Exercise 8: Visualizing Kernel Ridge Regression

CPSC 381/581: Machine Learning

Yale University

Instructor: Alex Wong

Prerequisites:

1. Enable Google Colaboratory as an app on your Google Drive account
2. Create a new Google Colab notebook, this will also create a "Colab Notebooks" directory under "MyDrive" i.e.

   ```
   /content/drive/MyDrive/Colab Notebooks
   ```

3. Create the following directory structure in your Google Drive

   ```
   /content/drive/MyDrive/Colab Notebooks/CPSC 381-581: Machine
   Learning/Exercises
   ```

4. Move the 08_exercise_visualizing_kernel_ridge_regression.ipynb into

   ```
   /content/drive/MyDrive/Colab Notebooks/CPSC 381-581: Machine
   Learning/Exercises
   ```

so that its absolute path is

```
/content/drive/MyDrive/Colab Notebooks/CPSC 381-581: Machine
Learning/Exercises/08_exercise_visualizing_kernel_ridge_regressio.ipynb
```

In this exercise, we will optimize a kernel ridge regression with different kernels and visualize the decision boundaries.

Submission:

1. Implement all TODOs in the code blocks below.
2. List any collaborators.

   ```
   Collaborators: None
   ```

Import packages

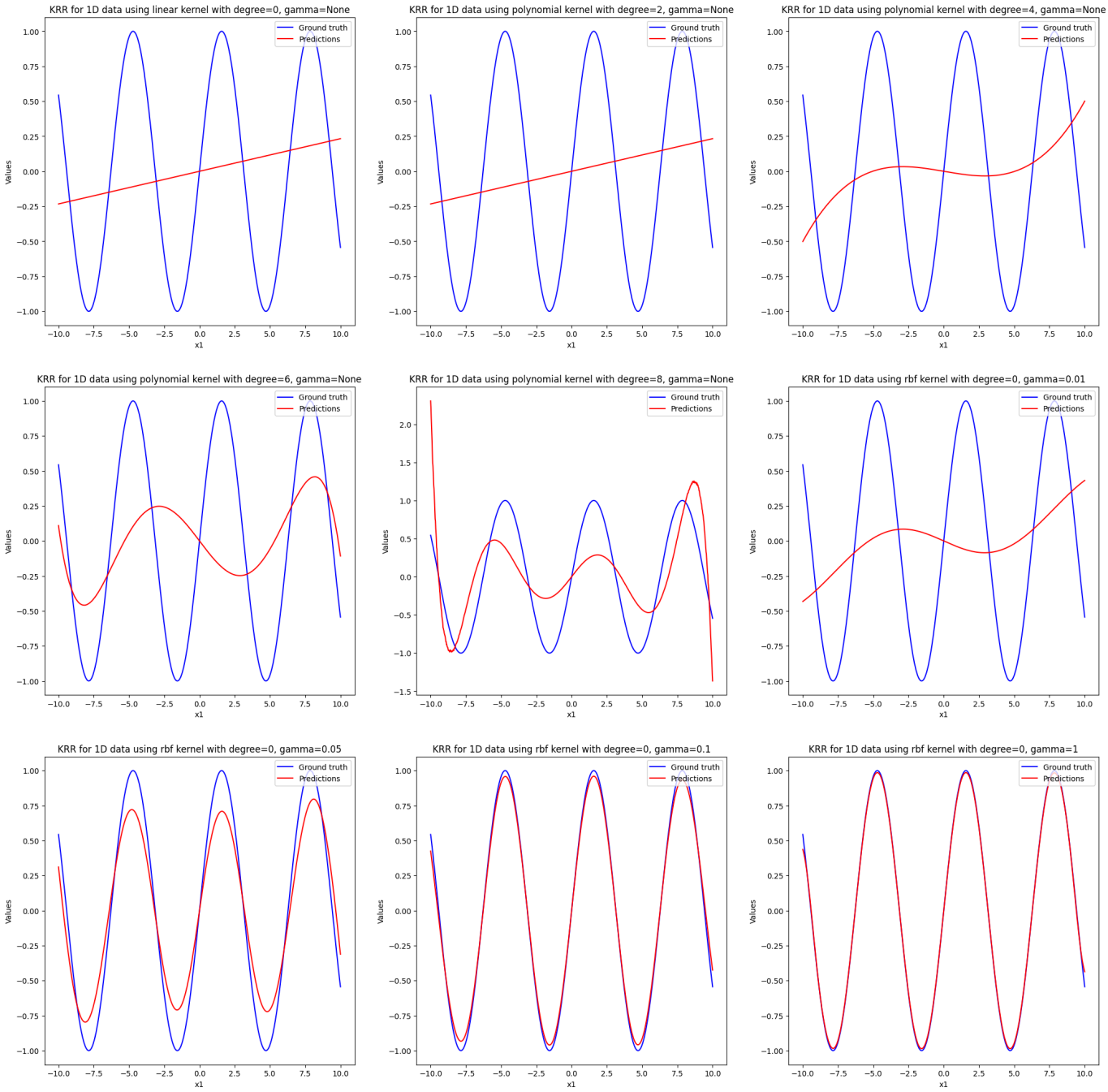
In [ ]:
```
import numpy as np
import sklearn.datasets as skdata
from sklearn.kernel_ridge import KernelRidge as KernelRidgeRegressionSciKit
import warnings
from matplotlib import pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

warnings.filterwarnings(action='ignore')
np.random.seed = 1
```

Kernel Ridge Regression Hyperparameters

In [ ]:
```
# Structured in form of [kernel_func, degree, gamma]
hyperparameters = [
    ['linear', 0, None],
    ['polynomial', 2, None],
    ['polynomial', 4, None],
    ['polynomial', 6, None],
    ['polynomial', 8, None],
    ['rbf', 0, 0.01],
    ['rbf', 0, 0.05],
    ['rbf', 0, 0.1],
    ['rbf', 0, 1],
]
```

Comparing linear, polynomial, and RBF kernels for 1D data

In [ ]:
```
# Create sine dataset
X = np.reshape(np.linspace(-10, 10, 1000), (-1, 1))
y = np.sin(X).ravel()

# TODO: Create figure with figsize=(25, 25)
fig = plt.figure(figsize=(25, 25))

# TODO: Enumerate through kernel ridge regression hyperparameters with index
for idx, (kernel_func, degree, gamma) in enumerate(hyperparameters):

    # TODO: Instantiate and fit Kernel Ridge Regression model from scikit
    # using different kernel functions and their parameters using alpha=1.0
    model = KernelRidgeRegressionSciKit(kernel=kernel_func, alpha=1.0, degree=degree,
    model.fit(X, y)

    # TODO: Predict target value from X
    y_hat = model.predict(X)

    # TODO: Instantiate axis for subplot of a 3 x 3 figure
    ax = fig.add_subplot(3, 3, idx + 1)

    # TODO: Plot the original data with x-axis being the X and y-axis being y with co
    ax.plot(X, y, color='blue', label='Ground truth')

    # TODO: Plot the Kernel Ridge Regression (KRR) predictions with x-axis being the
    ax.plot(X, y_hat, color='red', label='Predictions')

    # TODO: Set title to 'KRR for 1D data using {} kernel with degree={}, gamma={}'

    ax.set_title('KRR for 1D data using {} kernel with degree={}, gamma={}'.format(ke

    # TODO: Set xlabel to 'x1'
    ax.set_xlabel('x1')

    # TODO: Set ylabel to 'Values'
    ax.set_ylabel('Values')

    # TODO: Set legend with loc='upper right'

    ax.legend(loc='upper right')
plt.show()
```

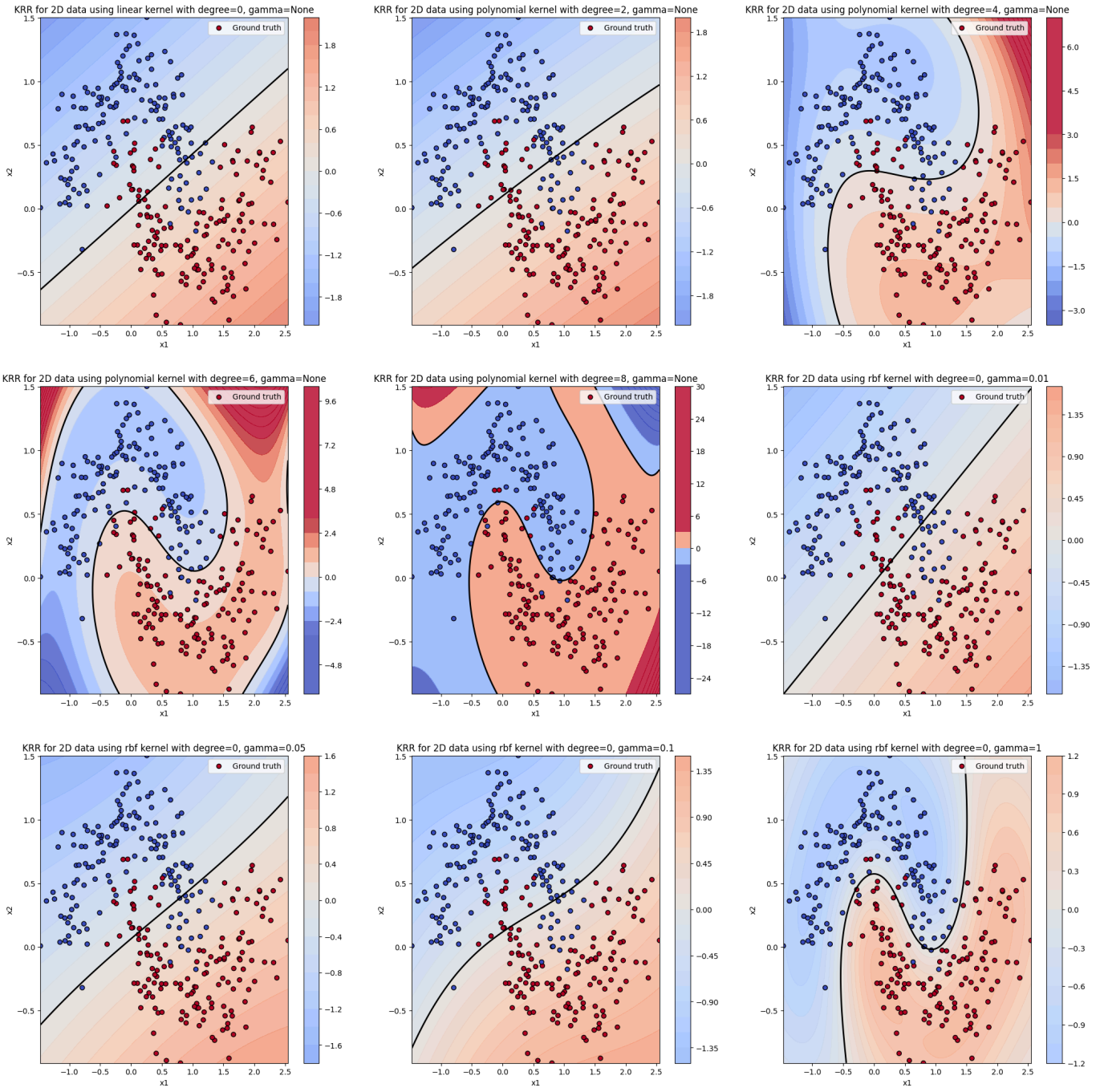


Comparing linear, polynomial, and RBF kernels for 2D data

In [ ]:

```
# Generate moons dataset for binary classification
X, y = skdata.make_moons(n_samples=300, noise=0.2, random_state=42)
y[y == 0] = -1

# TODO: Create figure with figsize=(25, 25)
fig = plt.figure(figsize=(25, 25))

# TODO: Enumerate through kernel ridge regression hyperparameters with index
for idx, (kernel_func, degree, gamma) in enumerate(hyperparameters):

    # TODO: Instantiate and fit Kernel Ridge Regression model from scikit
    # using different kernel functions and their parameters using alpha=1.0
    model = KernelRidgeRegressionSciKit(kernel=kernel_func, alpha=1.0, degree=degree,
    model.fit(X, y)

    # TODO: Get x1_min and x1_max (0-th dimension), and x2_min and x2_max (1-st dimen
    x1_min, x1_max = X[:, 0].min(), X[:, 0].max()
    x2_min, x2_max = X[:, 1].min(), X[:, 1].max()

    # TODO: Create 2 linspaces: one from x1_min to x1_max and the other from x1_min t
    x1_linspace = np.linspace(x1_min, x1_max, 500)
    x2_linspace = np.linspace(x2_min, x2_max, 500)
```

```
    # TODO: Create meshgrid for x1 and x2 using linspaces
    x1, x2 = np.meshgrid(x1_linspace, x2_linspace)

    # TODO: Predict values for every point in meshgrid
    all_Xs = np.stack([x1.ravel(), x2.ravel()], axis=-1)
    y_hat = model.predict(all_Xs)

    # TODO: Reshape y_hat to x1 or x2's shape
    y_hat = np.reshape(y_hat, x1.shape)

    # TODO: Instantiate axis for subplot of a 3 x 3 figure
    ax = fig.add_subplot(3, 3, idx + 1)

    # TODO: Plot Contour for predictions with levels=20, cmap='coolwarm', alpha=0.8,
    contour = ax.contourf(x1, x2, y_hat, levels=20, cmap='coolwarm', alpha=0.8, vmin=

    # TODO: Create colorbar for contour on axis and set its label to 'y_hat'
    cbar = fig.colorbar(contour, ax=ax)

    # TODO: Plot decision boundary using levels=[0], colors='black', linewidths=2
    decision_boundary = ax.contour(x1, x2, y_hat, levels=[0], colors='black', linewid

    # TODO: Create scatter plot for X and set its color to y with edgecolor='black',
    ax.scatter(X[:, 0], X[:, 1], c=y, edgecolor='black', cmap='coolwarm', label='Grou

    # TODO: Set title to 'KRR for 2D data using {} kernel with degree={}, gamma={}'
    ax.set_title('KRR for 2D data using {} kernel with degree={}, gamma={}'.format(ke

    # TODO: Set xlabel to 'x1'

    ax.set_xlabel('x1')

    # TODO: Set ylabel to 'x2'
    ax.set_ylabel('x2')

    # TODO: Set legend with loc='upper right'
    ax.legend(loc='upper right')


plt.show()
```

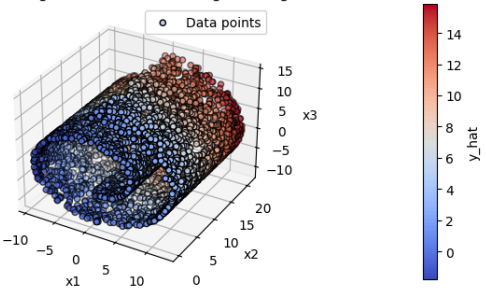


In [ ]:

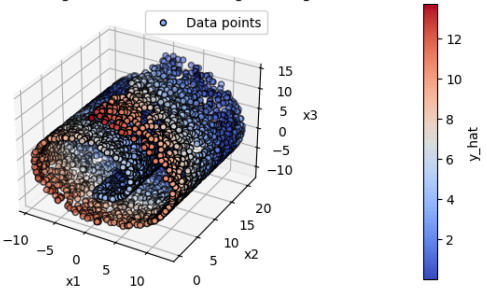
```
# Generate a 3-dimensional dataset
X, y = skdata.make_swiss_roll(n_samples=5000, noise=0.0, random_state=None, hole=Fals
# Optional you should try it on S curve as well
# X, y = skdata.make_s_curve(n_samples=5000, noise=0.0, random_state=None)

# TODO: Create figure with figsize=(40, 30)
fig = plt.figure(figsize=(40, 30))

# TODO: Enumerate through kernel ridge regression hyperparameters with index
for idx, (kernel_func, degree, gamma) in enumerate(hyperparameters):

    # TODO: Instantiate and fit Kernel Ridge Regression model from scikit
    # using different kernel functions and their parameters using alpha=1.0
    model = KernelRidgeRegressionSciKit(kernel=kernel_func, alpha=1.0, degree=degree,
    model.fit(X, y)

    # TODO: Predict for X
    y_hat = model.predict(X)

    # TODO: Instantiate axis for subplot of a 9 x 2 figure with projection='3d', acce
    ax1 = fig.add_subplot(9, 2, idx * 2 + 1, projection='3d')

    # TODO: Create scatter plot for X and set its color to y_hat with edgecolor='blac
    scatter1 = ax1.scatter(X[:, 0], X[:, 1], X[:, 2], c=y_hat, edgecolor='black', cma
```

```
    # TODO: Create colorbar for scatter plot on axis with ax=ax1 and set its label to
    cbar = fig.colorbar(scatter1, ax=ax1)
    cbar.set_label('y_hat')

    # TODO: Set title to 'KRR on 3D data using {} kernel with degree={}, gamma={}'
    ax1.set_title('KRR on 3D data using {} kernel with degree={}, gamma={}'.format(ke

    # TODO: Set xlabel to 'x1'
    ax1.set_xlabel('x1')

    # TODO: Set ylabel to 'x2'
    ax1.set_ylabel('x2')

    # TODO: Set zlabel to 'x3'
    ax1.set_zlabel('x3')

    # TODO: Set legend with loc='upper right'

    ax1.legend(loc='upper right')

    # TODO: Measure error for each prediction using absolute error
    y_error = np.abs(y_hat - y)

    # TODO: Instantiate axis for subplot of a 9 x 2 figure with projection='3d', acce
    ax2 = fig.add_subplot(9, 2, idx * 2 + 2, projection='3d')

    # TODO: Create scatter plot for X and set its color to y_error with edgecolor='bl
    scatter2 = ax2.scatter(X[:, 0], X[:, 1], X[:, 2], c=y_error, edgecolor='black', c

    # TODO: Create colorbar for scatter plot on axis with ax=ax2 and set its label to
    cbar = fig.colorbar(scatter2, ax=ax2)
    cbar.set_label('y_hat')

    # TODO: Set title to 'KRR Error on 3D data using {} kernel with degree={}, gamma=
    ax2.set_title('KRR Error on 3D data using {} kernel with degree={}, gamma={}'.for

    # TODO: Set xlabel to 'x1'
    ax2.set_xlabel('x1')

    # TODO: Set ylabel to 'x2'
    ax2.set_ylabel('x2')

    # TODO: Set zlabel to 'x3'
    ax2.set_zlabel('x3')

    # TODO: Set legend with loc='upper right'

    ax2.legend(loc='upper right')
fig.tight_layout(w_pad=-100.0)
plt.show()
```

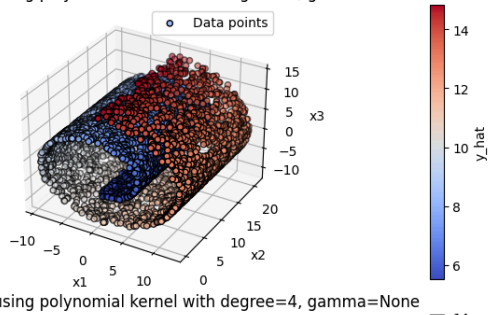
KRR on 3D data using linear kernel with degree=0, gamma=None



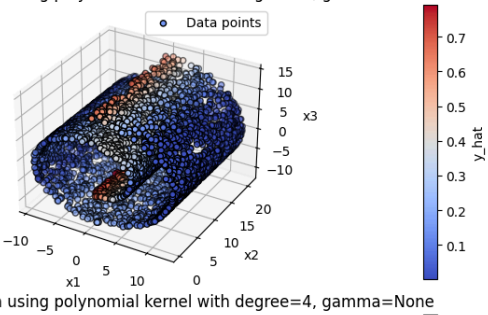
KRR Error on 3D data using linear kernel with degree=0, gamma=None



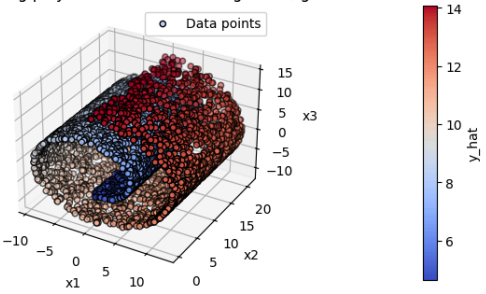
KRR on 3D data using polynomial kernel with degree=2, gamma=None



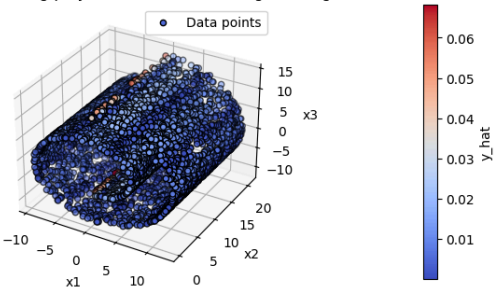
KRR Error on 3D data using polynomial kernel with degree=2, gamma=None



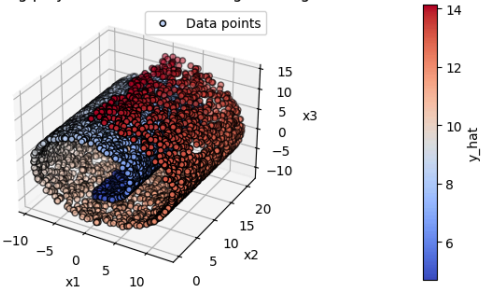
KRR on 3D data using polynomial kernel with degree=4, gamma=None



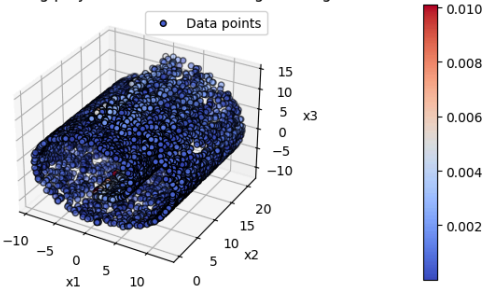
KRR Error on 3D data using polynomial kernel with degree=4, gamma=None



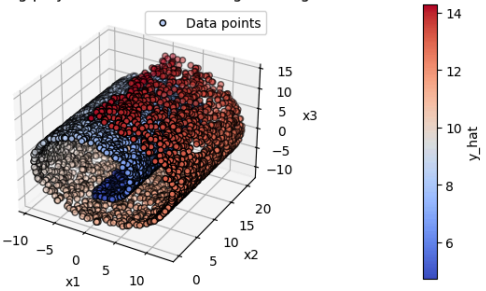
KRR on 3D data using polynomial kernel with degree=6, gamma=None



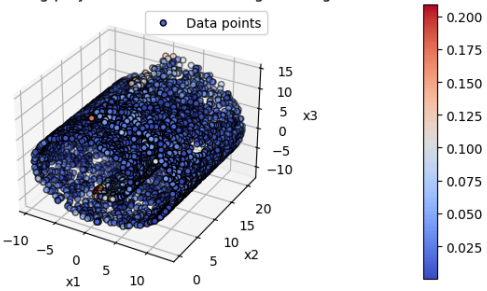
KRR Error on 3D data using polynomial kernel with degree=6, gamma=None



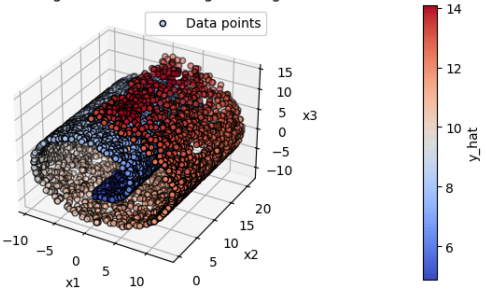
KRR on 3D data using polynomial kernel with degree=8, gamma=None



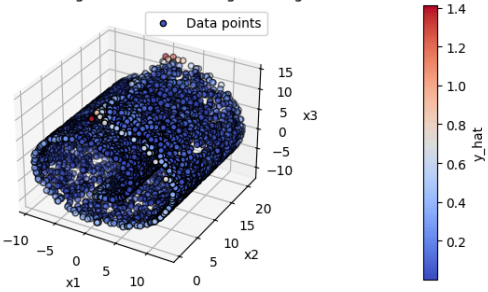
KRR Error on 3D data using polynomial kernel with degree=8, gamma=None



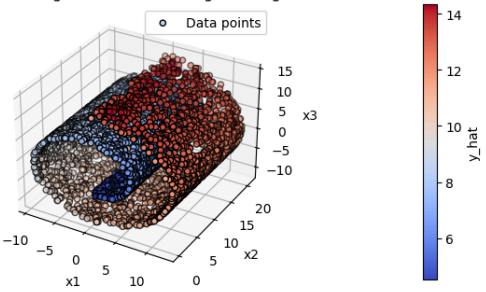
KRR on 3D data using rbf kernel with degree=0, gamma=0.01



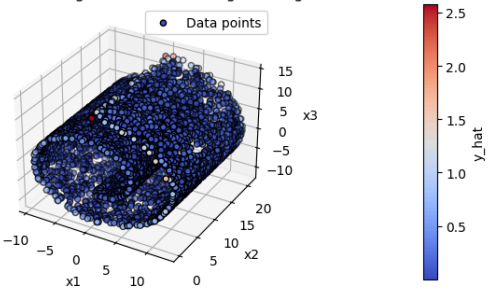
KRR Error on 3D data using rbf kernel with degree=0, gamma=0.01



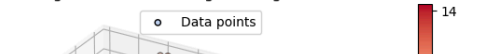
KRR on 3D data using rbf kernel with degree=0, gamma=0.05



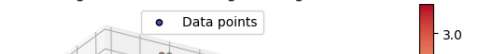
KRR Error on 3D data using rbf kernel with degree=0, gamma=0.05

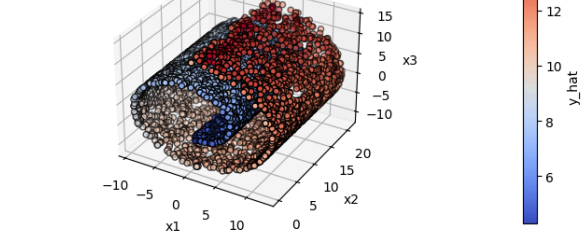


KRR on 3D data using rbf kernel with degree=0, gamma=0.1

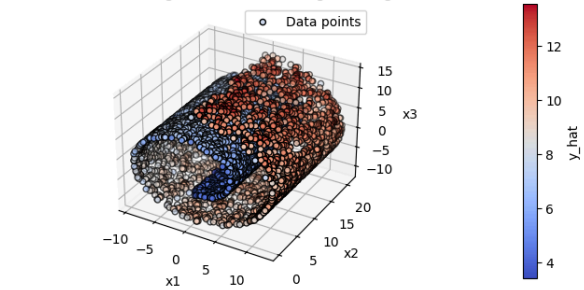


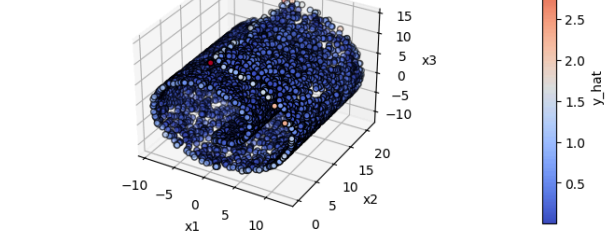
KRR Error on 3D data using rbf kernel with degree=0, gamma=0.1





KRR on 3D data using rbf kernel with degree=0, gamma=1





KRR Error on 3D data using rbf kernel with degree=0, gamma=1