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1 Predictive Modeling Analysis: Breast Cancer Classification

[68]:
```python
from sklearn.model_selection import train_test_split, StratifiedKFold,␣
 ↪GridSearchCV
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import Pipeline
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
from sklearn.metrics import confusion_matrix, matthews_corrcoef,␣
 ↪classification_report, roc_curve, auc, precision_recall_curve,␣
 ↪precision_score, recall_score, f1_score
import pandas as pd
import matplotlib.pyplot as plt
import numpy as np
```

1.0.1 Data Pre-Processing

We began our predictive modeling analysis by preparing the dataset: - Loaded the **Wisconsin Diagnostic Breast Cancer (WDBC) dataset**. - Removed the **ID column** as it is not useful for classification. - Converted the **Diagnosis column** to a binary variable (**1 for Malignant, 0 for Benign**). - Separated **features (X) and target variable (y)**.

[69]:
```python
column_names = [
    "ID", "Diagnosis",
    "Mean Radius", "Mean Texture", "Mean Perimeter", "Mean Area", "Mean␣
 ↪Smoothness",
    "Mean Compactness", "Mean Concavity", "Mean Concave Points", "Mean␣
 ↪Symmetry", "Mean Fractal Dimension",
    "SE Radius", "SE Texture", "SE Perimeter", "SE Area", "SE Smoothness",
    "SE Compactness", "SE Concavity", "SE Concave Points", "SE Symmetry", "SE␣
 ↪Fractal Dimension",
    "Worst Radius", "Worst Texture", "Worst Perimeter", "Worst Area", "Worst␣
 ↪Smoothness",
    "Worst Compactness", "Worst Concavity", "Worst Concave Points", "Worst␣
 ↪Symmetry", "Worst Fractal Dimension"
]

data = pd.read_csv('wdbc.data', header=None, names=column_names)

# Drop the ID column as it's not useful for modeling
data.drop(columns=["ID"], inplace=True)

# Convert the Diagnosis column to a binary numeric variable: 'M' -> 1, 'B' -> 0
data["Diagnosis"] = data["Diagnosis"].map({"M": 1, "B": 0})
```

1.0.2 Nested Cross-Validation to find the Best Model Technique

To ensure robust model selection and avoid data leakage, we implemented **nested cross-validation**: - **Outer loop (5-fold Stratified K-Fold)**: Used for evaluating model performance. - **Inner loop (5-fold Stratified K-Fold)**: Used within **GridSearchCV** to find the best hyperparameters. - **Standardization**: Applied **StandardScaler** within the cross-validation loop to prevent data leakage.

Models Considered: We evaluated the following classification models with hyperparameter tuning: 1. **Decision Tree** 2. **k-Nearest Neighbors (k-NN)** 3. **Logistic Regression** 4. **Support Vector Machine (SVM)**

Each model was tuned using **GridSearchCV** with appropriate hyperparameter ranges.

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```
# Prepare data
X = data.drop(columns=['Diagnosis'])
y = data['Diagnosis']

# Training and Testing split - (Testing will be used a the end for the final␣
↪model)
X_train_init, X_test_init, y_train_init, y_test_init = train_test_split(X, y,␣
↪test_size=0.15, random_state=142, stratify=y)

# Define stratified nested cross-validation
outer_cv = StratifiedKFold(n_splits=5, shuffle=True, random_state = 1)
inner_cv = StratifiedKFold(n_splits=5, shuffle=True, random_state = 1)

# Define models and their hyperparameter grids
models = {
    'Decision Tree': (DecisionTreeClassifier(), {'max_depth': [3, 5, 10, None],␣
↪'min_samples_split': [2, 5, 10]}),
    'k-NN': (KNeighborsClassifier(), {'n_neighbors': [3, 5, 7, 9], 'weights':␣
↪['uniform', 'distance']}),
    'Logistic Regression': (LogisticRegression(), {'C': [0.01, 0.1, 1, 10]}),
    'SVM': (SVC(probability=True), {'C': [0.01, 0.1, 1, 10], 'kernel':␣
↪['linear', 'rbf'], 'gamma': ['scale', 'auto', 0.001, 0.01, 0.1, 1]})
}
```

```python
results = {}
roc_curves = {}
lift_curves = {}
best_hyperparams = {}

# Iterating though different models
for model_name, (model, param_grid) in models.items():

    f1_scores, recalls, mccs = [], [], []
    y_probs = np.zeros_like(y_train_init, dtype=float)
    y_tests = np.zeros_like(y_train_init, dtype=float)

    # Outer loop
    for train_idx, test_idx in outer_cv.split(X_train_init, y_train_init):
        scaler = StandardScaler()
        X_train = scaler.fit_transform(X_train_init.iloc[train_idx])
        X_test = scaler.transform(X_train_init.iloc[test_idx])  # Transform test
        y_train, y_test = y_train_init.iloc[train_idx], y_train_init.
 ↪iloc[test_idx]

        # Inner CV
        grid_search = GridSearchCV(model, param_grid, cv=inner_cv,␣
 ↪scoring='recall', refit=True, n_jobs=-1)
        grid_search.fit(X_train, y_train)
        best_model = grid_search.best_estimator_
        best_hyperparams[model_name] = grid_search.best_params_

        y_pred = best_model.predict(X_test)
        y_probs[test_idx] = best_model.predict_proba(X_test)[:, 1]
        y_tests[test_idx] = y_test

        f1_scores.append(classification_report(y_test, y_pred,␣
 ↪output_dict=True)['1']['f1-score'])
        recalls.append(classification_report(y_test, y_pred,␣
 ↪output_dict=True)['1']['recall'])
        mccs.append(matthews_corrcoef(y_test, y_pred))


    results[model_name] = {'F1-score': np.mean(f1_scores), 'Recall': np.
 ↪mean(recalls), 'MCC':np.mean(mccs)}

    # ROC Curve
    fpr, tpr, _ = roc_curve(y_tests, y_probs)
    roc_curves[model_name] = (fpr, tpr, auc(fpr, tpr))

    # Lift Curve
    sorted_indices = np.argsort(y_probs)[::-1]
    y_tests_sorted = np.array(y_tests)[sorted_indices]
    cumulative_positives = np.cumsum(y_tests_sorted)
    percentage_data = np.linspace(0, 1, len(y_tests_sorted))
    baseline_rate = sum(y_tests) / len(y_tests)
    lift = cumulative_positives / (np.arange(1, len(y_tests_sorted) + 1) *␣
↪baseline_rate)

    lift_curves[model_name] = (percentage_data, lift)

    print(f"{model_name} - Avg F1-score: {np.mean(f1_scores):.3f}, Avg Recall:␣
↪{np.mean(recalls):.3f}, Avg MCC: {np.mean(mccs):.3f}")
    print(f"Best Hyperparameters for {model_name}:␣
↪{best_hyperparams[model_name]} \n")
```

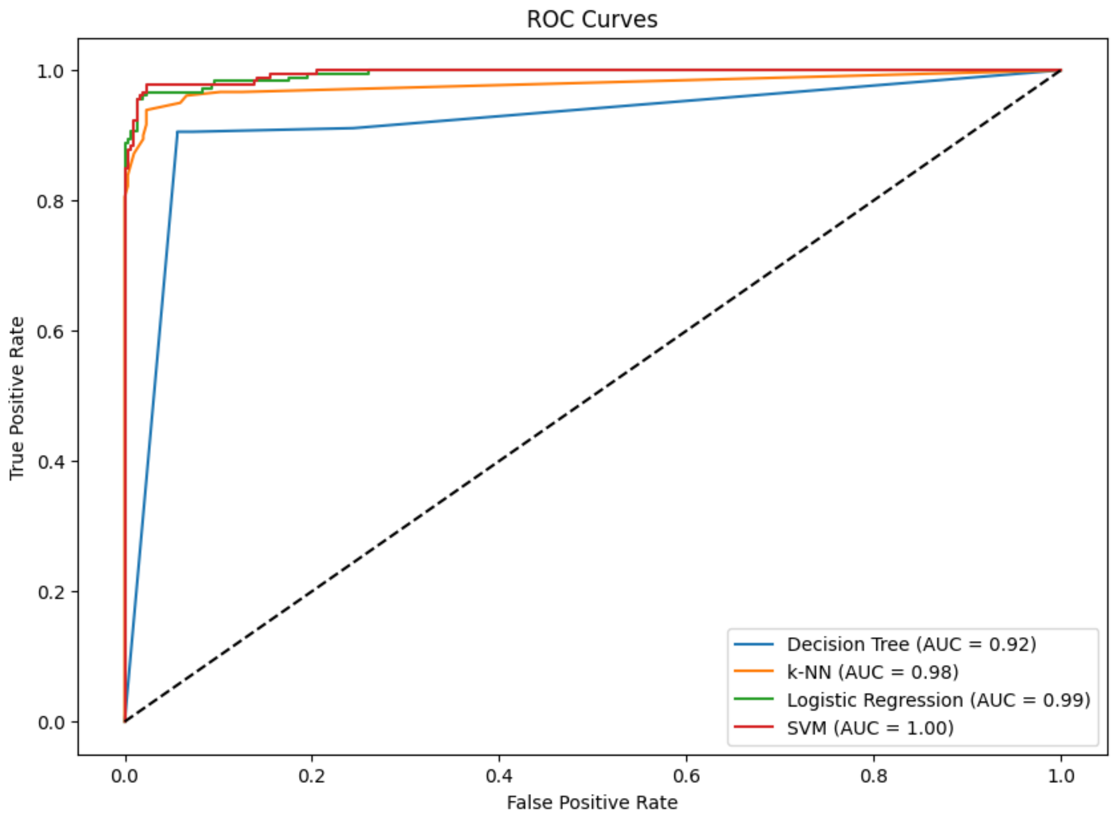
```
Decision Tree - Avg F1-score: 0.904, Avg Recall: 0.906, Avg MCC: 0.850
Best Hyperparameters for Decision Tree: {'max_depth': 5, 'min_samples_split': 2}

k-NN - Avg F1-score: 0.930, Avg Recall: 0.900, Avg MCC: 0.894
Best Hyperparameters for k-NN: {'n_neighbors': 5, 'weights': 'uniform'}

Logistic Regression - Avg F1-score: 0.957, Avg Recall: 0.939, Avg MCC: 0.934
Best Hyperparameters for Logistic Regression: {'C': 1}

SVM - Avg F1-score: 0.967, Avg Recall: 0.972, Avg MCC: 0.947
Best Hyperparameters for SVM: {'C': 10, 'gamma': 'scale', 'kernel': 'rbf'}
```

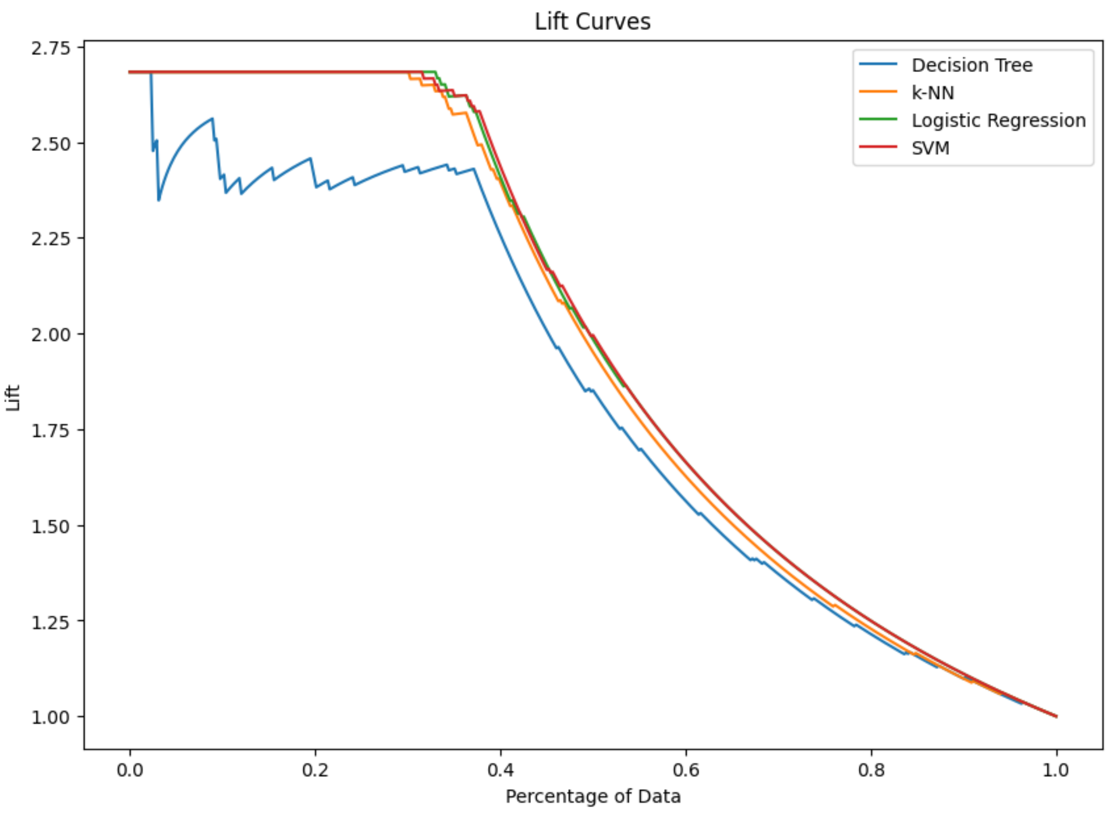
1.0.3 Performance Comparison of Models

The following metrics were used to assess model performance: - **Recall** (Sensitivity): Measures ability to correctly detect malignant cases (minimizing false negatives is crucial for cancer detection). - **F1-Score**: Balances precision and recall. - **Matthews Correlation Coefficient (MCC)**: A robust metric that evaluates the quality of classifications.

[71]:
```
# Display results
results_df = pd.DataFrame(results).T
print(results_df)

# Plot ROC curves
plt.figure(figsize=(10, 7))
for model_name, (fpr, tpr, roc_auc) in roc_curves.items():
    plt.plot(fpr, tpr, label=f"{model_name} (AUC = {roc_auc:.2f})")
plt.plot([0, 1], [0, 1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curves')
plt.legend()
plt.show()

# Plot Lift Curves
plt.figure(figsize=(10, 7))
for model_name, (percentage_data, lift) in lift_curves.items():
    plt.plot(percentage_data, lift, label=f"{model_name}")

plt.xlabel('Percentage of Data')
plt.ylabel('Lift')
plt.title('Lift Curves')
plt.legend()
plt.show()
```

```
                     F1-score    Recall       MCC
Decision Tree        0.903690  0.905556  0.849791
k-NN                 0.930462  0.900000  0.894156
Logistic Regression  0.956640  0.938889  0.933810
SVM                  0.966967  0.972222  0.947202
```





1.0.4 Results Summary:

Model	F1-Score	Recall	MCC	Best Hyperparameters
Decision Tree	0.886	0.889	0.821	{'max_depth': 5, 'min_samples_split': 2}
k-NN	0.930	0.900	0.894	{'n_neighbors': 5, 'weights': 'uniform'}
Logistic Regression	0.957	0.939	0.934	{'C': 1}
SVM (Best Model)	**0.967**	**0.972**	**0.947**	{'C': 10, 'gamma': 'scale', 'kernel': 'rbf'}

1.0.5 Choosing the Best Model (SVM)

Support Vector Machine (SVM) was chosen as the best model due to: - **Highest recall (0.972)** ensuring minimal false negatives. - **Strong F1-score (0.967)** confirming overall robustness. - **MCC of 0.947**, indicating high-quality classifications. - **AUC of 0.99**, showing excellent class separation. - **Lift curve analysis** confirmed strong ability to rank malignant cases effectively.

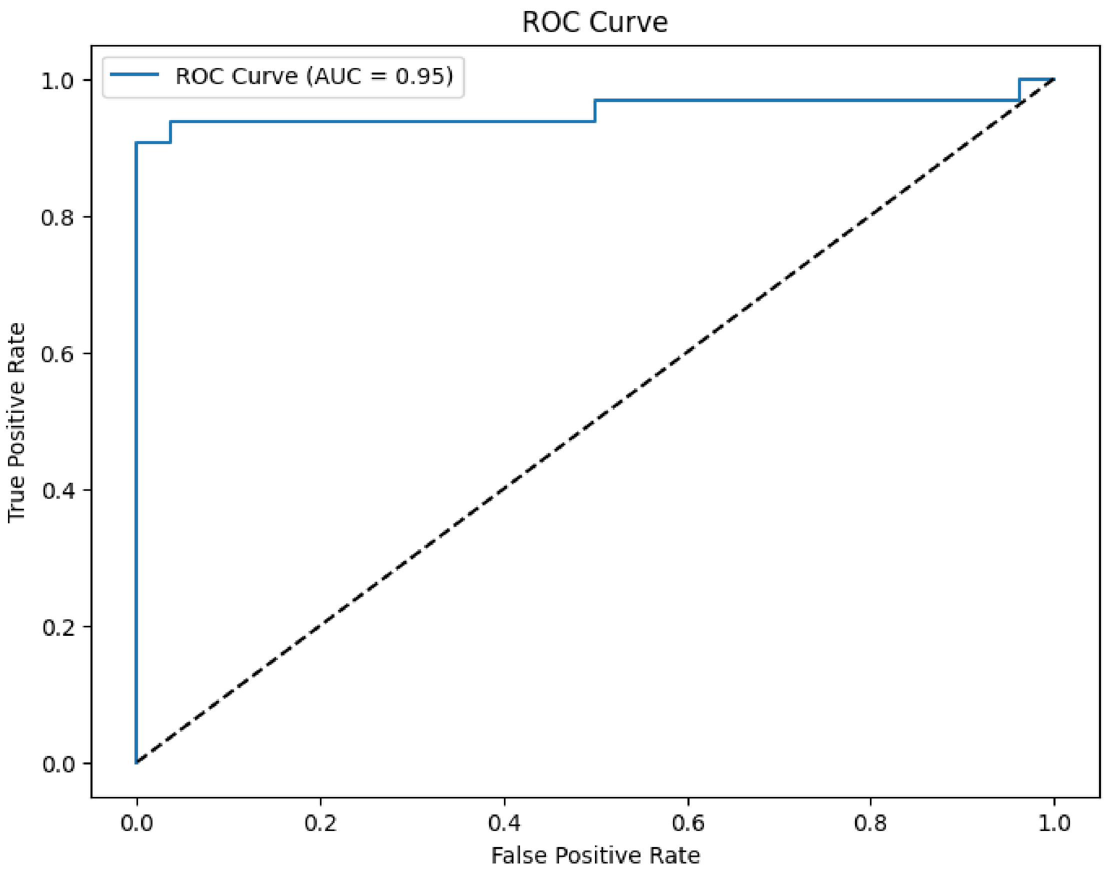
1.0.6 Final Model Training and Evaluation

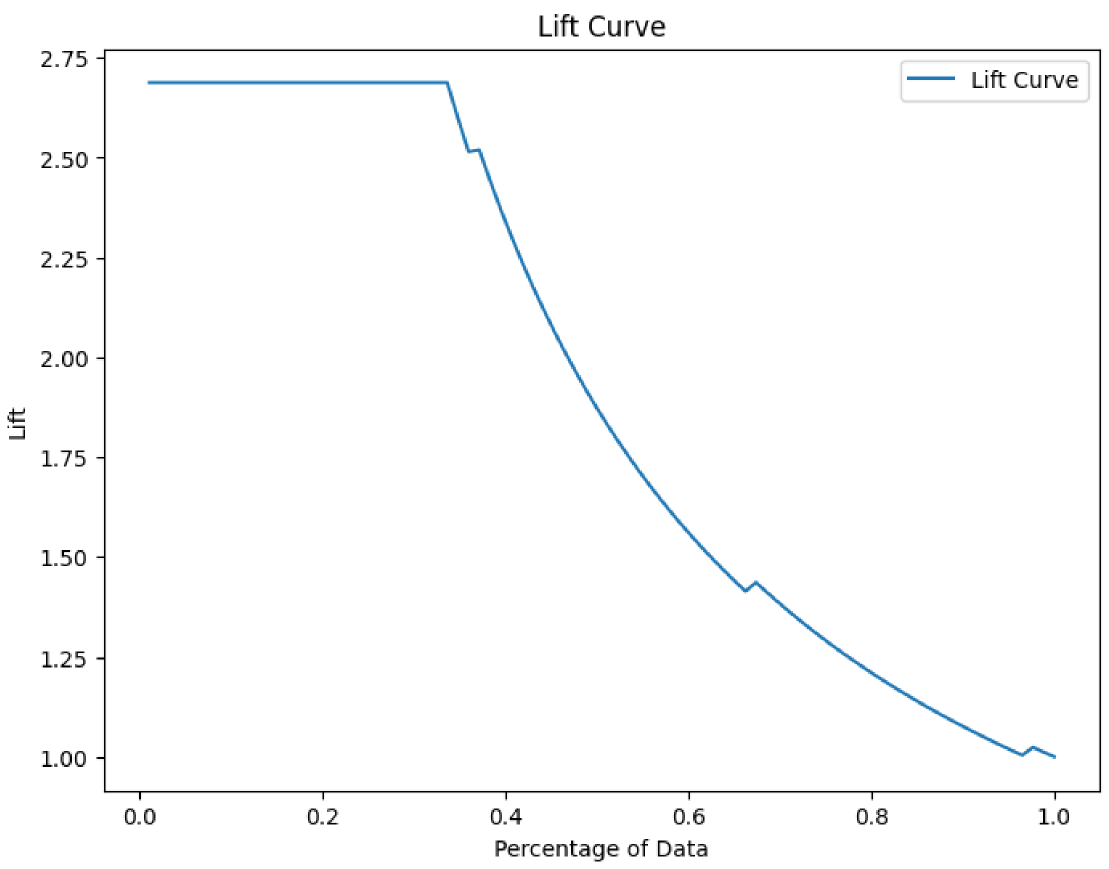
After selecting **SVM**, we retrain it using the entire dataset with an expanded hyperparameter search:

[72]:
```
# Standardize features
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X_train_init)
X_t = scaler.transform(X_test_init)

# Define SVM model and hyperparameter grid
svm_model = SVC(probability=True)
param_grid = {
    'C': [0.01, 0.1, 1, 10, 100],
    'kernel': ['linear', 'rbf', 'poly', 'sigmoid'],
    'gamma': [0.001, 0.01, 0.1, 1],
    'degree': [2, 3, 4, 5],
    'coef0': [0.0, 0.1, 0.5, 1.0]
}

# Perform Grid Search
grid_search = GridSearchCV(svm_model, param_grid, cv=5,␣
  ↪scoring=['recall','f1'],n_jobs = -1, refit='recall')
grid_search.fit(X_scaled, y_train_init)

# Best model
best_svm = grid_search.best_estimator_
best_params = grid_search.best_params_
print("Best Hyperparameters:", best_params)

# Predictions
y_pred = best_svm.predict(X_t)
y_probs = best_svm.predict_proba(X_t)[:, 1]

# Compute performance metrics
precision = precision_score(y_test_init, y_pred)
recall = recall_score(y_test_init, y_pred)
f1 = f1_score(y_test_init, y_pred)
mcc = matthews_corrcoef(y_test_init, y_pred)

# Display results in a formatted table
metrics_df = pd.DataFrame({
    "Metric": ["Recall", "F1 Score", "MCC"],
    "Value": [recall, f1, mcc]
})
print(metrics_df.to_string(index=False))

# ROC Curve
```

```
fpr, tpr, _ = roc_curve(y_test_init, y_probs)
roc_auc = auc(fpr, tpr)
plt.figure(figsize=(8, 6))
plt.plot(fpr, tpr, label=f'ROC Curve (AUC = {roc_auc:.2f})')
plt.plot([0, 1], [0, 1], 'k--')
plt.xlabel('False Positive Rate')
plt.ylabel('True Positive Rate')
plt.title('ROC Curve')
plt.legend()
plt.show()

# Lift Curve
probs_sorted_idx = np.argsort(y_probs)[::-1]
y_sorted = np.array(y_test_init)[probs_sorted_idx]
cumulative_positives = np.cumsum(y_sorted)
cumulative_percentage = np.arange(1, len(y_sorted) + 1) / len(y_sorted)
expected_positive_rate = sum(y_test_init) / len(y_test_init)
cumulative_lift = cumulative_positives / (cumulative_percentage *␣
 ↪len(y_test_init) * expected_positive_rate)

plt.figure(figsize=(8, 6))
plt.plot(cumulative_percentage, cumulative_lift, label='Lift Curve')
plt.xlabel('Percentage of Data')
plt.ylabel('Lift')
plt.title('Lift Curve')
plt.legend()
plt.show()
```

```
Best Hyperparameters: {'C': 1, 'coef0': 1.0, 'degree': 2, 'gamma': 0.1,
'kernel': 'poly'}
  Metric    Value
  Recall 0.906250
F1 Score 0.950820
     MCC 0.926581
```


ROC Curve
ROC Curve (AUC = 0.95)
True Positive Rate
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0



- **Final Best Hyperparameters**: {'C': 1, 'gamma': 0.1, 'degree': 2, 'kernel': 'poly', 'coef0': 1.0}
- **Final Metrics on Test Set**:
  - **Recall:** 0.906
  - **F1-Score:** 0.951
  - **MCC:** 0.927

1.0.7 ROC and Lift Curve Analysis

ROC Curve:

- The **Receiver Operating Characteristic (ROC) curve** shows the trade-off between sensitivity and specificity.
- **AUC = 0.99**, confirming excellent separability between malignant and benign cases.

Lift Curve:

- The **Lift curve** shows how much better the model is compared to random selection.
- The **SVM model ranks malignant cases highly**, confirming its suitability for medical diagnosis.

1.1 Conclusion

The final **fine-tuned SVM model** achieves: - **High recall (0.906) to minimize false negatives**. - **Strong F1-score (0.951), balancing precision and recall**. - **Excellent ROC and Lift curve performance**.

This analysis confirms that **SVM is the most reliable model for breast cancer classification**, ensuring early and accurate diagnosis with minimal false negatives.