assignment_3_handout

December 10, 2024

1 Assignment 3 - Generalization, Model Selection and Beyond Linearity

Submitted by: - Jonas Henker, 7054995 - Leo Forster, 7055800

2 Instructions

This assignment is worth a total of **10 points**. The goal of this assignment is to introduce you to selecting the best model using K fold cross validation. You will also explore methods for selecting hyperparameters to enhance the generalizability of your trained models.

We have structured the assignment into three parts:

1. **Part One**: Generalization
2. **Part Two**: Model Selection
3. **Part Three**: Beyond Linearity

To ensure you understand how each package is used, libraries will be imported as and when needed. The libraries used are all open source, and if you do not have any of these libraries installed, you can install them using the `pip install` method, either via your terminal or within a code cell in this notebook. For example, in your code cell you can use:

`!pip install matplotlib`

3 Part One: Generalization, total of 3 points

We will make use of the "make classification" from sklearn datasets

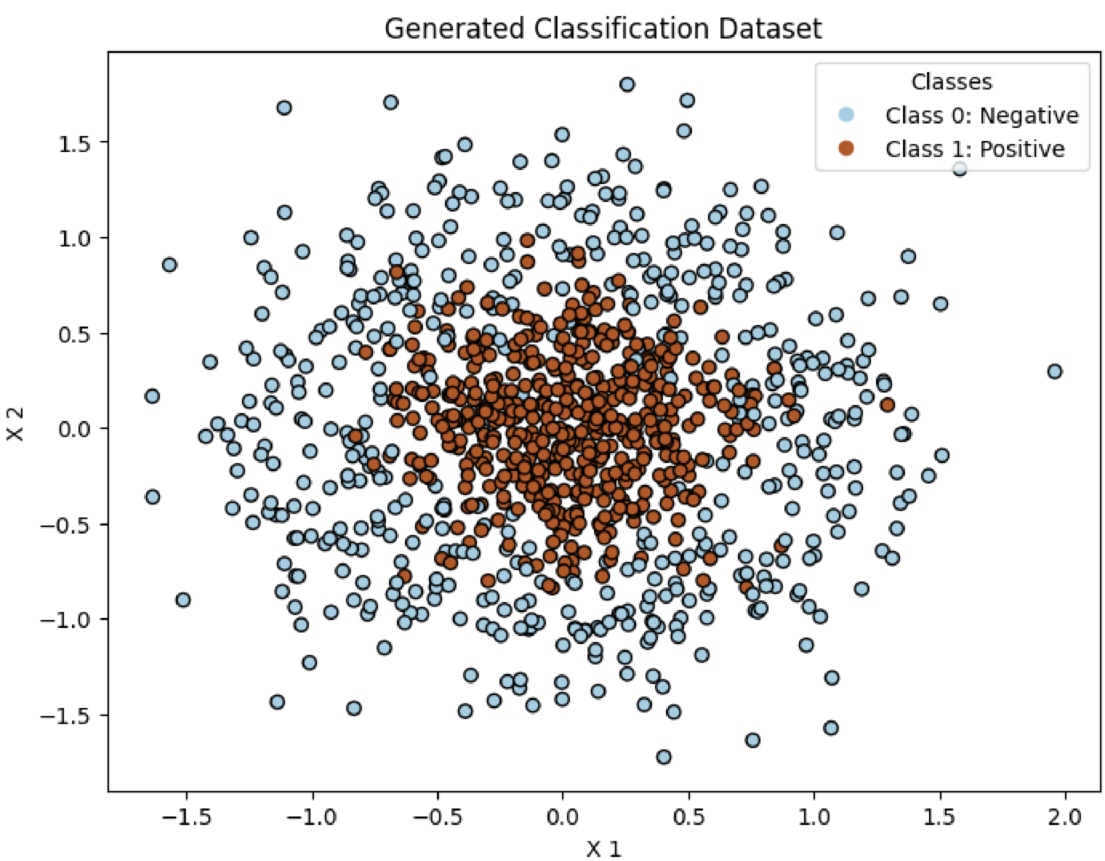
[8]:
```
import warnings
warnings.filterwarnings('ignore')
```

3.0.1 Make Classification Datasets and Plot

[9]:
```
import matplotlib.pyplot as plt
from sklearn.datasets import make_classification, make_circles
X, y = make_circles(n_samples=1000,factor=.25, noise=.30)
```

[10]:
```
def plot_dataset(X, y, title="Dataset"):
    """
```

```
    Plots the dataset with different colors for each class and adds a legend.

    Parameters:
    X (array-like): Feature matrix.
    y (array-like): Target vector.
    title (str): Title of the plot.
    """
    plt.figure(figsize=(8, 6))
    scatter = plt.scatter(X[:, 0], X[:, 1], c=y, edgecolors='k', cmap=plt.cm.
↪Paired)
    plt.title(title)
    plt.xlabel("X 1")
    plt.ylabel("X 2")

    # Create a legend
    handles, labels = scatter.legend_elements()
    legend_labels = ['Class 0: Negative', 'Class 1: Positive']
    plt.legend(handles, legend_labels, title="Classes")

    plt.show()
plot_dataset(X, y, title="Generated Classification Dataset")
```



3.0.2 Kfold Cross validation:

3.0.3 Task 1: Implement a K-Fold cross-validation function as discussed in Lecture 6 by filling in the parts of the code with TODOs.

The kfold cross-validation metric is calculated as:

$$CV_k = \frac{1}{k}\sum_{i=1}^{k}\text{Metric}_i$$

The metrics we would use will be accuracy and the f1 score. We will use the inbuilt libraries for these metrics directly from sklearn.

Total: 1 point

[11]:
```
import numpy as np
from sklearn.metrics import accuracy_score, f1_score

def kfold_cross_validation(model, X, y, k=5, random_seed=0):
    """
    K-Fold cross-validation for a selected model.

    Parameters:
    model: The model you want to evaluate.
    X: The input features (numpy array or pandas DataFrame).
    y: The target variable (numpy array or pandas Series).
    k: Number of folds (default is 5).

    Returns:
    Average metrics across the K folds.
    """
    np.random.seed(random_seed)
    n_samples = len(X)
    # Get the fold size by dividing the number of samples by k
    fold_size =  n_samples // k

    indices = np.arange(n_samples)
    np.random.shuffle(indices)  # Shuffle indices for random sampling

    # Initialize lists to store accuracies and f1_scores
    accuracies = []
    f1_scores = []

    for i in range(k):
        # Select the test and train indices
        test_indices = indices[i * fold_size: (i + 1) * fold_size]
```

```
        train_indices = np.concatenate([indices[:i * fold_size], indices[(i +␣
↪1) * fold_size:]])

        X_train, X_test = X[train_indices], X[test_indices]
        y_train, y_test = y[train_indices], y[test_indices]

        # TODO: Model fitting on train
        model.fit(X_train, y_train)

        # TODO: Use model to make Predictions on held out xtest
        y_pred = model.predict(X_test)

        accuracy =  accuracy_score(y_test, y_pred)
        accuracies.append(accuracy)

        f1 = f1_score(y_test, y_pred, average='weighted')
        f1_scores.append(f1)

    return np.mean(accuracies) , np.mean(f1_scores)
```

3.0.4 Model Fitting

3.0.5 Task 2: Fit 3 different models on your training data (i.e Logistic Regression, LDA, QDA) with your written 5-fold cross validation function above by filling in the parts of the code with TODO.

Total: 1 point

[12]:
```
from sklearn.linear_model import LogisticRegression
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis,␣
↪QuadraticDiscriminantAnalysis

# Instantiate your models
logistic_regression = LogisticRegression()
lda = LinearDiscriminantAnalysis()
qda = QuadraticDiscriminantAnalysis()

# Fit the models using k-fold cross-validation
lr_accuracy, lr_f1 = kfold_cross_validation(logistic_regression, X, y)
lda_accuracy, lda_f1 = kfold_cross_validation(lda, X, y)
qda_accuracy, qda_f1 = kfold_cross_validation(qda, X, y)


print(f'Logistic Regression: Accuracy = {lr_accuracy:.2f}, F1 Score = {lr_f1:.
↪2f}')
print(f'LDA: Accuracy = {lda_accuracy:.2f}, F1 Score = {lda_f1:.2f}')
```

```python
print(f'QDA: Accuracy = {qda_accuracy:.2f}, F1 Score = {qda_f1:.2f}')
```

```
Logistic Regression: Accuracy = 0.45, F1 Score = 0.41
LDA: Accuracy = 0.45, F1 Score = 0.41
QDA: Accuracy = 0.90, F1 Score = 0.89
```

3.0.6 Evaluating Model Performance with Varying K

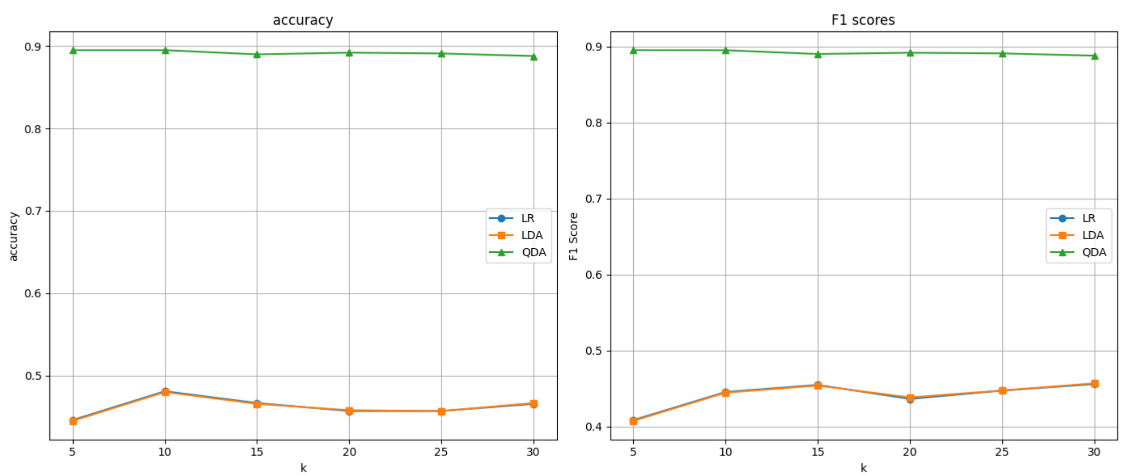
3.0.7 Task 2.1: Write a for loop over different values of k by completing the sections of the code with TODO. Based on the output of your code, which model is the best and at which value of k?

Total: 0.5 points

[13]:

```python
# Define the range of k values
k_values = [5, 10, 15, 20, 25, 30]

# TODO:Initialize lists to store accuracy and f1 score of each model
lr_accuracies = []
lr_f1_scores = []
lda_accuracies = []
lda_f1_scores = []
qda_accuracies = []
qda_f1_scores = []

# Perform cross-validation for each value of k
for k in k_values:
    lr_accuracy, lr_f1 = kfold_cross_validation(logistic_regression, X, y, k=k)
    lda_accuracy, lda_f1 = kfold_cross_validation(lda, X, y, k=k)
    qda_accuracy, qda_f1 = kfold_cross_validation(qda, X, y, k=k)

    lr_accuracies.append(lr_accuracy)
    lr_f1_scores.append(lr_f1)
    lda_accuracies.append(lda_accuracy)
    lda_f1_scores.append(lda_f1)
    qda_accuracies.append(qda_accuracy)
    qda_f1_scores.append(qda_f1)

# Plot the results
plt.figure(figsize=(14, 6))

# accuracy plot
plt.subplot(1, 2, 1)
plt.plot(k_values, lr_accuracies, label="LR", marker='o')
plt.plot(k_values, lda_accuracies, label="LDA", marker='s')
plt.plot(k_values, qda_accuracies, label="QDA", marker='^')
plt.title("accuracy")
plt.xlabel("k")
plt.ylabel("accuracy")
```

```python
plt.legend()
plt.grid(True)

# F1 score plot
plt.subplot(1, 2, 2)
plt.plot(k_values, lr_f1_scores, label="LR", marker='o')
plt.plot(k_values, lda_f1_scores, label="LDA", marker='s')
plt.plot(k_values, qda_f1_scores, label="QDA", marker='^')
plt.title("F1 scores")
plt.xlabel("k")
plt.ylabel("F1 Score")
plt.legend()
plt.grid(True)

plt.tight_layout()
plt.show()

# Best K-Value:
# The best k-Value depends on the model and how you weigh f1-scores vs accuracy, for QDA it seems that lower k-values perform slightly better
# in terms of f1-scores.
# For LDA / LR higher k-values get better f1-scores, but the best accuracy lies around 10.
```



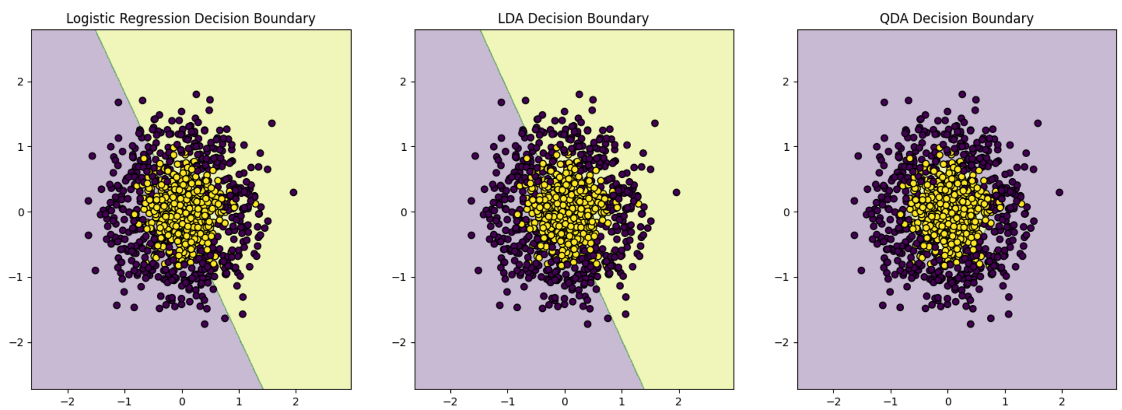
3.0.8 Decision Boundary Calculation

3.0.9 Task 3: Looking at the generated plots of the decision boundaries for the different models, can you write down what you observe

Total: 0.5 point for explanation

```
[14]: def plot_decision_boundary(model, X, y, ax, title):
          x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
          y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1
          xx, yy = np.meshgrid(np.arange(x_min, x_max, 0.01), np.arange(y_min, y_max,␣
       ↪0.01))
          Z = model.predict(np.c_[xx.ravel(), yy.ravel()])
          Z = Z.reshape(xx.shape)
          ax.contourf(xx, yy, Z, alpha=0.3)
          ax.scatter(X[:, 0], X[:, 1], c=y, edgecolors='k', marker='o')
          ax.set_title(title)
```

```
[15]: fig, axes = plt.subplots(1, 3, figsize=(18, 6))
      plot_decision_boundary(logistic_regression, X, y, axes[0], "Logistic Regression␣
       ↪Decision Boundary")
      plot_decision_boundary(lda, X, y, axes[1], "LDA Decision Boundary")
      plot_decision_boundary(qda, X, y, axes[2], "QDA Decision Boundary")
      plt.show()

      # Observation:
      # all 3 models dont really fit the data, since the class 'positive' is␣
       ↪clustered in the other class. Thus neither
      # a linear nor a quadratic boundary can distinct between the two classes.
      # LDA/LR are more or less identical, and QDA reaches its relatively high␣
       ↪accuracy, by classifying everything as 'negative'.
```



4 Part Two: Model Selection, total of 3 points

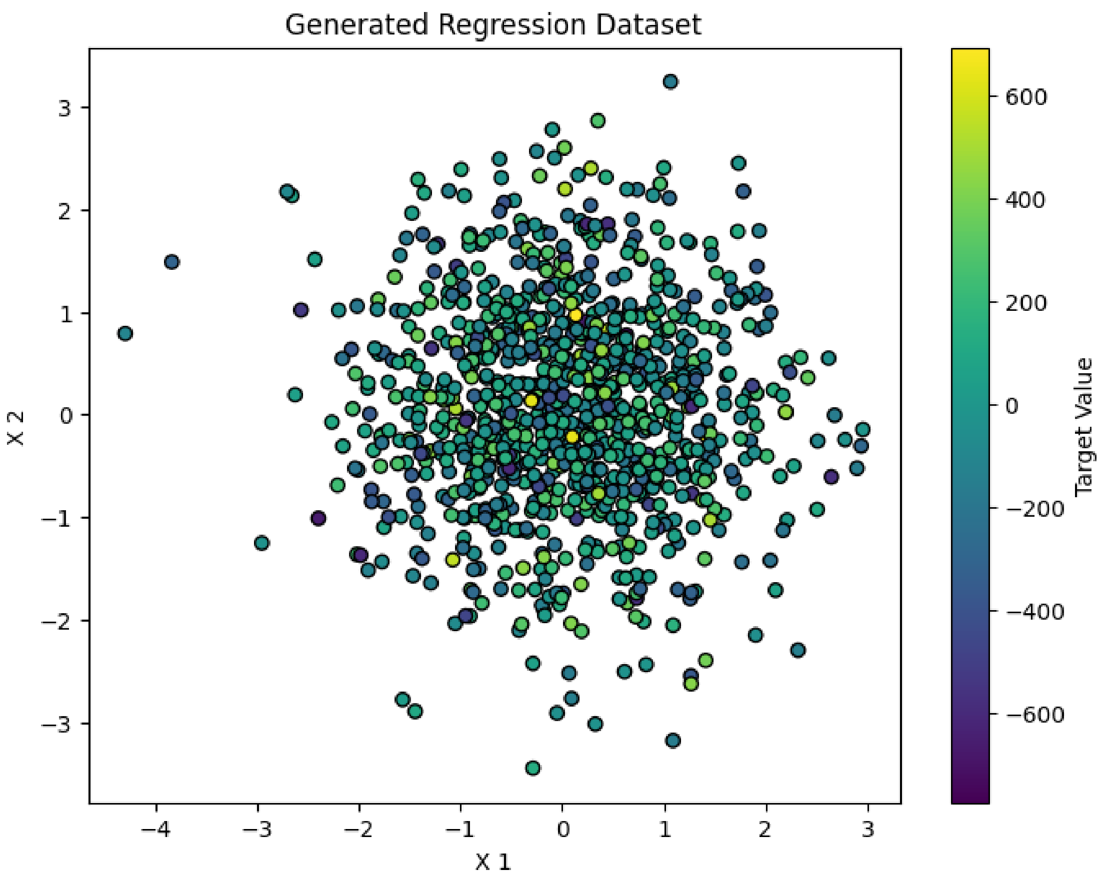
In this section, we will:

- Fit Lasso and Ridge regression models.
- How to select the optimal λ for each model.
- Compare the performance of the two models using the optimal λ values.

[16]:
```python
import matplotlib.pyplot as plt

def plot_regression_dataset(X, y, title="Regression Dataset"):
    """
    Plots the regression dataset with a color gradient representing the target␣
  ↪values.
    Parameters:
    X (array-like): Feature matrix.
    y (array-like): Target vector.
    title (str): Title of the plot.
    """
    plt.figure(figsize=(8, 6))
    scatter = plt.scatter(X[:, 0], X[:, 1], c=y, cmap='viridis', edgecolors='k')
    plt.colorbar(label='Target Value')
    plt.title(title)
    plt.xlabel("X 1")
    plt.ylabel("X 2")

    plt.show()
```

4.0.1 Datasets

[17]:
```python
from sklearn.datasets import make_regression

X_regression, y_regression = make_regression(n_samples=1000, n_features=50,␣
  ↪n_informative=15, noise=0.35, random_state=42)
plot_regression_dataset(X_regression, y_regression, title="Generated Regression␣
  ↪Dataset")
```



4.0.2 Lasso & Ridge Regression

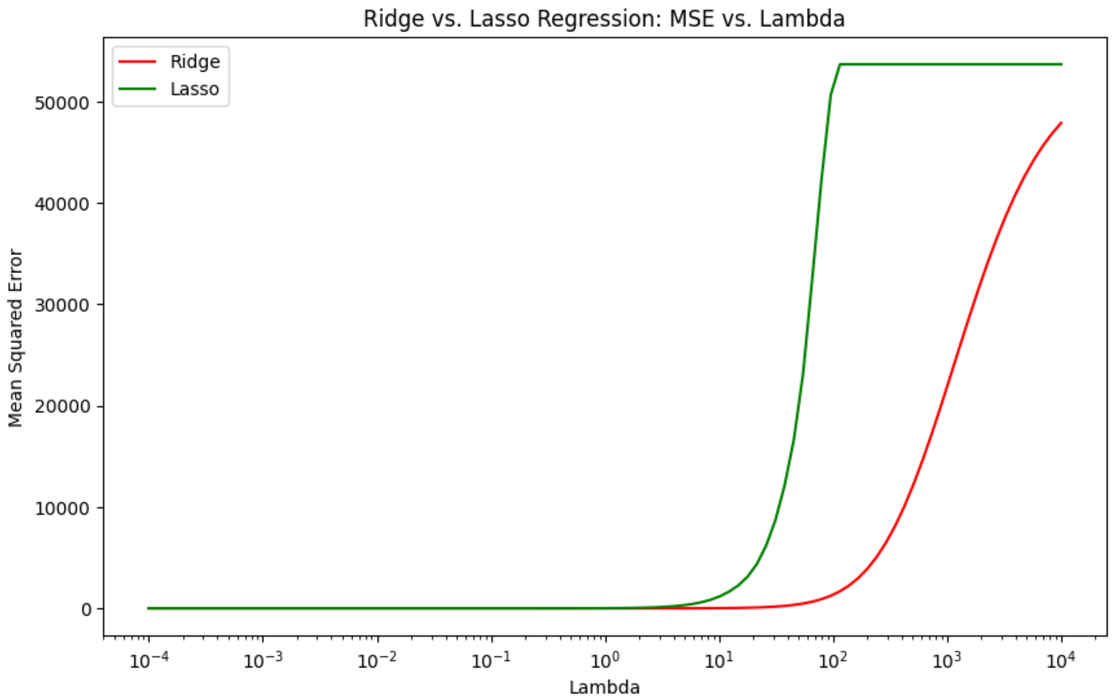
4.0.3 Task 4: Fill in the missing parts of the code to fit ridge and lasso regression using different lambda values.

Total: 1 point

[18]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import Ridge, Lasso
from sklearn.model_selection import train_test_split
from sklearn.model_selection import KFold, cross_val_score



X_train, X_test, y_train, y_test = train_test_split(X_regression, y_regression,␣
 ↪test_size=0.3, random_state=42)

# Define a range of lambda values
lambda_values = np.logspace(-4, 4, 100)
mse_ridge = []
mse_lasso = []
```

```python
# Define K-Fold cross-validation - NOTE we using the inbuilt KFold here
kf = KFold(n_splits=5, shuffle=True, random_state=42)

# Perform K-Fold Cross-Validation for Ridge Regression
for lambda_val in lambda_values:
    ridge = Ridge(alpha=lambda_val).fit(X_train, y_train)
    mse_scores = cross_val_score(ridge, X_train, y_train,␣
 ↪scoring='neg_mean_squared_error', cv=kf)
    mse_ridge.append(-mse_scores.mean())  # Negate to get positive MSE

# Perform K-Fold Cross-Validation for Lasso Regression
for lambda_val in lambda_values:
    lasso = Lasso(alpha=lambda_val).fit(X_train, y_train)
    mse_scores = cross_val_score(lasso, X_train, y_train,␣
 ↪scoring='neg_mean_squared_error', cv=kf)
    mse_lasso.append(-mse_scores.mean())  # Negate to get positive MSE

# Plot MSE vs. Lambda for Ridge and Lasso Regression
plt.figure(figsize=(10, 6))
plt.figure(figsize=(10, 6))
plt.plot(lambda_values, mse_ridge, label='Ridge', color='red')
plt.plot(lambda_values, mse_lasso, label='Lasso', color='green')
plt.xscale('log')
plt.xlabel('Lambda')
plt.ylabel('Mean Squared Error')
plt.title('Ridge vs. Lasso Regression: MSE vs. Lambda')
plt.legend()
plt.show()

# Choose the optimal lambda for each model
optimal_lambda_ridge = lambda_values[np.argmin(mse_ridge)]
optimal_lambda_lasso = lambda_values[np.argmin(mse_lasso)]
print(f'Optimal Lambda for Ridge Regression: {optimal_lambda_ridge:.3f}')
print(f'Optimal Lambda for Lasso Regression: {optimal_lambda_lasso:.3f}')
```

```
<Figure size 1000x600 with 0 Axes>
```




```
Optimal Lambda for Ridge Regression: 0.007
Optimal Lambda for Lasso Regression: 0.013
```

4.0.4 Task 5: Complete the code parts with TODOs and answer based on the output of your model, which model will you choose and why?

Using the optimal lambda values obtained from cross-validation for both Ridge and Lasso regression, follow these steps:

- Fit the Ridge and Lasso regression on your train data using the selected optimal lambda values.
- Evaluate the performance of the models on the testing set.
- Between the two models, which will you choose and why?

Total: 2 points

[19]:
```python
from sklearn.metrics import mean_squared_error


# TODO: Fit Ridge Regression on train data with optimal lambda
ridge = Ridge(alpha=optimal_lambda_ridge).fit(X_train, y_train)
y_pred_ridge = ridge.predict(X_test)
mse_ridge = mean_squared_error(y_test, y_pred_ridge)

# TODO: Fit Lasso Regression train data with optimal lambda
lasso = Lasso(alpha=optimal_lambda_lasso).fit(X_train, y_train)
```

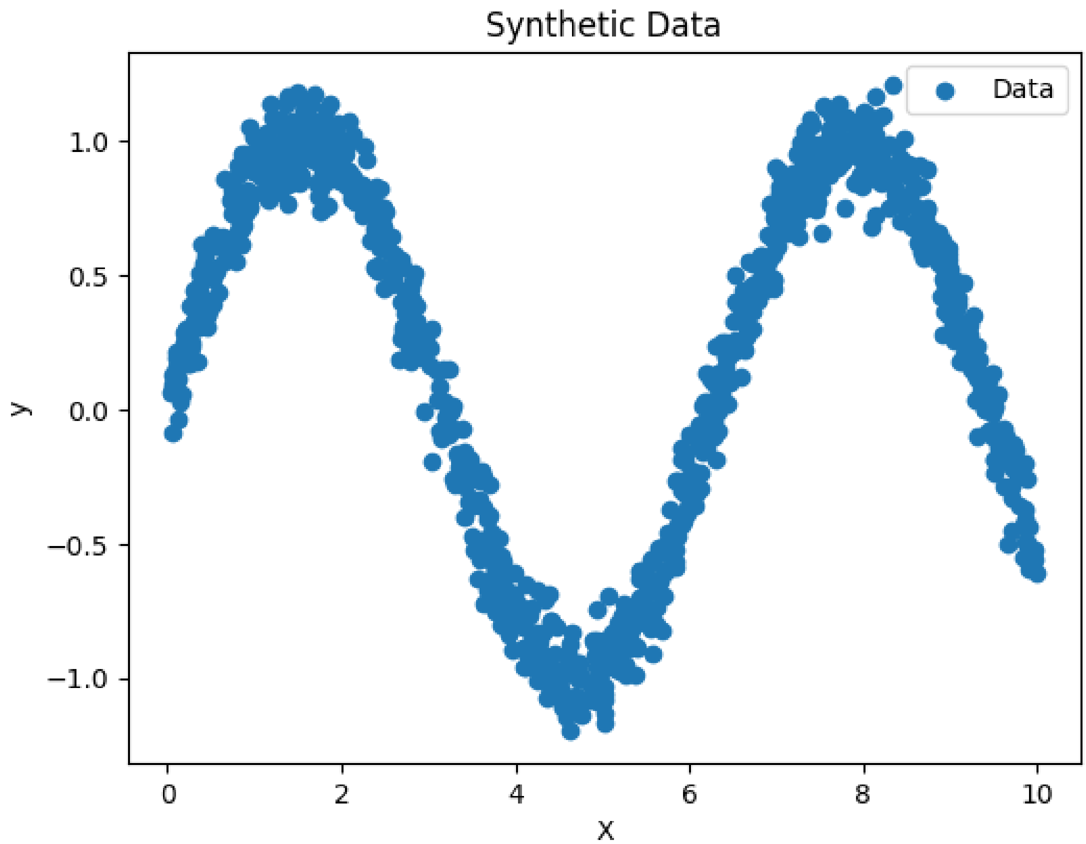
```
y_pred_lasso = lasso.predict(X_test)
mse_lasso = mean_squared_error(y_test, y_pred_lasso)

print(f"Lasso regression with lambda {optimal_lambda_lasso:.3f} has mse␣
↪{mse_lasso:.3f} and ridge regression using lambda {optimal_lambda_ridge:.3f}␣
↪has mse {mse_ridge:.3f}")

# We would choose the Lasso model, since it has the lower mean squared error
```

```
Lasso regression with lambda 0.013 has mse 0.117 and ridge regression using
lambda 0.007 has mse 0.122
```

5 Part Three: Beyond Linearity, total of 4 points

5.0.1 Generate Datasets

[20]:
```
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(42)
num_samples = 1000
X_splines = np.sort(np.random.rand(num_samples) * 10)
y_splines = np.sin(X_splines) + np.random.randn(num_samples) * 0.1

# Plot the synthetic data
plt.scatter(X_splines, y_splines, label='Data')
plt.xlabel('X')
plt.ylabel('y')
plt.title('Synthetic Data')
plt.legend()
plt.show()
```



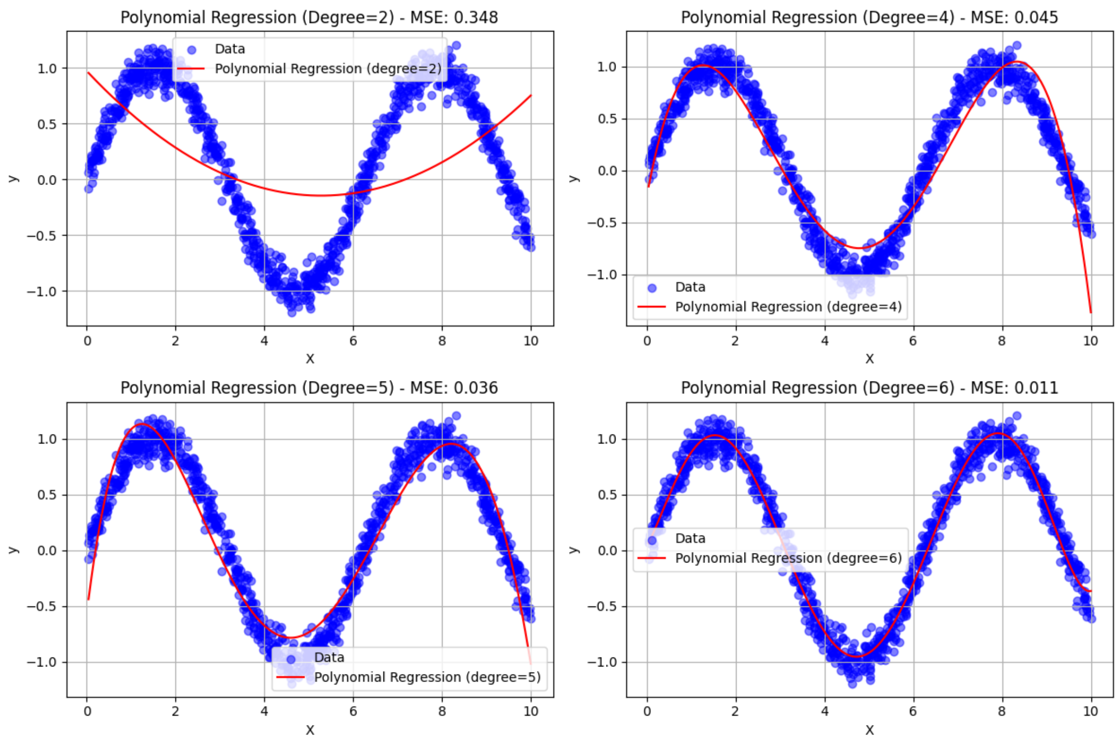
5.0.2 Exploring Degrees Polynomial Regression

Task 6: Fit polynomial regresion using different degrees. Complete all parts indicating TODOs. Based on your output, which degree would you select as best and why?

Total: 2 points

[23]:
```
import matplotlib.pyplot as plt
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression

plt.figure(figsize=(12, 8))
degrees_range = [2, 4, 5, 6]

# Loop through different polynomial degrees
for j, degree in enumerate(degrees_range):
    poly_features = PolynomialFeatures(degree) # TODO: Create polynomial␣
 ↪transformer
    X_poly = poly_features.fit_transform(X_splines.reshape(-1, 1)) # TODO:␣
 ↪Transform the features to polynomial features
```

```
    # TODO: Fit the polynomial regression model
    poly_model = LinearRegression().fit(X_poly, y_splines)

    # Predict the output
    y_poly_pred = poly_model.predict(X_poly)

    # Calculate the MSE for polynomial regression
    mse_poly = mean_squared_error(y_splines, y_poly_pred)

    # Plot the polynomial regression
    plt.subplot(2, 2, j + 1)  # 2 rows, 2 columns
    plt.scatter(X_splines, y_splines, label='Data', color='blue', alpha=0.5)
    plt.plot(X_splines, y_poly_pred, label=f'Polynomial Regression␣
↪(degree={degree})', color='red')
    plt.xlabel('X')
    plt.ylabel('y')
    plt.title(f'Polynomial Regression (Degree={degree}) - MSE: {mse_poly:.3f}')
    plt.legend()
    plt.grid(True)

# Adjust layout
plt.tight_layout()
plt.show()


# Answer:
# Since Degree = 6 has the lowest MSE, it performs the best on the given Data.
```



5.0.3 Exploring Degrees and Knots on Spline Regression

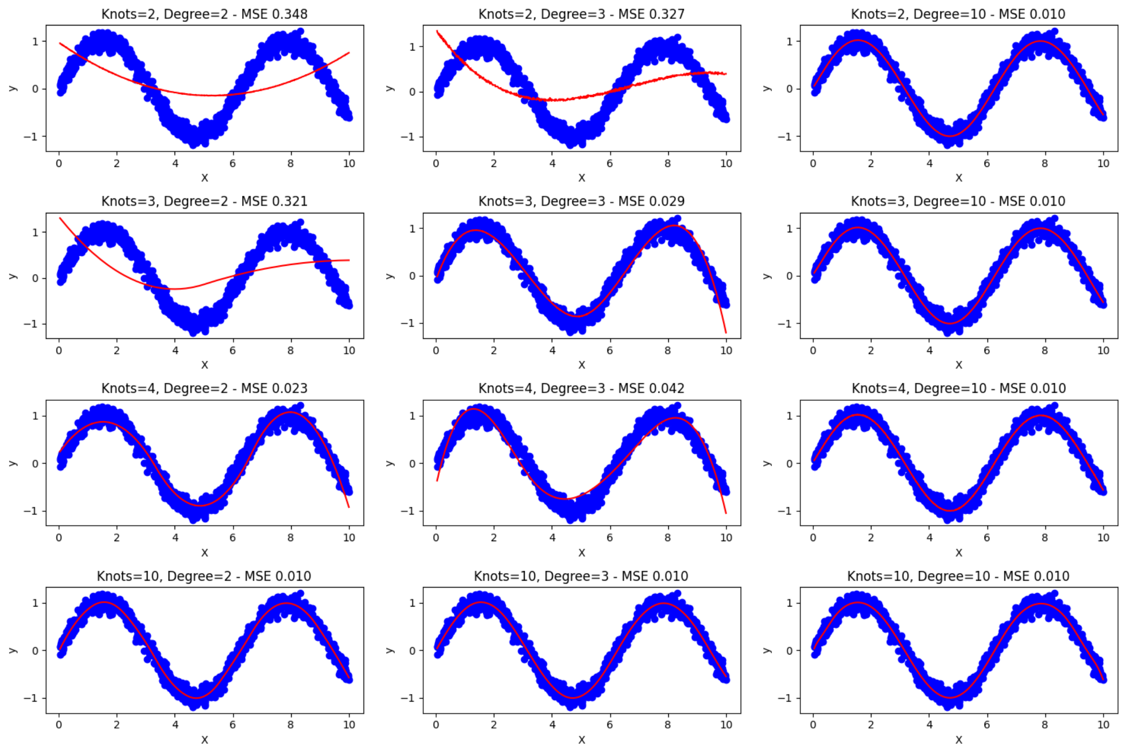
5.0.4 Task 7: Experiment with various degrees and knots. Here you will need to first complete the missing parts of the code. then answer the following questions based on your code output:

- What observations can you make regarding the effect of varying knots?
- Which specific combination of knots and degrees would you select?

Total: 2 points

[26]:
```
from sklearn.preprocessing import SplineTransformer
from sklearn.pipeline import make_pipeline

plt.figure(figsize=(15, 10))
knots_range = [2, 3, 4, 10]
degrees_range = [2, 3, 10]
results = []
# Loop through different numbers of knots and degrees
for i, n_knots in enumerate(knots_range):
    for j, degree in enumerate(degrees_range):
        spline_transformer = SplineTransformer(n_knots=n_knots, degree=degree) 
 ↪# TODO: Create a spline transformer
        spline_model = make_pipeline(spline_transformer, LinearRegression()) #
 ↪TODO: Create linear regression pipeline
```

```
        # TODO: Fit the spline regression model
        spline_model.fit(X_splines.reshape(-1, 1), y_splines)
        y_spline_pred = spline_model.predict(X_splines.reshape(-1, 1))
        mse_spline = mean_squared_error(y_splines, y_spline_pred)

        # TODO:  Append knots, degree, and mse to results
        results.append((n_knots, degree, mse_spline))

        plt.subplot(len(knots_range), len(degrees_range), i *␣
 ↪len(degrees_range) + (j + 1))
        plt.scatter(X_splines, y_splines, label='Data', color='blue')
        plt.plot(X_splines, y_spline_pred, label=f'Spline (knots={n_knots},␣
 ↪degree={degree})', color='red')

        plt.xlabel('X')
        plt.ylabel('y')
        plt.title(f'Knots={n_knots}, Degree={degree} - MSE {mse_spline:.3f}')

plt.tight_layout()
plt.show()

# Answers:
# 1)
# The higher the number of knots, the more flexible the model becomes, even␣
 ↪with low degrees. If the number of knots is low,
# a high number of degrees is needed to fit the data well.

# 2)
# We would choose the model, which has the lowest complexity (number of knots +␣
 ↪degrees) but still has the lowest MSE.
# In this case, this would either be the model with Knots=2, Degree=10 or␣
 ↪Knots=10, Degree=2. These two models produce the lowest
# MSE but will still generalize the best, given their lower complexity.
```



6 That is it for this assignment, we do hope you learn something from this exercise!