Cognitive Algorithms - Assignment 4 (30 points)

Cognitive Algorithms
Summer term 2018
Technische Universität Berlin
Fachgebiet Maschinelles Lernen

Due on June 20, 2018 10am via ISIS

After completing all tasks, run the whole notebook so that the content of each cell is properly displayed. Make sure that the code was ran and the entire output (e.g. figures) is printed. Print the notebook as a PDF file and again make sure that all lines are readable - use line breaks in the Python Code '\' if necessary. Points will be deducted, if code or content is not readable!

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Part 1: Theory (8 points)

Let φ be a function, that maps the input data $x_1, \ldots, x_n \in \mathbb{R}^d$ to some finite or infinite dimensional $\mathbb{R}$-vector space (so-called *feature space*). The *representer theorem* states that if a function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a *valid kernel*, then it defines the scalar product of the input data in that feature space

$$k(x, x') \;=\; \langle \varphi(x), \varphi(x') \rangle \qquad \text{for all} \;\; x, x' \in \mathbb{R}^d$$

The function k is a *valid kernel*, iff it satisfies the *Mercer's condition*, which verifies that for any input data $x_1, \ldots, x_n \in \mathbb{R}^d$ and coefficients $c_1, \ldots, c_n \in \mathbb{R}$ the inequality

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) \geq 0$$

is satisfied.

A) (4 points) Show that the sum of two valid kernels k_1 and k_2 is again a valid kernel, i.e. that

$$k(x, x') := k_1(x, x') + k_2(x, x')$$

satisfies the Mercer's condition.

Solution

Since $k_1(x, x')$ and $k_2(x, x')$ are valid kernels, it holds true that $\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k_1(x_i, x_j) \geq 0$ and $\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k_2(x_i, x_j) \geq 0$.

Therefore, inserting $k(x, x') := k_1(x, x') + k_2(x, x')$ into $\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j)$ yields

$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) = \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k_1(x_i, x_j) + \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k_2(x_i, x_j)$.

Since both terms in the right hand side are ≥ 0, it is clear that $\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) \geq 0$, so $k(x, x')$ is a valid Kernel.

B) (4 point) Let $\varphi_1 : \mathbb{R}^d \to \mathbb{R}^{h_1}$ and $\varphi_2 : \mathbb{R}^d \to \mathbb{R}^{h_2}$ the feature mappings of k_1 and k_2. Give the feature mapping for the kernel k, i.e. a mapping φ such that

$$k(x, x') \;=\; k_1(x, x') + k_2(x, x') \;=\; \langle \varphi(x), \varphi(x') \rangle$$

and show that it fulfills the representer theorem.

Solution

The feature map φ can be defined as $\varphi : \mathbb{R}^d \to \mathbb{R}^{h_1 + h_2}$ by vertically stacking the feature maps φ_1 and φ_2 in a vector $(\varphi_1(x); \varphi_2(x))$ (the semicolon here indicates vertical concatenation).

Hence, expading the inner product $\langle \varphi(x), \varphi(x') \rangle$:

$$\langle \varphi(x), \varphi(x') \rangle = \langle \varphi_1(x), \varphi_1(x') \rangle + \langle \varphi_2(x), \varphi_2(x') \rangle$$

and therefore $k(x, x') \;=\; k_1(x, x') + k_2(x, x')$. Again, since k_1 and k_2 are valid kernels, the resulting kernel k is a valid kernel and can be expressed as a scalar product in the feature space, therefore fulfilling the representer theorem.

Part 2: Programming (22 points)

The application in this assignment is the same as in assignment 4. You will predict two dimensional hand positions $y \in \mathbb{R}^2$ from electromyographic (EMG) recordings $x \in \mathbb{R}^{192}$ obtained with high-density electrode arrays on the lower arm.
Labels are 2D positions of the hand during different hand movements.

Remember that even after 'linearizing' the EMG-hand position relationship by computing the log of the EMG features, the relationship is not exactly linear. Also we do not know the exact non-linearity; it might not be the same for all regions in EMG space and for all electrodes. So we can hope to gain something from using a non-parametric and non-linear method like kernel ridge regression.

The criterion to evaluate the model and select optimal parameters is the so called coefficient of determination, or r^2 index

$$r^2 = 1 - \frac{\sum_{d=1}^{D} \mathbb{V}(\hat{y}_d - y_d)}{\sum_{d=1}^{D} \mathbb{V}(y_d)}$$

where D is the dimensionality of the data labels, y are the true labels and $\hat{y}$ the estimated labels. This score is 1 for perfect predictions and smaller otherwise.

Use the data set `myo_data.mat` from the last assignment.

In [2]:
```
import pylab as pl
import scipy as sp
from numpy.linalg import inv
from numpy.linalg import solve
from scipy.io import loadmat
import numpy as np
from scipy.spatial.distance import cdist
%matplotlib inline
```

In [14]:
```
def load_data(fname):
    ''' Loads EMG data from <fname> '''
    # load the data
    data = loadmat(fname)
    # extract data for training
    X_train = data['training_data']
    X_train = sp.log(X_train)
    X_train = X_train[:, :1000]
    # extract hand positions
    Y_train = data['training_labels']
    Y_train = Y_train[:, :1000]
    return X_train,Y_train

def GaussianKernel(X1, X2, kwidth):
    ''' Compute Gaussian Kernel
    Input: X1    - DxN1 array of N1 data points with D features
           X2    - DxN2 array of N2 data points with D features
           kwidth - Kernel width
    Output K     - N1 x N2 Kernel matrix
    '''
    assert(X1.shape[0] == X2.shape[0])
    K = cdist(X1.T, X2.T, 'euclidean')
    K = np.exp(-(K ** 2) / (2. * kwidth ** 2))
    return K

def train_krr(X_train, Y_train,kwidth,llambda):
    ''' Trains kernel ridge regression (krr)
    Input:       X_train  -  DxN array of N data points with D features
                 Y        -  D2xN array of length N with D2 multiple labels
                 kwdith   -  kernel width
                 llambda    -  regularization parameter
    Output:      alphas   -  NxD2 array, weighting of training data used for a
pply_krr
    '''
    # your code here
    D,N = X_train.shape
    K = GaussianKernel(X_train,X_train,kwidth)
    return inv(K + llambda*np.eye(N)).dot(np.transpose(Y_train))

def apply_krr(alphas, X_train, X_test, kwidth):
    ''' Applys kernel ridge regression (krr)
    Input:      alphas      -  NtrxD2 array trained in train_krr
                X_train     -  DxNtr array of Ntr train data points with D fea
tures
                X_test      -  DxNte array of Nte test data points with D feat
ures
                kwidht      -  Kernel width
    Output:     Y_test      -  D2xNte array
    '''
    # your code here
    K = GaussianKernel(X_test,X_train,kwidth)
    return np.transpose(K.dot(alphas))

def train_ols(X_train, Y_train):
    ''' Trains ordinary least squares (ols) regression
    Input:       X_train  -  DxN array of N data points with D features
```

```
                Y        -  D2xN array of length N with D2 multiple labels
    Output:     W        -  DxD2 array, linear mapping used to estimate label
s
                            with sp.dot(W.T, X)
    '''
    #W = sp.dot(inv(sp.dot(X_train,X_train.T)),sp.dot(X_train,Y_train.T))
    W = solve(sp.dot(X_train,X_train.T),sp.dot(X_train,Y_train.T))
    return W

def apply_ols(W, X_test):
    ''' Applys ordinary least squares (ols) regression
    Input:      X_test    -  DxN array of N data points with D features
                W        -  DxD2 array, linear mapping used to estimate label
s
                            trained with train_ols
    Output:     Y_test    -  D2xN array
    '''
    Y_test = sp.dot(W.T, X_test)
    return Y_test

def test_handpositions():
    X,Y = load_data('myo_data.mat')
    print (crossvalidate_krr(X,Y))

def test_sine_toydata(kwidth = 1, llambda = 1):
    #Data generation
    X_train = sp.arange(0,10,.01)
    X_train = X_train[None,:]
    Y_train = sp.sin(X_train) + sp.random.normal(0,.5,X_train.shape)
    #Linear Regression
    w_est = train_ols(X_train, Y_train)
    Y_est_lin = apply_ols(w_est,X_train)
    #Kernel Ridge Regression
    alphas = train_krr(X_train,Y_train,kwidth,llambda)
    Y_est_krr = apply_krr(alphas,X_train,X_train,kwidth)

    #Plot result
    pl.figure()
    pl.plot(X_train.T, Y_train.T, '+k', label = 'Train Data')
    pl.plot(X_train.T, Y_est_lin.T, '-.', linewidth = 2, label = 'OLS')
    pl.plot(X_train.T, Y_est_krr.T,  'r', linewidth = 2, label = 'KRR')
    pl.xlabel('x')
    pl.ylabel('y')
    pl.title(r'$\lambda$ = ' + str(llambda) + '   $\sigma$ = ' + str(kwidth))
    pl.legend(loc = 'lower right')


def crossvalidate_krr(X,Y,f=5, kwidths=10.0**np.array([0, 1, 2]), llambdas=10.
0**np.array([-4, -2, 0])):
    '''
    Test generalization performance of kernel ridge regression with gaussian k
ernel
    Input:      X   data (dims-by-samples)
                Y   labels (dims2-by-samples)
                f   number of cross-validation folds
                kwidths width of gaussian kernel function
                llambdas regularizer (height of ridge on kernel matrix)
```

```
    '''
    #N = f*(X.shape[-1]/f)
    #idx = sp.reshape(sp.random.permutation(sp.arange(N)),(f,N/f))
    N = f*(X.shape[-1]//f)
    idx = sp.reshape(sp.arange(N),(f,N//f))
    r2_outer = sp.zeros((f))
    r2_linear = sp.zeros((f))
    r2_inner = sp.zeros((f-1,kwidths.shape[-1],llambdas.shape[-1]))

    # to outer cross-validation (model evaluation)
    for ofold in range(f):
        # split in training and test (outer fold)
        otestidx = sp.zeros((f),dtype=bool)
        otestidx[ofold] = 1
        otest = idx[otestidx,:].flatten()
        otrain = idx[~otestidx,:]

        # inner cross-validation (model selection)
        for ifold in range(f-1):
            # split in training and test (inner fold)
            itestidx = sp.zeros((f-1),dtype=bool)
            itestidx[ifold] = 1
            itest = otrain[itestidx,:].flatten()
            itrain = otrain[~itestidx,:].flatten()

            # do inner cross-validation (model selection)
            for illambda in range(llambdas.shape[-1]):
                for ikwidth in range(kwidths.shape[-1]):
                    #compute kernel for all data points
                    alphas = train_krr(X[:,itrain],Y[:,itrain],kwidths[ikwidth
],llambdas[illambda])
                    yhat = apply_krr(alphas, X[:,itrain], X[:,itest],kwidths[i
kwidth])
                    r2_inner[ifold,ikwidth,illambda] = compute_rsquare(yhat,Y
[:,itest])

        #train again using optimal parameters
        r2_across_folds = r2_inner.mean(axis=0)
        optkwidthidx, optllambdaidx = np.unravel_index(r2_across_folds.flatten
().argmax(),r2_across_folds.shape)
        #evaluate model on outer test fold
        alphas = train_krr(X[:,otrain.flatten()],Y[:,otrain.flatten()], kwidth
s[optkwidthidx],llambdas[optllambdaidx])
        yhat = apply_krr(alphas, X[:,otrain.flatten()],X[:,otest], kwidths[opt
kwidthidx])
        r2_outer[ofold] = compute_rsquare(yhat,Y[:,otest])

        # for comparison: predict with linear model
        w_est = train_ols(X[:,otrain.flatten()], Y[:,otrain.flatten()])
        y_est_lin = apply_ols(w_est,X[:,otest])
        r2_linear[ofold] = compute_rsquare(y_est_lin,Y[:,otest])

        print('Fold %d'%ofold + ' best kernel width %f'%kwidths[optkwidthidx]
 +\
        ' best regularizer %f'%llambdas[optllambdaidx] + \
        ' rsquare %f'%r2_outer[ofold] + \
        ' rsquare linear %f'%r2_linear[ofold])
```

```
    pl.figure()
    pl.boxplot(sp.vstack((r2_outer,r2_linear)).T)
    pl.ylabel('$r^2$')
    pl.xticks((1,2),('KRR','Lin'))
    #pl.savefig('krr_vs_lin_comparison.pdf')
    return r2_outer,r2_linear

def compute_rsquare(yhat,Y):
    '''compute coefficient of determination'''
    return 1 - (sp.var((yhat - Y),axis=1).sum()/sp.var(Y,axis=1).sum())
```

A) (6 points) Implement Kernel Ridge Regression (KRR) by completing the function stubs `krr_train` and `krr_apply`. We use the notation from assignment 4,

$$X_{\text{train}} \in \mathbb{R}^{D_X \times N_{tr}},\ Y_{\text{train}} \in \mathbb{R}^{D_Y \times N_{tr}},\ X_{\text{test}} \in \mathbb{R}^{D_X \times N_{te}}$$

In `krr_train`, you estimate a linear combination of the input vectors α,

$$\alpha = (K + \lambda I)^{-1} Y_{\text{train}}^T$$

where λ is the regularization parameter and K is the $N_{tr} \times N_{tr}$ Gaussian Kernel matrix with Kernel width σ, $K_{ij} = \exp\left(-\frac{\|X^i_{\text{train}} - X^j_{\text{train}}\|^2}{\sigma^2}\right)$. You can compute K with the provided function `GaussianKernel`.

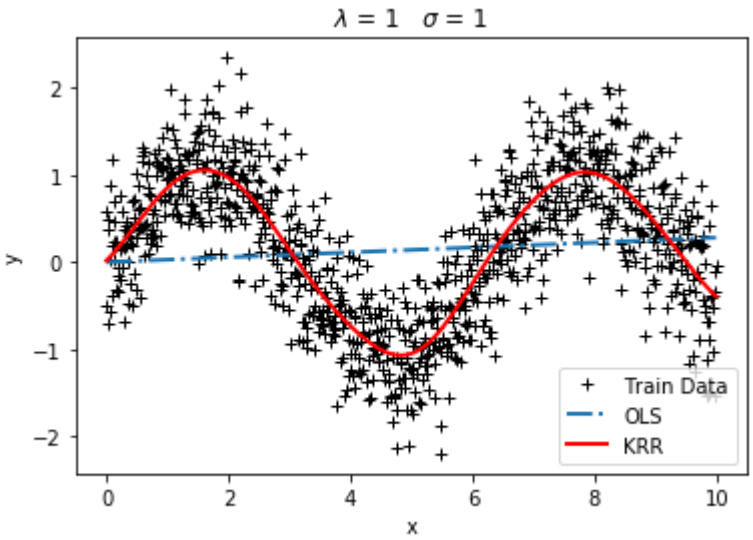
The function `krr_apply` than uses the weights α to predict the (unknown) hand positions of new test data X_{test}

$$Y_{\text{test}} = (\mathbf{k}\alpha)^T.$$

where $\mathbf{k}$ is the $N_{\text{test}} \times N_{\text{train}}$ matrix $\mathbf{k}_{ij} = \exp\left(-\frac{\|X^i_{\text{test}} - X^j_{\text{train}}\|^2}{\sigma^2}\right)$.

The function `test_sine_toydata` helps you to debug your code. It generates toy data that follows a sine function, $x_i \in \{0, 0.01, 0.02, \ldots, 10\}, y_i = \sin(x_i) + \epsilon, \epsilon \sim \mathcal{N}(0, 0.5)$. The result of KRR should resemble the sine function.

In [9]:
```
test_sine_toydata()
```



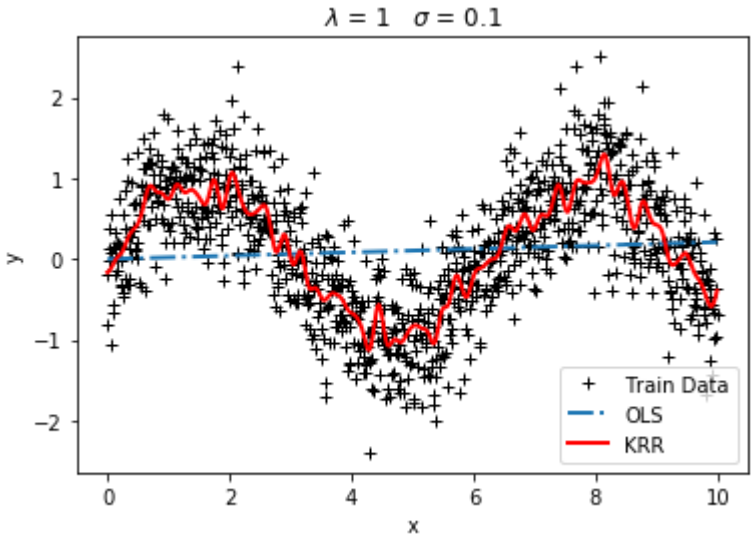
B) (5 points) We want to analyse how the Kernel Ridge solution depends on its hyperparameters, the kernel width σ and the regularization parameter λ.

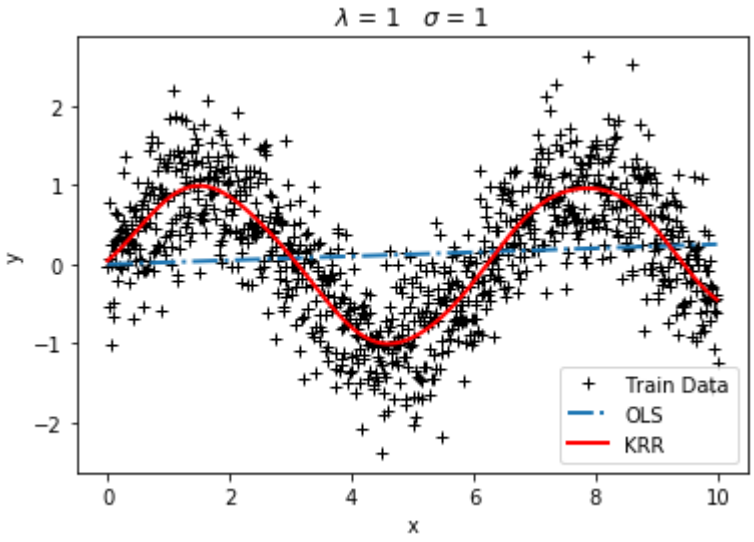
- Call the function `test_sine_toydata` with λ = 1 for three different Kernel widths, $\sigma = \{0.1, 1, 10\}$. How does the Kernel width affect the solution? Explain the observed behaviour.
- Call the function `test_sine_toydata` with σ = 1 for three different regularization parameters, $\lambda = \{10^{-10}, 1, 500\}$. How does the regularization parameter affect the solution? Explain the observed behaviour.

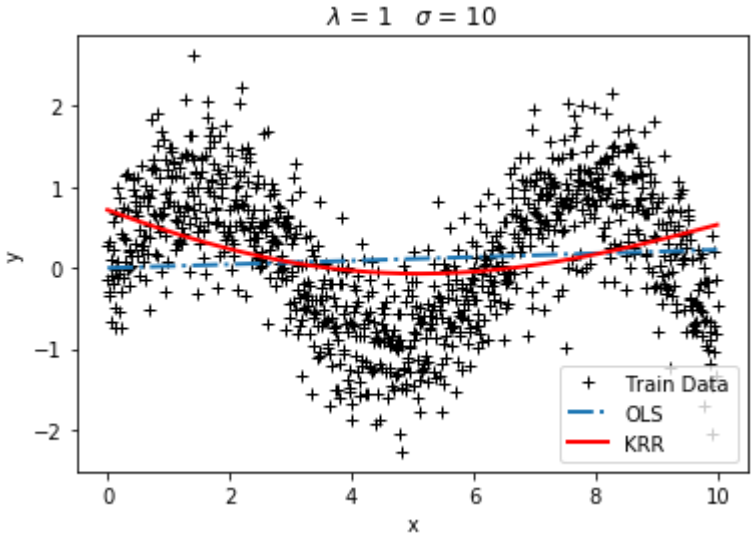
Solution

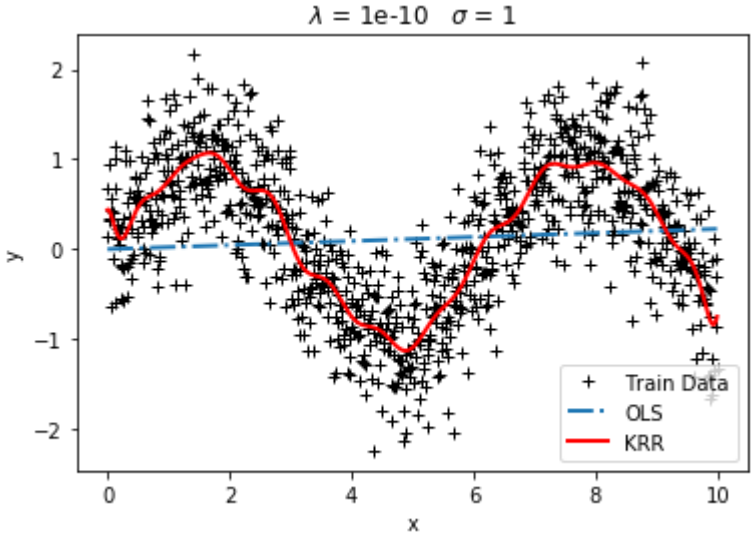
- The Kernel width can be interpreted as a window containing training points considered when making a prediction. With a small σ the number of training examples considered around the test point is small, so the prediction is likely to pose a local behavior, being possible to end up with overfitting. When σ is increased, more training points are used for the prediction and therefore a smoother behaviour is expected. If σ is too large, too many points will be considered for the prediction and the result is likely to lack complexity. This is the behavior observed in the following figures.
- The regularization parameter λ determines the complexity of the solution by enforcing the model parameters to take relatively small values. For small λ, the regularization is negligible and we can run into overfitting if the model allows it. For moderate λ, the model parameters are significantly affected by the regularization and the solution smoothly reproduces the behavior of the data. For high values of λ the model parameters are forced to take relatively small values, and this might cause lack of complexity for our model. This behavior can be found in the following figures.

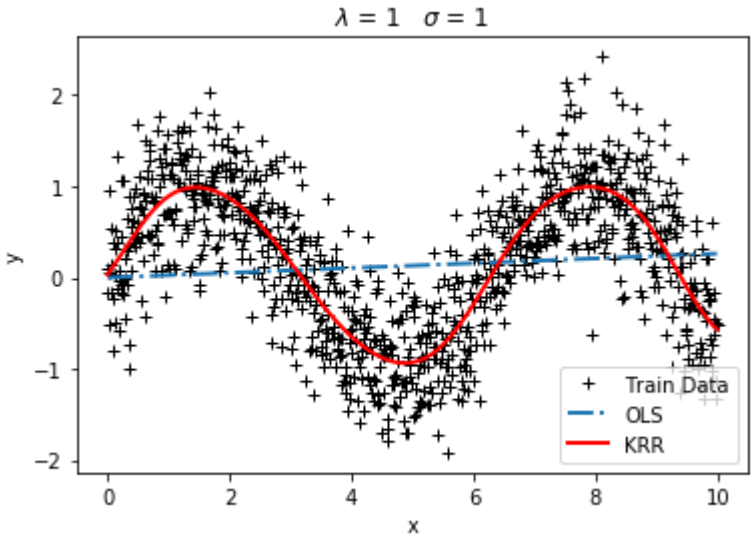
In [5]:
```
test_sine_toydata(kwidth = 0.1, llambda = 1)
test_sine_toydata(kwidth = 1, llambda = 1)
test_sine_toydata(kwidth = 10, llambda = 1)
test_sine_toydata(kwidth = 1, llambda = 1e-10)
test_sine_toydata(kwidth = 1, llambda = 1)
test_sine_toydata(kwidth = 1, llambda = 500)
```

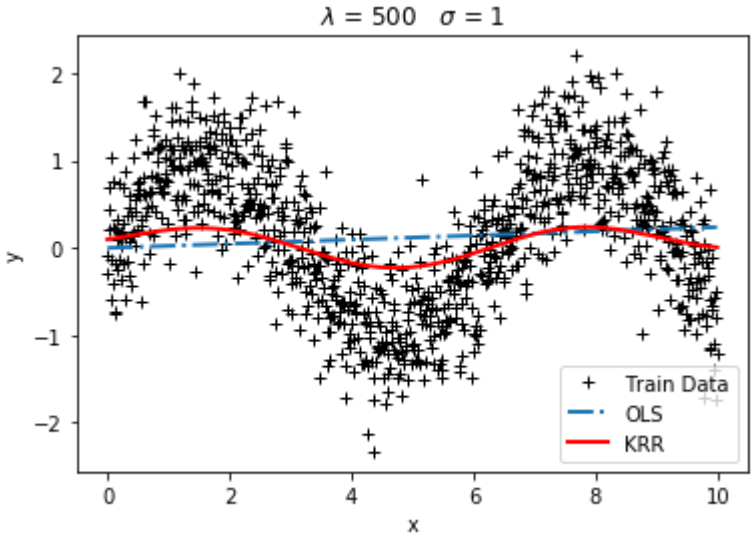

$\lambda = 1 \quad \sigma = 0.1$
Train Data
OLS
KRR
x
y


$\lambda = 1 \quad \sigma = 1$
Train Data
OLS
KRR
x
y


$\lambda = 1 \quad \sigma = 10$
Train Data
OLS
KRR
x
y







C) (4 points) Briefly explain in your own words how nested-crossvalidation is done. To do so, you can examine the function `crossvalidate_krr`.Explain briefly how λ and σ are chosen within the function.

Solution

NCV first splits the dataset D in subsets D_i. On each of these subsets, normal CV is performed (assuming a single nesting). This means each subest D_i is split into smaller subsets D_{ij}. Then, iterating over j, a model is trained with data from D_{ij} for each possible combination of paramters and then evaluated on the set D_i/D_{ij}. The evaluation score is then averaged over all j which yields an average score for each parameter configuration. From this, the best configuration is chosen and a model is trained on D_i using this configuration and validated on D/D_i. The outer loop does not do any parameter selection and only acts as a validator for the selection method. If the model paramters are not stable over iterations i this can indicate a bad model fitting procedure in the inner loop or insufficient training data.

D) (6 points) Predict two dimensional hand positions with Kernel Ridge Regression by calling the function `test_handpositions`. It shows a boxplot for the linear regression and the Kernel Ridge Regression. What does a boxplot show? (check the help function in python or the wikipedia article). Do we gain something from Kernel Ridge Regression as compared to simple linear regression?

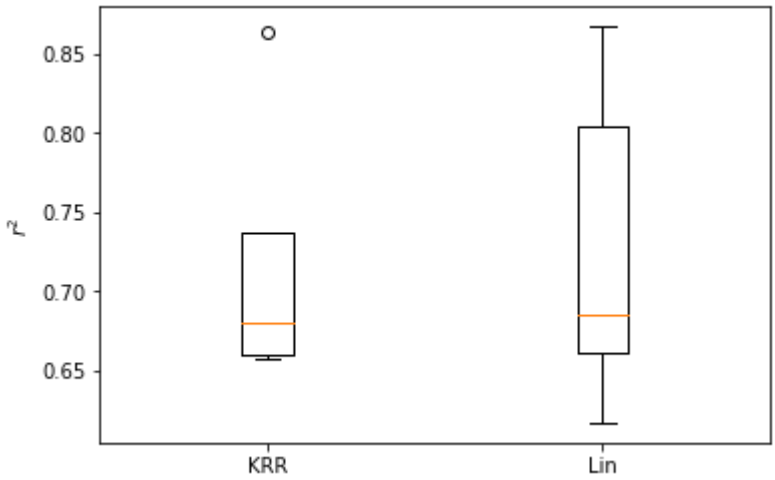
Solution

Per definition in their decomentation, the boxplot from [matpplotlib] works as follows: The box extends from the lower (Q1) to the upper (Q3) quartile. The whiskers (by default) extend to Q1 - 1.5 *IQR and Q3 + 1.5* IQR respectively (IQR = Q3 - Q1). Any other datapoints are plotted seperatly (here as little circles) and can be considered outliers. The mean is plotted inside the box as an orange line.

In our case (limited data, low number of iterations) the boxplot shows a smaller variance for the KRR with the same mean. This may indicate a more stable model, even though it shows a nasty outlier. Increasing the number of loaded data points to 2000 however, has KRR perform very stable across all iterations without any noticable fluctuation in the parameter configuration, while consistently outperforming the linear regression. This suggests that the plot we see is not indicative of the KRR procedure in general. In any case we have a lower variance in performance compared to the linear regression but considering there are only 5 iterations, the Quartiles are not large enough themselves to support a definite proposition.

In [15]:
```
print (test_handpositions())
```

```
Fold 0 best kernel width 100.000000 best regularizer 0.000100 rsquare 0.73689
8 rsquare linear 0.661384
Fold 1 best kernel width 100.000000 best regularizer 0.010000 rsquare 0.65664
9 rsquare linear 0.685375
Fold 2 best kernel width 100.000000 best regularizer 0.000100 rsquare 0.65951
0 rsquare linear 0.616657
Fold 3 best kernel width 10.000000 best regularizer 1.000000 rsquare 0.680160
rsquare linear 0.804902
Fold 4 best kernel width 100.000000 best regularizer 0.000100 rsquare 0.86377
8 rsquare linear 0.867395
(array([0.73689792, 0.65664944, 0.6595102 , 0.68015994, 0.86377778]), array
([0.66138387, 0.68537513, 0.6166573 , 0.8049023 , 0.86739507]))
None
```



E) (1 point) In the last task, we have applied the function `test_handpositions` only to the first 1000 data points out of the 10255 available data points. Why did we do so in this exercice?

Solution

Training with a significantly higher number of data points increases computation time quadratically as K is an $N \times N$ matrix. This can lead to infeasible computation costs.