.500175	1.929798	-0.790229	-1.300509	2.173076	...	0.135289	1.291674
2	1.0	1.768051	-0.226015	-1.334685	1.382299	0.217815	0.470495	-0.552574	0.669846	0.000000	...	1.217127	1.470911
3	0.0	0.716481	-0.800656	-1.245352	0.648034	0.972671	0.600302	0.714921	1.638340	0.000000	...	-0.047932	0.899351
4	0.0	0.327586	1.395643	1.130114	1.191988	0.713228	0.883368	0.884250	-1.577697	2.173076	...	-0.337754	-0.480818

5 rows × 29 columns

1.2 Exploratory Data Analysis (EDA)

Analyze the dataset, and visualize feature distributions.

In [ ]:
```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 110000 entries, 0 to 109999
Data columns (total 28 columns):
 #   Column      Non-Null Count   Dtype  
---  ------      --------------   -----  
 0   feature_1   110000 non-null  float64
 1   feature_2   110000 non-null  float64
 2   feature_3   110000 non-null  float64
 3   feature_4   110000 non-null  float64
 4   feature_5   110000 non-null  float64
 5   feature_6   110000 non-null  float64
 6   feature_7   110000 non-null  float64
 7   feature_8   110000 non-null  float64
 8   feature_9   110000 non-null  float64
 9   feature_10  110000 non-null  float64
 10  feature_11  110000 non-null  float64
 11  feature_12  110000 non-null  float64
 12  feature_13  110000 non-null  float64
 13  feature_14  110000 non-null  float64
 14  feature_15  110000 non-null  float64
 15  feature_16  110000 non-null  float64
 16  feature_17  110000 non-null  float64
 17  feature_18  110000 non-null  float64
 18  feature_19  110000 non-null  float64
 19  feature_20  110000 non-null  float64
 20  feature_21  110000 non-null  float64
 21  feature_22  110000 non-null  float64
 22  feature_23  110000 non-null  float64
 23  feature_24  110000 non-null  float64
 24  feature_25  110000 non-null  float64
 25  feature_26  110000 non-null  float64
 26  feature_27  110000 non-null  float64
 27  feature_28  110000 non-null  float64
dtypes: float64(28)
memory usage: 23.5 MB
```

In [ ]:
```
data.describe()  # summary statistics
```

Out[ ]:

	feature_1	feature_2	feature_3	feature_4	feature_5	feature_6	feature_7	feature_8	11(
count	110000.000000	110000.000000	110000.000000	110000.000000	110000.000000	110000.000000	110000.000000	110000.000000	
mean	0.993285	-0.005985	-0.002650	0.998366	0.001416	0.990549	0.003786	-0.006673	
std	0.569758	1.007981	1.004571	0.603324	1.007990	0.476472	1.012672	1.007398	
min	0.274697	-2.434976	-1.742508	0.001690	-1.743932	0.157473	-2.969725	-1.741237	
25%	0.591119	-0.746114	-0.872486	0.575659	-0.871000	0.679084	-0.687245	-0.879738	
50%	0.852639	-0.007846	-0.003570	0.889777	0.000287	0.894270	0.005916	-0.008257	
75%	1.238789	0.734318	0.864890	1.291532	0.877119	1.167351	0.692145	0.861660	
max	8.790659	2.434868	1.743236	11.531485	1.743257	7.419452	2.966703	1.741454	

8 rows × 28 columns

In [ ]:
```
data.nunique()  # number of unique values in each column
```

Out[ ]:

	0
feature_1	13435
feature_2	4934
feature_3	6284
feature_4	103448
feature_5	103560
feature_6	21082
feature_7	5768
feature_8	6284
feature_9	3
feature_10	16990
feature_11	5859
feature_12	6284
feature_13	3
feature_14	12757
feature_15	5937
feature_16	6284
feature_17	3
feature_18	9613
feature_19	5987
feature_20	6284
feature_21	3
feature_22	99448
feature_23	74371
feature_24	49334

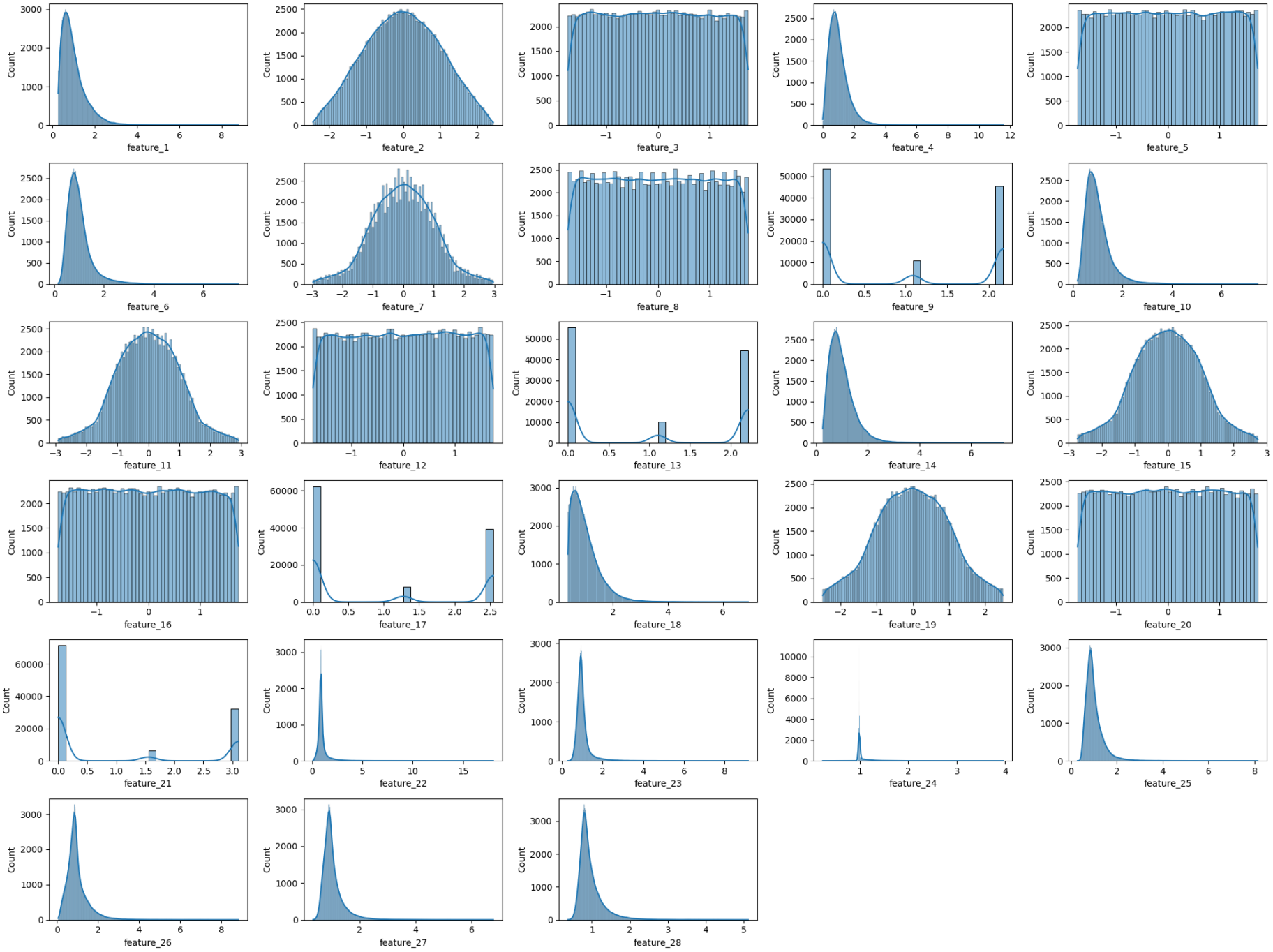
	0
feature_25	84054
feature_26	90893
feature_27	91767
feature_28	95000

dtype: int64

Histogram

Show the frequency distribution of each feature. Ideal for identifying skewness and modality.

In [ ]:
```
def beautiful_plot(df):
    plt.figure(figsize=(20, 15))
    rows, cols = (df.shape[1] + 4) // 5, 5

    for idx, column in enumerate(df.columns):
        plt.subplot(rows, cols, idx + 1)
        sns.histplot(df[column], kde=True)

    plt.tight_layout()
    plt.show()


beautiful_plot(data)
```


Count
feature_1
feature_2
feature_3
feature_4
feature_5
feature_6
feature_7
feature_8
feature_9
feature_10
feature_11
feature_12
feature_13
feature_14
feature_15
feature_16
feature_17
feature_18
feature_19
feature_20
feature_21
feature_22
feature_23
feature_24
feature_25
feature_26
feature_27
feature_28

Covariance Matrix

- The covariance matrix ($n \times n$) contains the covariances between each pair of elements in a dataset (with n variables).

$$\begin{bmatrix} \text{Var}(X) & \text{Cov}(X,Y) & \text{Cov}(X,Z) \\ \text{Cov}(Y,X) & \text{Var}(Y) & \text{Cov}(Y,Z) \\ \text{Cov}(Z,X) & \text{Cov}(Z,Y) & \text{Var}(Z) \end{bmatrix}$$

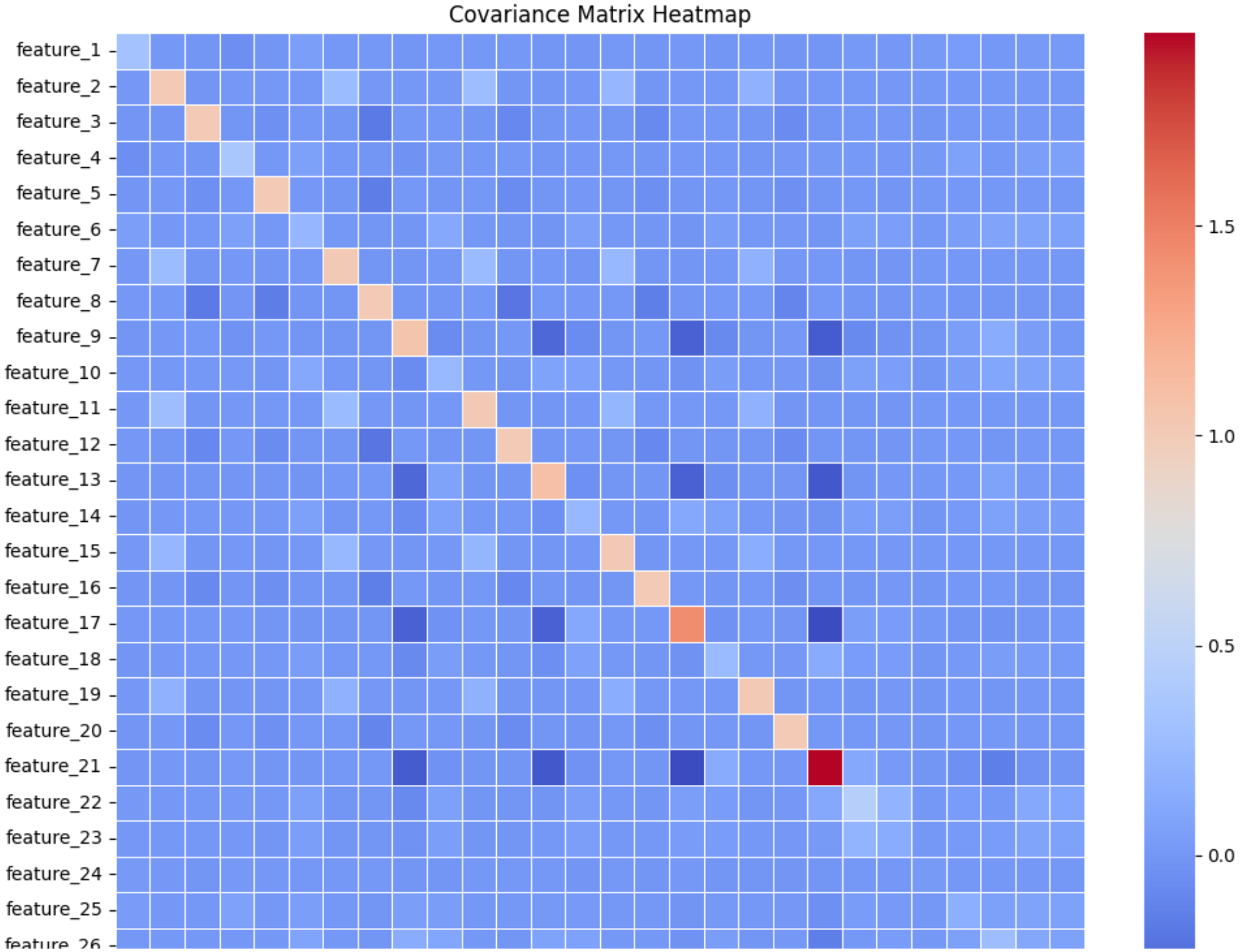
- The covariance between two variables X and Y is calculated as:

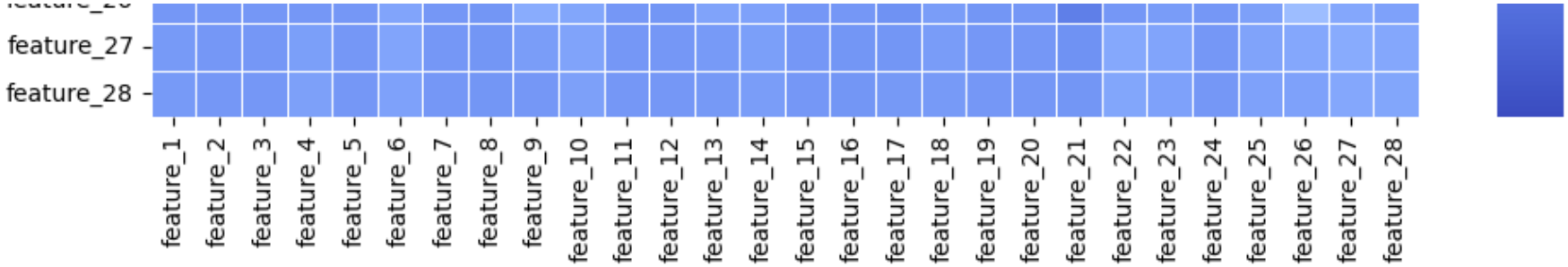
$$\text{Cov}(X,Y) = \frac{1}{N-1}\sum_{i=1}^{N}(X_i - \bar{X})(Y_i - \bar{Y})$$

Where $\bar{X}$ and $\bar{Y}$ are the means of X and Y, and N is the number of observations.

- A positive covariance indicates that as one variable increases, the other variable tends to increase, while a negative covariance indicates an inverse relationship.
- The covariance matrix is symmetric and provides insights into the data's distribution, variability, and correlation.

In [ ]:
```
# Calculate the covariance matrix
cov_matrix = data.cov()

# Set up the figure size
plt.figure(figsize=(12, 10))

# Create the heatmap
sns.heatmap(cov_matrix, annot=False, fmt=".2f", cmap="coolwarm", linewidths=0.5)
plt.title("Covariance Matrix Heatmap")
plt.xticks(rotation=90)
plt.yticks(rotation=0)
plt.show()
```


Covariance Matrix Heatmap
feature_1
feature_2
feature_3
feature_4
feature_5
feature_6
feature_7
feature_8
feature_9
feature_10
feature_11
feature_12
feature_13
feature_14
feature_15
feature_16
feature_17
feature_18
feature_19
feature_20
feature_21
feature_22
feature_23
feature_24
feature_25
feature_26
1.5
1.0
0.5
0.0



Outliers

Identify outliers/anomalies and clean the data accordingly.

- Check for missing values.
- After visualizing the data, it can be concluded that the features can be broadly divided into normal and skewed. Apply outlier detection method accordingly.

Z-Score (for normal distribution)

1. Calculate mean and standard deviation.
2. Calculate Z-Score for each point:

$$Z_i = \frac{x_i - \mu}{\sigma}$$

3. Data points are considered outliers if their Z-score satisfies the condition:

$$|Z_i| > threshold$$

IQR (Interquartile Range) Method

1. Compute the first quartile (Q_1) and the third quartile (Q_3) of the dataset.
2. Calculate the IQR as:

$$\text{IQR} = Q_3 - Q_1$$

3. Define the lower and upper bounds for outliers:

$$\text{Lower Bound} = Q_1 - threshold \times \text{IQR}$$

$$\text{Upper Bound} = Q_3 + threshold \times \text{IQR}$$

4. Data points outside these bounds are considered outliers.

In [ ]:
```
data.isnull().sum()  # number of missing values in each column
```

Out[ ]:

	0
feature_1	0
feature_2	0
feature_3	0
feature_4	0
feature_5	0
feature_6	0
feature_7	0
feature_8	0
feature_9	0
feature_10	0
feature_11	0
feature_12	0
feature_13	0
feature_14	0
feature_15	0
feature_16	0
feature_17	0
feature_18	0
feature_19	0
feature_20	0
feature_21	0
feature_22	0
feature_23	0
feature_24	0

	0
feature_25	0
feature_26	0
feature_27	0
feature_28	0

dtype: int64

In [ ]:
```
print(f"Shape before removing outliers: {data.shape}")

outliers = {}
outlier_indices = set()

for column in data.columns:
    skewness = data[column].skew()

    if abs(skewness) < 0.5:  # Approximately normal - Use Z-score
        threshold = 3
        z_scores = zscore(data[column].dropna())
        outliers[column] = data[column][np.abs(z_scores) > threshold]
        outlier_indices.update(outliers[column].index)
        print(f"{column}: Z-score method detected {len(outliers[column])} outliers")
    else:  # Skewed or non-normal - Use IQR
        threshold = 4.5
        Q1 = data[column].quantile(0.25)
        Q3 = data[column].quantile(0.75)
        IQR = Q3 - Q1
        outliers[column] = data[column][
            (data[column] < Q1 - threshold * IQR) | (data[column] > Q3 + threshold * IQR)
        ]
        outlier_indices.update(outliers[column].index)
        print(f"{column}: IQR method detected {len(outliers[column])} outliers")

# Remove rows with outliers
data_cleaned = data.drop(index=outlier_indices)
target = target.drop(index=outlier_indices)
```

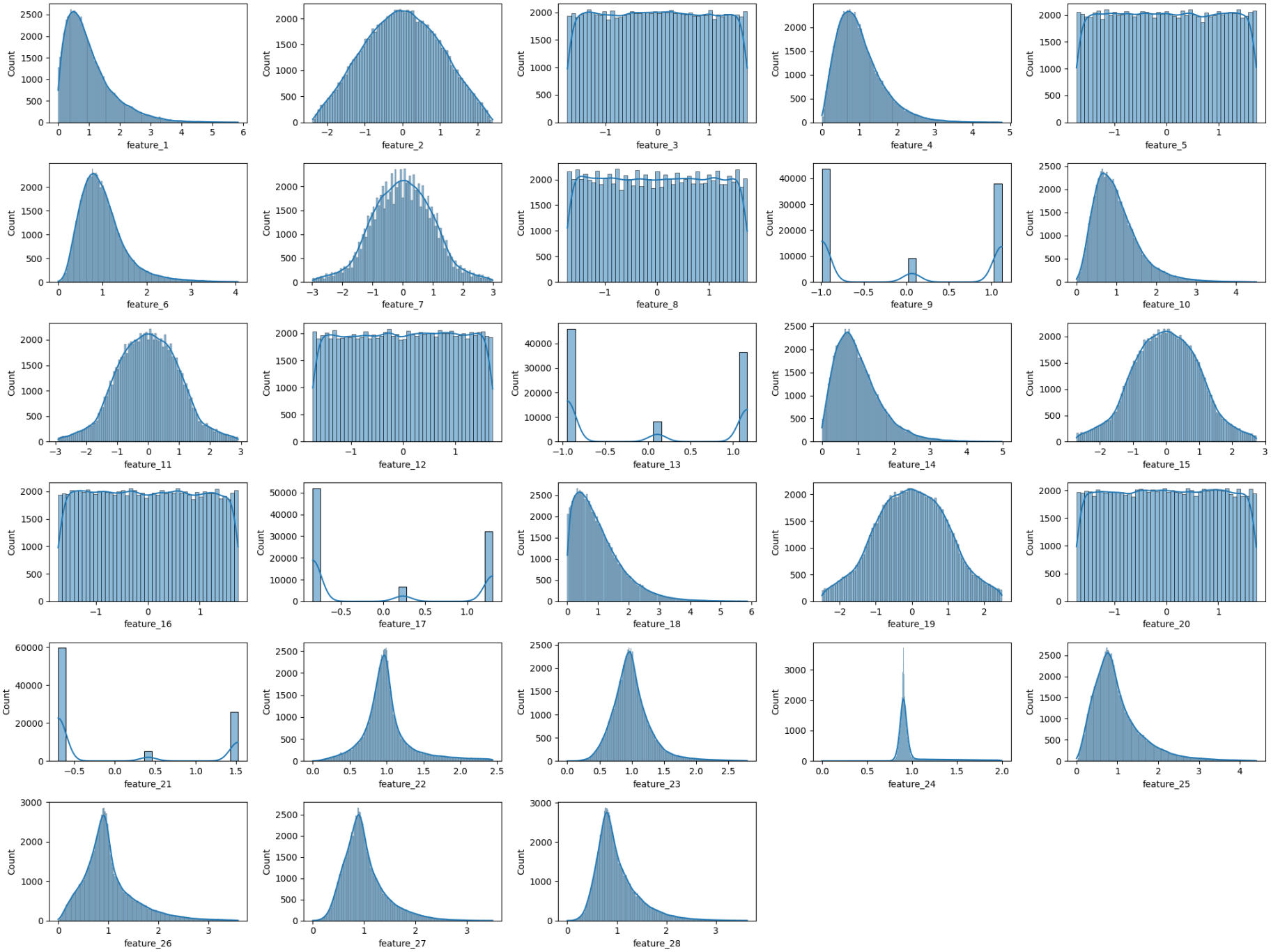
```
print(f"Shape after removing outliers: {data_cleaned.shape}")
```

```
Shape before removing outliers: (110000, 28)
feature_1: IQR method detected 161 outliers
feature_2: Z-score method detected 0 outliers
feature_3: Z-score method detected 0 outliers
feature_4: IQR method detected 114 outliers
feature_5: Z-score method detected 0 outliers
feature_6: IQR method detected 281 outliers
feature_7: Z-score method detected 0 outliers
feature_8: Z-score method detected 0 outliers
feature_9: Z-score method detected 0 outliers
feature_10: IQR method detected 224 outliers
feature_11: Z-score method detected 0 outliers
feature_12: Z-score method detected 0 outliers
feature_13: Z-score method detected 0 outliers
feature_14: IQR method detected 120 outliers
feature_15: Z-score method detected 0 outliers
feature_16: Z-score method detected 0 outliers
feature_17: Z-score method detected 0 outliers
feature_18: IQR method detected 122 outliers
feature_19: Z-score method detected 0 outliers
feature_20: Z-score method detected 0 outliers
feature_21: IQR method detected 0 outliers
feature_22: IQR method detected 5105 outliers
feature_23: IQR method detected 2165 outliers
feature_24: IQR method detected 12847 outliers
feature_25: IQR method detected 625 outliers
feature_26: IQR method detected 677 outliers
feature_27: IQR method detected 759 outliers
feature_28: IQR method detected 664 outliers
Shape after removing outliers: (90806, 28)
```

1.3 Data Normalization/Standardization

> "Input features were standardized over the entire train/test set with mean zero and standard deviation one, except for those features with values strictly greater than zero – these we scaled so that the mean value was one."
> — *Searching for Exotic Particles in High-Energy Physics with Deep Learning*

In [ ]:
```
# Identify columns with strictly positive values
positive_only_columns = [col for col in data_cleaned.columns if (data_cleaned[col] > 0).all()]

# Separate data into positive-only and other columns
data_positive_only = data_cleaned[positive_only_columns]
data_other = data_cleaned.drop(columns=positive_only_columns)

# Standardize columns with both positive and negative values
scaler = StandardScaler()
data_other_scaled = scaler.fit_transform(data_other)
data_other_scaled = pd.DataFrame(data_other_scaled, columns=data_other.columns)

# Scale positive-only columns so the mean is 1
scaler_positive = MinMaxScaler()
data_positive_only_scaled = scaler_positive.fit_transform(data_positive_only)
data_positive_only_scaled = pd.DataFrame(
    data_positive_only_scaled, columns=data_positive_only.columns
)
data_positive_only_scaled = data_positive_only_scaled * (
    1 / data_positive_only_scaled.mean()
)

# Combine both scaled parts back into a single DataFrame
data_scaled = pd.concat([data_other_scaled, data_positive_only_scaled], axis=1)
data_scaled = data_scaled[data.columns]  # Reorder columns to match original data order

# Plot the histograms of each feature
beautiful_plot(data_scaled)
```


Count
feature_1
feature_2
feature_3
feature_4
feature_5
feature_6
feature_7
feature_8
feature_9
feature_10
feature_11
feature_12
feature_13
feature_14
feature_15
feature_16
feature_17
feature_18
feature_19
feature_20
feature_21
feature_22
feature_23
feature_24
feature_25
feature_26
feature_27
feature_28

1.4 Feature Engineering

Polynomial features can capture non-linear relationships. **Interaction terms** can help capture the combined effects of multiple features. Generate interaction terms from the scaled dataset using the `PolynomialFeatures` with degree 2.

In [ ]:
```
# Generate only interaction terms (no powers)
interaction = PolynomialFeatures(degree=2, interaction_only=True, include_bias=False)
interaction_features = interaction.fit_transform(data_scaled)

# Convert to DataFrame
interaction_feature_names = interaction.get_feature_names_out(data_scaled.columns)
data_interactions = pd.DataFrame(interaction_features, columns=interaction_feature_names)
```

In [ ]:
```
# Combine original and interaction features
data_engineered = pd.concat([data_scaled, data_interactions], axis=1)

print(f"Shape of engineered data: {data_engineered.shape}")
```

```
Shape of engineered data: (90806, 434)
```

1.5 Feature Selection

Remove duplicate columns and use `SelectKBest` to identify the most important features for classification, reducing dimensionality.

SelectKBest

- **Scoring**: It applies a statistical scoring function (such as ANOVA F-value, mutual information, or chi-squared) to evaluate the importance of each feature in relation to the target.
- **Selection**: It selects the (k) features with the highest scores, effectively filtering out the less informative features.

In [ ]:
```
# Check for duplicate column names in the data_engineered DataFrame
duplicate_columns = data_engineered.columns[data_engineered.columns.duplicated()]

# Remove duplicates
data_engineered = data_engineered.loc[:, ~data_engineered.columns.duplicated()]

print(f"Shape of engineered data after removing duplicates: {data_engineered.shape}")
```

```
Shape of engineered data after removing duplicates: (90806, 406)
```

In [ ]:
```
select_kbest = SelectKBest(score_func=f_classif, k=20)
select_kbest.fit(data_engineered, target)

# Get the selected features
selected_features_kbest = data_engineered.columns[select_kbest.get_support()]
data_reduced = data_engineered[list(selected_features_kbest)]

print(f"Shape of reduced data: {data_reduced.shape}")
```

```
Shape of reduced data: (90806, 20)
```

2. Linear SVM Implementation

2.1 SVM with a linear kernel (mini-batch learning)

- A **Linear Support Vector Machine (SVM)** is a supervised machine learning algorithm used for classification tasks. It seeks to find the optimal linear boundary, or hyperplane, that best separates data points of different classes.
- A SVM model is initialized using `SVC` and is evaluated by performing cross-validation (using `StratifiedKFold` strategy) on a small sample extracted from the data.

In [ ]:
```
# Sample 1% of the data for the mini batch, keeping class distribution
data_sampled, _, target_sampled, _ = train_test_split(data_reduced, target, train_size=0.01, stratify=target, rando
```

In [ ]:
```
# Initialize the linear SVM model
svm = SVC(kernel='linear', probability=True, random_state=42)

# Define cross-validation strategy
```

```
cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)

# Define the scoring metrics
scoring = {
    'accuracy': make_scorer(accuracy_score),
    'precision': make_scorer(precision_score, average='weighted'),
    'recall': make_scorer(recall_score, average='weighted'),
    'f1': make_scorer(f1_score, average='weighted'),
    'roc_auc': make_scorer(roc_auc_score, average='weighted', multi_class='ovr', response_method="predict_proba")
}

# Perform cross-validation
cv_results = cross_validate(svm, data_sampled, target_sampled, cv=cv, scoring=scoring)

# Calculate and print mean metrics across all folds
print("SVM (Linear Kernel) Performance Metrics:")
print(f"Accuracy: {cv_results['test_accuracy'].mean():.4f}")
print(f"Precision: {cv_results['test_precision'].mean():.4f}")
print(f"Recall: {cv_results['test_recall'].mean():.4f}")
print(f"F1 Score: {cv_results['test_f1'].mean():.4f}")
print(f"AUC (Area Under the ROC Curve): {cv_results['test_roc_auc'].mean():.4f}")
```

```
SVM (Linear Kernel) Performance Metrics:
Accuracy: 0.6277
Precision: 0.6499
Recall: 0.6277
F1 Score: 0.6012
AUC (Area Under the ROC Curve): 0.6530
```

2.2 Stochastic Gradient Descent (SGD)

- **SGD** is an optimization method that updates model parameters incrementally with each training example rather than in batches. Each iteration updates the model's weights based on a single example, which is computationally efficient and allows handling of large-scale datasets.
- `SGDClassifier(loss='hinge')` configures the classifier to minimize the **hinge loss**, which is the loss function used by linear SVMs.

In [ ]:
```
# Initialize the SGDClassifier with a linear SVM loss function
sgd_clf = SGDClassifier(loss='hinge', random_state=42, max_iter=1000)
```

```python
# Define cross-validation strategy
cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=42)

# Define the scoring metrics
scoring = {
    'accuracy': make_scorer(accuracy_score),
    'precision': make_scorer(precision_score, average='weighted'),
    'recall': make_scorer(recall_score, average='weighted'),
    'f1': make_scorer(f1_score, average='weighted')
}

# Perform cross-validation
cv_results = cross_validate(sgd_clf, data_reduced, target, cv=cv, scoring=scoring)

# Calculate and print mean metrics across all folds
print("SGDClassifier Performance Metrics:")
print(f"Accuracy: {cv_results['test_accuracy'].mean():.4f}")
print(f"Precision: {cv_results['test_precision'].mean():.4f}")
print(f"Recall: {cv_results['test_recall'].mean():.4f}")
print(f"F1 Score: {cv_results['test_f1'].mean():.4f}")
```

```
SGDClassifier Performance Metrics:
Accuracy: 0.6228
Precision: 0.6525
Recall: 0.6228
F1 Score: 0.5909
```

Key Classification Metrics

1. Accuracy

The proportion of correct predictions (both true positives and true negatives) out of the total predictions.

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

2. Precision

The ratio of correctly predicted positive observations to the total predicted positives.

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

3. Recall (Sensitivity or True Positive Rate)

The ratio of correctly predicted positive observations to all actual positives.

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

4. F1-Score

The harmonic mean of precision and recall, balancing the two metrics.

$$\text{F1-Score} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

5. AUC (Area Under the ROC Curve)

Represents the area under the Receiver Operating Characteristic (ROC) curve, plotting the true positive rate (recall) against the false positive rate.

Range: 0 to 1, where 1 is a perfect model.

3. Comparison and Time Complexity Analysis of SVM with various Kernels

In [ ]:
```
# Sample 80% of data for training and 20% for testing, keeping class distribution
data_train, data_test, target_train, target_test = train_test_split(
    data_sampled, target_sampled, train_size=0.8, stratify=target_sampled, random_state=42
)
```

In [ ]:
```
# Function to evaluate the model and capture computation time
def evaluate_model(model, data_train, target_train, data_test, target_test):

    # Training
    start_time = time()
    model.fit(data_train, target_train)
    end_time = time()
    training_time = end_time - start_time
```

```
    # Prediction
    start_time = time()
    predictions = model.predict(data_test)
    end_time = time()
    prediction_time = end_time - start_time

    # Performance Metrics
    accuracy = accuracy_score(target_test, predictions)
    precision = precision_score(target_test, predictions)
    recall = recall_score(target_test, predictions)
    f1 = f1_score(target_test, predictions)
    auc = roc_auc_score(target_test, model.decision_function(data_test))

    return {
        'accuracy': accuracy,
        'precision': precision,
        'recall': recall,
        'f1_score': f1,
        'auc': auc,
        'training_time': training_time,
        'prediction_time': prediction_time
    }
```

In [ ]:
```
# Function to print performance metrics
def print_metrics(metrics):
  print("Metrics:")
  print(f"  Accuracy: {metrics['accuracy']:.4f}")
  print(f"  Precision: {metrics['precision']:.4f}")
  print(f"  Recall: {metrics['recall']:.4f}")
  print(f"  F1 Score: {metrics['f1_score']:.4f}")
  print(f"  AUC: {metrics['auc']:.4f}")
  print(f"  Training Time: {metrics['training_time']:.4f} seconds")
  print(f"  Prediction Time: {metrics['prediction_time']:.4f} seconds")
```

Grid Search

- `GridSearchCV` is a hyperparameter tuning technique that automates the process of finding the optimal combination of hyperparameters for a given model.
- `param_grid` : grid of possible hyperparameter values

- Performance metric used for scoring: **accuracy**

3.1 Polynomial Kernel

In [ ]:
```
from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC

# Polynomial Kernel with varying degrees and parameter tuning
poly_results = {}
param_grid = {
    'C': [0.1, 1, 10, 100],
    'degree': [2, 3, 4]
}

poly_svm = SVC(kernel='poly', random_state=42)
grid_search = GridSearchCV(poly_svm, param_grid, scoring='accuracy', cv=5)
grid_search.fit(data_train, target_train)

# Capture results and performance metrics for the best model
best_model = grid_search.best_estimator_
poly_results['best_params'] = grid_search.best_params_
poly_results['metrics'] = evaluate_model(best_model, data_train, target_train, data_test, target_test)
metrics = poly_results['metrics']

# Print the results
print("Polynomial Kernel")
print(f"Best Parameters: C={grid_search.best_params_['C']}, Degree={grid_search.best_params_['degree']}")
print_metrics(metrics)
```

```
Polynomial Kernel
Best Parameters: C=100, Degree=2
Metrics:
  Accuracy: 0.6484
  Precision: 0.6429
  Recall: 0.7500
  F1 Score: 0.6923
  AUC: 0.6846
  Training Time: 0.4298 seconds
  Prediction Time: 0.0041 seconds
```

3.2 RBF Kernel

In [ ]:
```
# RBF Kernel with varying gamma and parameter tuning
rbf_results = {}

# Define the parameter grid to include both C and gamma
param_grid = {
    'C': [0.1, 1, 10, 100],
    'gamma': [0.01, 0.1, 1, 10]
}

# Initialize the RBF SVM and perform grid search
rbf_svm = SVC(kernel='rbf', random_state=42)
grid_search = GridSearchCV(rbf_svm, param_grid, scoring='accuracy', cv=5)
grid_search.fit(data_train, target_train)

# Capture results and performance metrics for the best model
best_model = grid_search.best_estimator_
rbf_results['best_params'] = grid_search.best_params_
rbf_results['metrics'] = evaluate_model(best_model, data_train, target_train, data_test, target_test)
metrics = rbf_results['metrics']

# Print the results
print("RBF Kernel")
print(f"Best Parameters: C={grid_search.best_params_['C']}, Gamma={grid_search.best_params_['gamma']}")
print_metrics(metrics)
```

```
RBF Kernel
Best Parameters: C=100, Gamma=0.01
Metrics:
  Accuracy: 0.6648
  Precision: 0.6549
  Recall: 0.7708
  F1 Score: 0.7081
  AUC: 0.6797
  Training Time: 0.0360 seconds
  Prediction Time: 0.0073 seconds
```

3.3 Custom Hybrid Kernel

$$HybridKernel(X, Y) = \alpha \cdot RBF(X, Y) + (1 - \alpha) \cdot Linear(X, Y)$$

In [ ]:
```python
# Define a custom kernel class with set_params and get_params
class HybridKernel:
    def __init__(self, gamma=0.1, alpha=0.5):
        self.gamma = gamma
        self.alpha = alpha

    def __call__(self, X, Y):
        rbf_part = rbf_kernel(X, Y, gamma=self.gamma)
        linear_part = linear_kernel(X, Y)
        return self.alpha * rbf_part + (1 - self.alpha) * linear_part

    # Allow GridSearchCV to set parameters
    def set_params(self, **params):
        for param, value in params.items():
            setattr(self, param, value)
        return self

    # Allow GridSearchCV to get parameters
    def get_params(self, deep=True):
        return {"gamma": self.gamma, "alpha": self.alpha}

# Define the parameter grid including C, gamma, and alpha
param_grid = {
    'C': [0.1, 1, 10, 100],
    'kernel__gamma': [0.01, 0.1, 1],
    'kernel__alpha': [0.3, 0.5, 0.7]
}

# Initialize the custom kernel and SVC with custom kernel
custom_kernel = HybridKernel()
custom_svm = SVC(kernel=custom_kernel, random_state=42)

# Use GridSearchCV with the custom kernel and parameter grid
grid_search = GridSearchCV(custom_svm, param_grid, scoring='accuracy', cv=5)
grid_search.fit(data_train, target_train)

# Capture results and performance metrics for the best model
```

```
best_model = grid_search.best_estimator_
custom_results = evaluate_model(best_model, data_train, target_train, data_test, target_test)
metrics = custom_results

# Print the results
print("Custom Hybrid Kernel")
print(f"Best Parameters: C={grid_search.best_params_['C']}, Gamma={grid_search.best_params_['kernel__gamma']}, Alph
print_metrics(metrics)
```

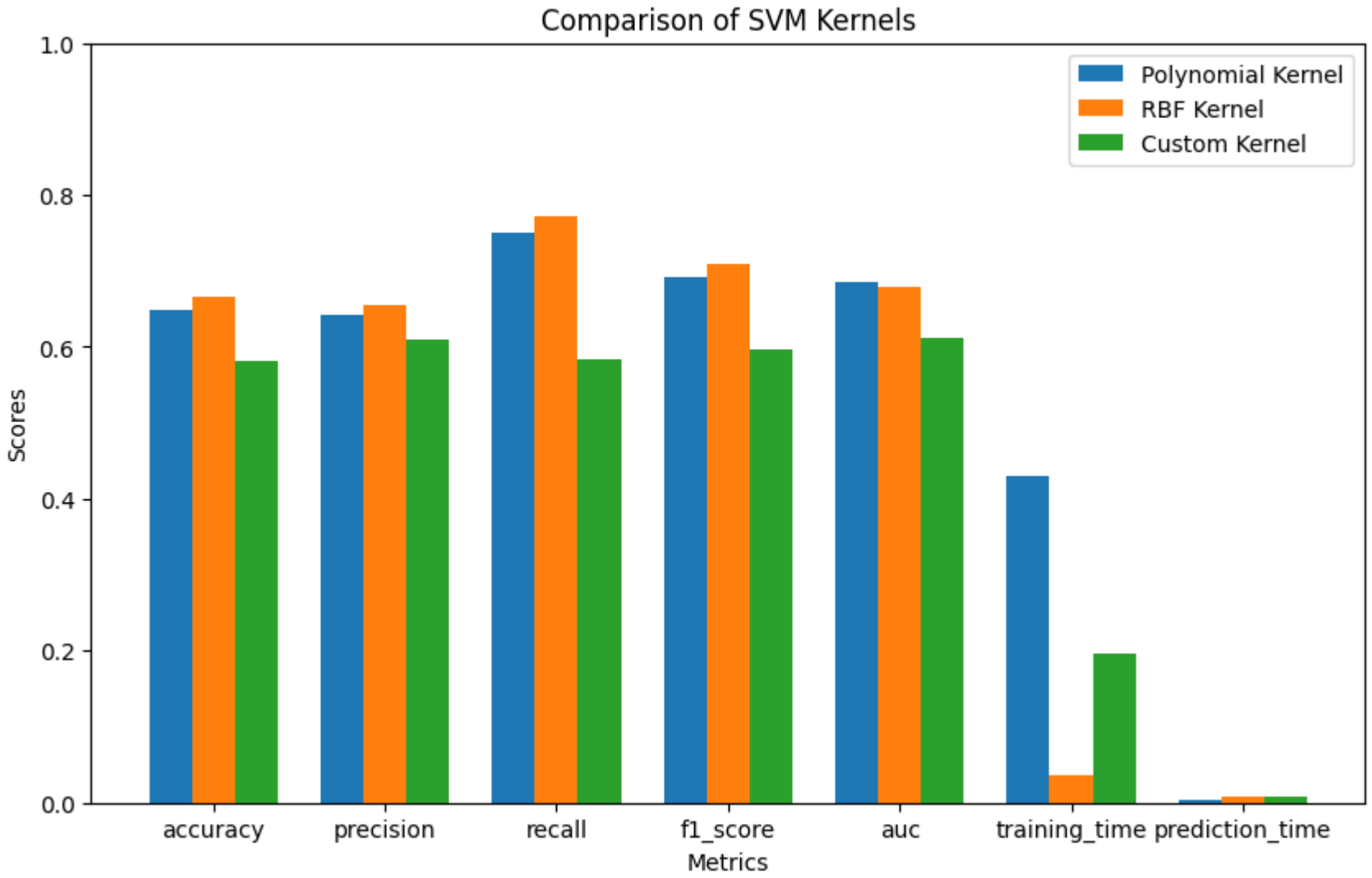
```
Custom Hybrid Kernel
Best Parameters: C=10, Gamma=1, Alpha=0.5
Metrics:
  Accuracy: 0.5824
  Precision: 0.6087
  Recall: 0.5833
  F1 Score: 0.5957
  AUC: 0.6118
  Training Time: 0.1951 seconds
  Prediction Time: 0.0083 seconds
```

3.4 Comparison of the Kernels' Performance

In [ ]:

```
# Extract metric names and corresponding values
metrics = list(poly_results['metrics'].keys())
poly_values = list(poly_results['metrics'].values())
rbf_values = list(rbf_results['metrics'].values())
custom_values = list(custom_results.values())

# Set up bar width and positions for each kernel
bar_width = 0.25
x = np.arange(len(metrics))

# Plotting the bars for each kernel
plt.figure(figsize=(10, 6))
plt.bar(x - bar_width, poly_values, width=bar_width, label='Polynomial Kernel')
plt.bar(x, rbf_values, width=bar_width, label='RBF Kernel')
plt.bar(x + bar_width, custom_values, width=bar_width, label='Custom Kernel')

# Adding labels and title
plt.xlabel('Metrics')
```

```
plt.ylabel('Scores')
plt.title('Comparison of SVM Kernels')
plt.xticks(x, metrics)
plt.ylim(0, 1)  # Assuming scores are between 0 and 1
plt.legend()

# Display the plot
plt.show()
```



4. Hyperparameter Tuning

- Chosen SVM Kernel: **RBF**
- Advanced methods such as Bayesian Optimization and Random Search are used for tuning hyperparameters (C and gamma), and analysing sensitivity of the SVM performance to different hyperparameters.

4.1 Bayesian Optimization

`BayesSearchCV` is an implementation of Bayesian Optimization, a probabilistic model-based approach for optimizing hyperparameters.

- Uses a **surrogate model** (often a Gaussian Process) to approximate the objective function.
- Utilizes an **acquisition function** to balance exploration and exploitation of the hyperparameter space.
- Iteratively updates the model based on previously evaluated hyperparameters.

In [ ]:
```
# Define the search space for Bayesian Optimization
search_space = {
    'C': (1e-3, 1e3, 'uniform'),  # C values from 0.001 to 1000
    'gamma': (1e-4, 1e1, 'log-uniform'),  # gamma values from 0.0001 to 10
}

# Bayesian Optimization for RBF Kernel
bayes_search_rbf = BayesSearchCV(SVC(kernel='rbf', random_state=42), search_space, n_iter=20, scoring='accuracy', c
bayes_search_rbf.fit(data_train, target_train)

# Capture optimal values and performance metrics
best_bayes_rbf_model = bayes_search_rbf.best_estimator_
bayes_rbf_results = evaluate_model(best_bayes_rbf_model, data_train, target_train, data_test, target_test)
optimal_c = bayes_search_rbf.best_params_['C']
optimal_gamma = bayes_search_rbf.best_params_['gamma']
metrics = bayes_rbf_results

print(f"Optimal Parameters for RBF Kernel:\n"
      f"  C: {optimal_c}\n"
      f"  Gamma: {optimal_gamma}\n")
print_metrics(metrics)
```

```
Optimal Parameters for RBF Kernel:
  C: 1000.0
  Gamma: 0.005534265789348691

Metrics:
  Accuracy: 0.6593
  Precision: 0.6604
  Recall: 0.7292
  F1 Score: 0.6931
  AUC: 0.6789
  Training Time: 0.1260 seconds
  Prediction Time: 0.0075 seconds
```

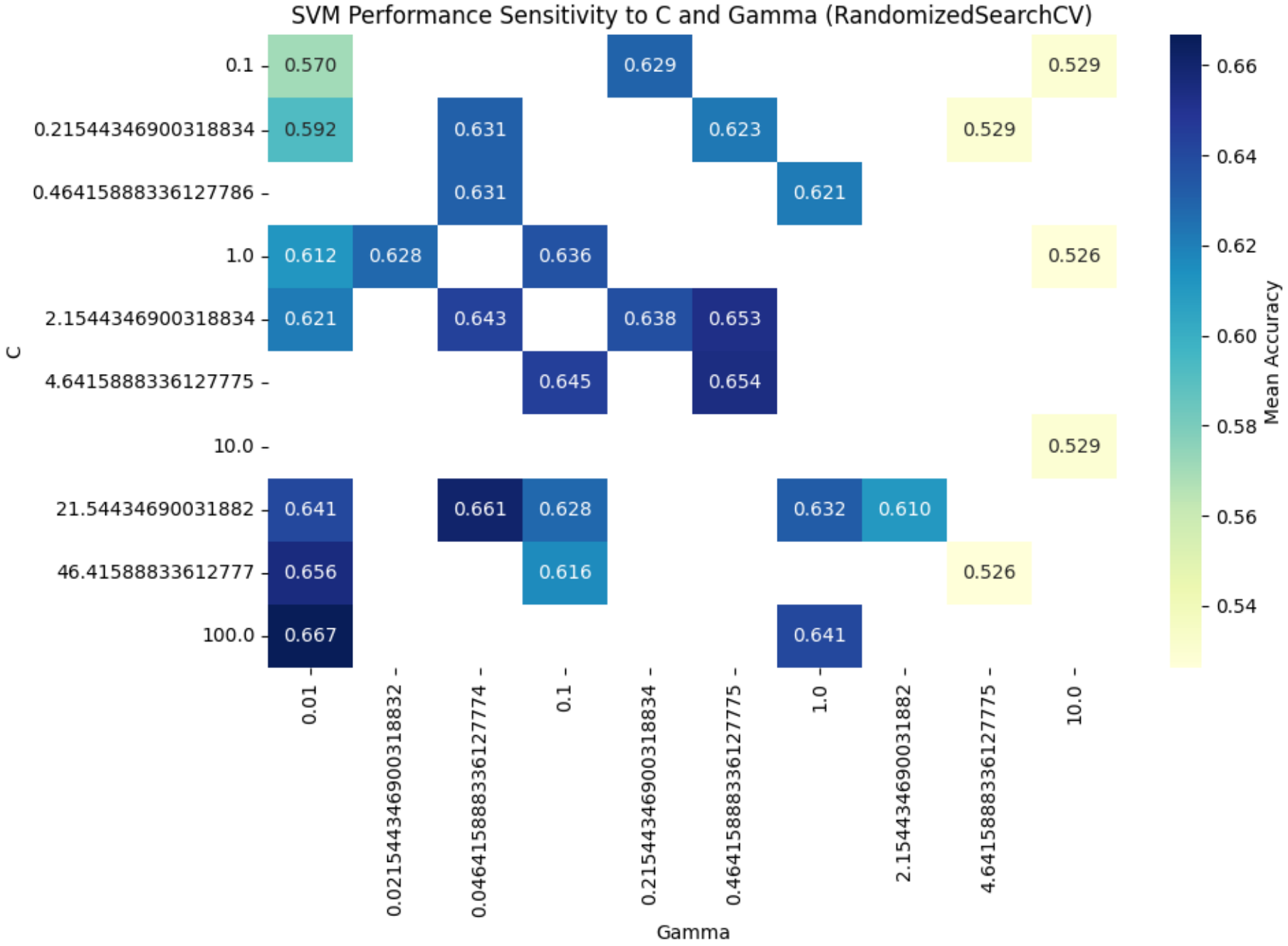
4.2 Hyperparameter Sensitivity Analysis

`RandomizedSearchCV` is a hyperparameter tuning method that samples from a specified distribution for each hyperparameter, allowing for a random selection of combinations to evaluate.

- Evaluates a fixed number of parameter settings (defined by `n_iter`) rather than all possible combinations.

In [ ]:
```
# Define the parameter distribution for C and gamma
param_dist = {
    'C': np.logspace(-1, 2, num=10),  # C values from 0.1 to 100
    'gamma': np.logspace(-2, 1, num=10) # gamma values from 0.01 to 10
}

# Initialize the SVC model
svm = SVC(kernel='rbf', random_state=42)

# Perform RandomizedSearchCV
random_search = RandomizedSearchCV(svm, param_distributions=param_dist, n_iter=30, scoring='accuracy', cv=5, n_jobs
random_search.fit(data_train, target_train)

# Extract results into a DataFrame
results = pd.DataFrame(random_search.cv_results_)

# Create a pivot table for heatmap visualization
heatmap_data = results.pivot(index='param_C', columns='param_gamma', values='mean_test_score')
```

```
# Plot the heatmap
plt.figure(figsize=(10, 6))
sns.heatmap(heatmap_data, annot=True, fmt=".3f", cmap="YlGnBu", cbar_kws={'label': 'Mean Accuracy'})
plt.title('SVM Performance Sensitivity to C and Gamma (RandomizedSearchCV)')
plt.xlabel('Gamma')
plt.ylabel('C')
plt.show()

# Print the best parameters and classification report
print(f"Best Parameters: {random_search.best_params_}")
best_model = random_search.best_estimator_
y_pred = best_model.predict(data_test)
print(classification_report(target_test, y_pred))
```


SVM Performance Sensitivity to C and Gamma (RandomizedSearchCV)
C
0.1
0.21544346900318834
0.46415888336127786
1.0
2.1544346900318834
4.6415888336127775
10.0
21.54434690031882
46.41588833612777
100.0
0.570 0.629 0.529
0.592 0.631 0.623 0.529
0.631 0.621
0.612 0.628 0.636 0.526
0.621 0.643 0.638 0.653
0.645 0.654
0.529
0.641 0.661 0.628 0.632 0.610
0.656 0.616 0.526
0.667 0.641
0.01
0.021544346900318832
0.046415888336127774
0.1
0.21544346900318834
0.46415888336127775
1.0
2.1544346900318834
4.6415888336127775
10.0
Gamma
Mean Accuracy
0.66
0.64
0.62
0.60
0.58
0.56
0.54

```
Best Parameters: {'gamma': 0.01, 'C': 100.0}
              precision    recall  f1-score   support

         0.0       0.68      0.55      0.61        86
         1.0       0.65      0.77      0.71        96

    accuracy                           0.66       182
   macro avg       0.67      0.66      0.66       182
weighted avg       0.67      0.66      0.66       182
```

5. Analysis and Report

Kernel	Max Accuracy Achieved
Linear	62.77%
Polynomial	64.84%
RBF	66.48%
Custom (RBF + Linear)	58.24%

- RBF Kernel achieved the highest accuracy, suggesting it may best capture the dataset's structure among the tested kernels. Polynomial Kernel followed closely, making it a viable option for some non-linear data patterns.
- Custom Kernel, designed to combine RBF and Linear characteristics, resulted in a lower accuracy, possibly due to overfitting or an inappropriate combination of these two kernels for this dataset.