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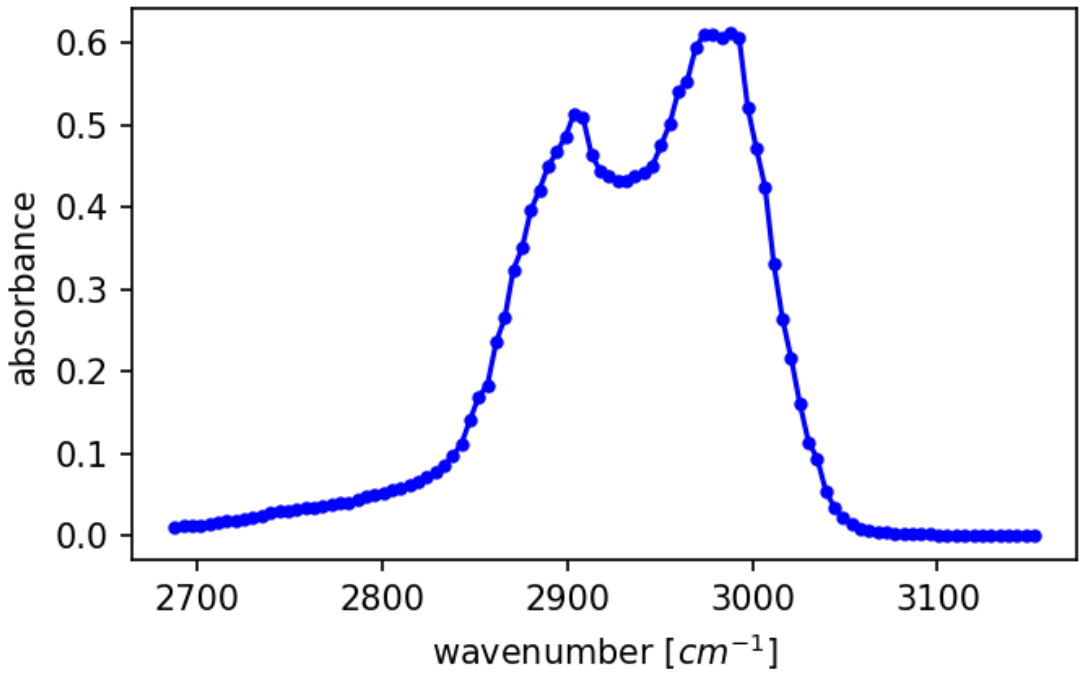
Regression - Assignment 2

Data and Package Import

In [1]:
```
%matplotlib inline
import numpy as np
import pandas as pd
import pylab as plt
```

In [2]:
```
df = pd.read_csv('data/ethanol_IR.csv')
x_all = df['wavenumber [cm^-1]'].values
y_all = df['absorbance'].values

x_peak = x_all[475:575]
y_peak = y_all[475:575]

fig, ax = plt.subplots(figsize = (5, 3), dpi = 150)
ax.plot(x_peak, y_peak, '-b', marker = '.')
ax.set_xlabel('wavenumber [$cm^{-1}$]')
ax.set_ylabel('absorbance');
```



Mean Absolute Errors

Write a function that computes the mean absolute error (MAE).

In [3]:
```
def MAE(actual, prediction):
    mae = abs(actual - prediction).mean()
```

```
    return mae
```

Use 8-fold cross-validation to compute the average and standard deviation of the MAE on the spectra dataset.

Use a `LinearRegression` model and an `rbf` kernel with σ=100.

Make sure to pass `shuffle = True` argument when you make a `KFold` object.

In [4]:
```
def rbf(x_train, x_test = None, gamma = 1):
    if x_test is None:
        x_test = x_train
    N = len(x_test)
    M = len(x_train)
    X = np.zeros((N, M))
    for i in range(N):
        for j in range(M):
            X[i, j] = np.exp(-gamma * (x_test[i] - x_train[j])**2)

    return X
```

In [5]:
```
from sklearn.model_selection import KFold
from sklearn.linear_model import LinearRegression

kfold = KFold(n_splits = 8, shuffle = True)
sigma = 100
gamma = 1. / 2 / sigma**2

listMAE = []

for train_index, test_index in kfold.split(x_peak):
    x_train, x_test = x_peak[train_index], x_peak[test_index]
    y_train, y_test = y_peak[train_index], y_peak[test_index]

    X_train = rbf(x_train, gamma = gamma)

    model = LinearRegression()
    model.fit(X_train, y_train)

    X_test = rbf(x_train, x_test, gamma = gamma)

    yhat = model.predict(X_test)

    mae = MAE(y_test, yhat)
    listMAE.append(mae)

listMAE = np.array(listMAE)
mean = listMAE.mean()
std = listMAE.std()

print('Mean of MAE: {}'.format(mean))
print('Standard deviation of MAE: {}'.format(std))
```

```
Mean of MAE: 0.007426851366487635
Standard deviation of MAE: 0.00506196808615005
```

Determine the optimum σ that results in the lowest mean of MAE based on 8-fold cross validation.

Vary the width of an `rbf` kernel with σ = [1, 10, 50, 100, 150].

In [6]:
```
sigmas = np.array([1, 10, 50, 100, 150])
gammas = 1. / 2 / sigmas**2

findOptimum = []
for gamma in gammas:
    listMAE = []
    for train_index, test_index in kfold.split(x_peak):
```

```
        x_train, x_test = x_peak[train_index], x_peak[test_index]
        y_train, y_test = y_peak[train_index], y_peak[test_index]

        X_train = rbf(x_train, gamma = gamma)

        model = LinearRegression()
        model.fit(X_train, y_train)

        X_test = rbf(x_train, x_test, gamma = gamma)

        yhat = model.predict(X_test)

        mae = MAE(y_test, yhat)
        listMAE.append(mae)

    listMAE = np.array(listMAE)
    mean = listMAE.mean()
    findOptimum.append(mean)

minIndex = findOptimum.index(min(findOptimum))
optGamma = gammas[minIndex]
optSigma = sigmas[minIndex]

print(findOptimum)

print('Optimal gamma: {}'.format(optGamma))
print('Optimal sigma: {}'.format(optSigma))
```

```
[0.20038408530712962, 0.5784814793872782, 0.015588800599666802, 0.008753082948173892, 0.016254
492921130473]
Optimal gamma: 5e-05
Optimal sigma: 100
```

Hyperparameter Tuning

Reshape x_peak and y_peak into 2D arrayx.

In [7]:
```
x_peak = x_peak.reshape(-1, 1)
y_peak = y_peak.reshape(-1, 1)
```

Do a train/test split with test_size=0.3 for the spectra data.

In [8]:
```
from sklearn.model_selection import train_test_split

x_train, x_test, y_train, y_test = train_test_split(x_peak, y_peak, test_size = 0.3)
```

Use a for loop to determine the optimum regularization strength α of a KRR model.

Use an rbf kernel with σ=20.

Determine the optimum value of α out of [1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1].

In [9]:
```
from sklearn.kernel_ridge import KernelRidge

alphas = np.array([1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1])

sigma = 20
gamma = 1. / 2 / sigma**2

listR2 = []
for alpha in alphas:
    KRR = KernelRidge(alpha = alpha, kernel = 'rbf', gamma = gamma)
    KRR.fit(x_train, y_train)

    yhat = KRR.predict(x_test)
```

```
    r2 = KRR.score(x_test, y_test)
    listR2.append(r2)

maxIndex = listR2.index(max(listR2))
optAlpha = alphas[maxIndex]

print(listR2)
print('Optimal alpha: {}'.format(optAlpha))
```

```
[0.9984200372983285, 0.9984430064066064, 0.9983755583531992, 0.998370537316032, 0.9981447116555
068, 0.9699372172069529]
Optimal alpha: 0.0001
```

3. GridSearchCV

Import a LASSO model.

In [10]:
```
from sklearn.linear_model import Lasso
```

Shuffle the `x_peak` and `y_peak`.

You can get a shuffled array when you run `x_shuffle, y_shuffle = shuffle(x, y)`.

The reason why we shuffle the data is that `GridSearchCV` does not have an option to shuffle the input data. Note that we automatically shuffled the data using the `shuffle=True` argument in the `Kfold` function.

In [11]:
```
from sklearn.utils import shuffle

x_peak_shuffle, y_peak_shuffle = shuffle(x_peak, y_peak)
```

Build a `GridSearchCV` model that optimizes the hyperparameters of a LASSO model for the spectra data.

Search over $\alpha \in$ [1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1] and $\sigma \in$ [5, 10, 15, 20, 25, 30, 35, 40].

Use 3-fold cross-validation.

Hint: You will need to use a `for` loop over σ values. Unlike KRR, LASSO models do not take `gamma` or `sigma` as a parameter. Therefore, you have to make an `rbf` kernel manually and input it to a LASSO model.

Obtain the optimum α and the best score for each σ value. Use `GridSearchCV.best_score_` as an accuracy metric.

In [12]:
```
#Let's ignore the warnings
import warnings
warnings.simplefilter('ignore')
```

In [13]:
```
# not valid but acceptable answer
from sklearn.model_selection import GridSearchCV

alphas = np.array([1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1])
sigmas = np.array([5, 10, 15, 20, 25, 30, 35, 40])

listEstimator = []
listScore = []
for sigma in sigmas:
    gamma = 1. / 2 / sigma**2

    x_train, x_test, y_train, y_test = train_test_split(x_peak_shuffle, y_peak_shuffle, test_size = 0.3)

    X_train = rbf(x_train, gamma = gamma)
    X_test = rbf(x_train, x_test, gamma = gamma)
```

```
    lasso = Lasso()
    param_grid = {'alpha': alphas}
    lasso_search = GridSearchCV(lasso, param_grid, cv = 3)
    lasso_search.fit(X_train, y_train)

    listEstimator.append(lasso_search.best_estimator_)

    score = lasso_search.best_estimator_.score(X_test, y_test)
    listScore.append(score)

maxIndex = listScore.index(max(listScore))
optAlpha = listEstimator[maxIndex].alpha
optSigma = sigmas[maxIndex]

print('Optimal alpha: {}'.format(optAlpha))
print('Optimal sigma: {}'.format(optSigma))
```

```
Optimal alpha: 0.0001
Optimal sigma: 30
```

In [14]:
```
# Using 2 for loops
alphas = np.array([1e-5, 1e-4, 1e-3, 1e-2, 1e-1, 1])
sigmas = np.array([5, 10, 15, 20, 25, 30, 35, 40])

x_train, x_test, y_train, y_test = train_test_split(x_peak, y_peak, test_size = .3)

findAlpha =[]
for alpha in alphas:
    findSigma = []
    for sigma in sigmas:
        gamma = 1. / 2 / sigma**2

        X_train = rbf(x_train, gamma = gamma)
        X_test = rbf(x_train, x_test, gamma = gamma)

        lasso = Lasso(alpha = alpha)

        lasso.fit(X_train, y_train)
        r2 = lasso.score(X_test, y_test)

        findSigma.append(r2)
    optSigmaIndex = findSigma.index(max(findSigma))
    suboptSigma = sigmas[optSigmaIndex]
    submaxR2 = max(findSigma)

    findAlpha.append((submaxR2, suboptSigma))

optAlphaIndex = findAlpha.index(max(findAlpha))
optAlpha = alphas[optAlphaIndex]
optSigma = findAlpha[optAlphaIndex][1]
maxR2 = findAlpha[optAlphaIndex][0]

print(findAlpha)
```

```
[(0.9984186501247988, 15), (0.9984826818030107, 30), (0.9968090612710975, 30), (0.9296158632378431, 30), (-0.011856591089540292, 5), (-0.011856591089540292, 5)]
```

In [15]:
```
# Working on using pipeline...
```

What is the optimum σ and α?

In [16]:
```
print('Optimal alpha: {}'.format(optAlpha))
print('Optimal sigma: {}'.format(optSigma))
```

```
Optimal alpha: 0.0001
Optimal sigma: 30
```

Optional Task

Check what happens if the input data is not shuffled before the `GridSearchCV`.

In [ ]:

Ensemble Kernel Ridge Regression

In this problem you will combine ideas from k-fold cross-validation and bootstrapping with KRR to create an **ensemble** of KRR models.

Reshape `x_peak` and `y_peak` into 2D array.

In [17]:
```
x_peak = x_peak.reshape(-1, 1)
y_peak = y_peak.reshape(-1, 1)
```

Use 5-fold cross-validation with the spectra data to construct a series of 5 KRR models with a `rbf` kernel with γ=0.0005 and α=0.01.

Each model will be trained with 80% of the data, but the exact training points will vary each time so the models will also vary.

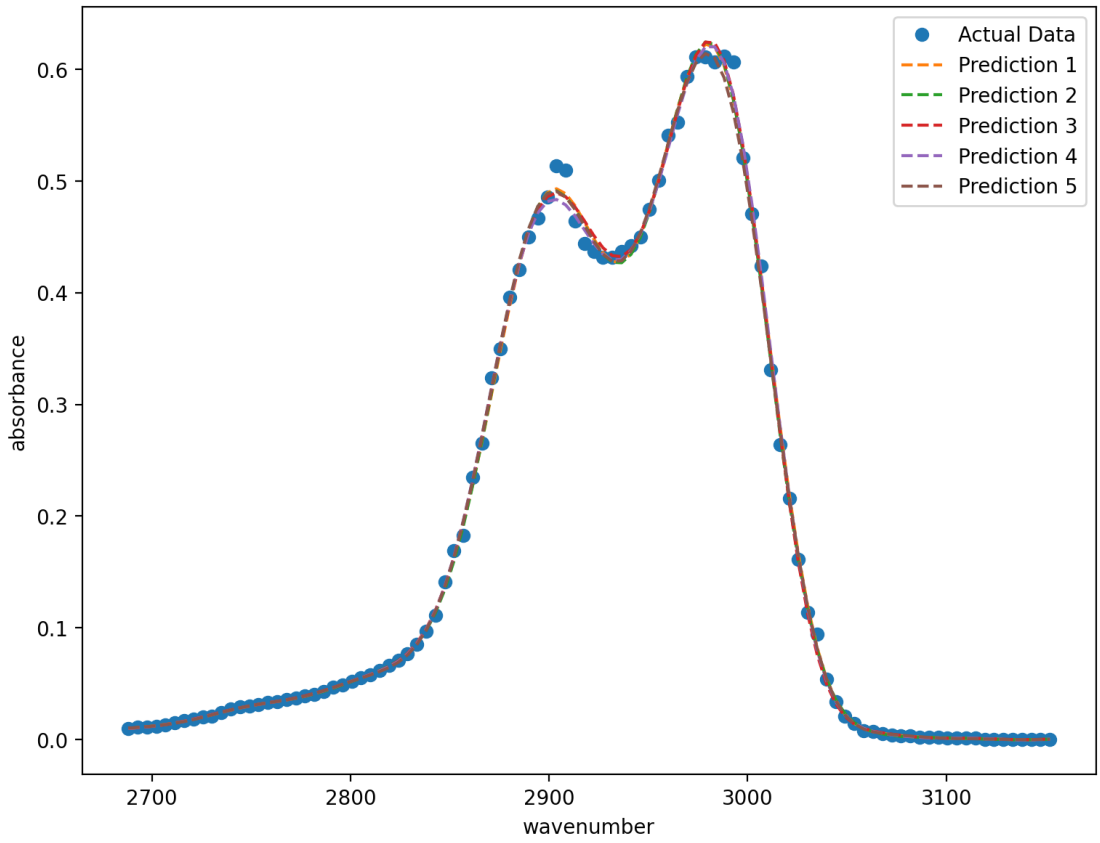
You can use all of the data points in the `x_peak` for generating the predictions (in other words, predict on both the training and testing data).

In [18]:
```
kfold = KFold(n_splits = 5, shuffle = True)

yhatList = []

for train_index, test_index in kfold.split(x_peak):
    x_train, x_test = x_peak[train_index], x_peak[test_index]
    y_train, y_test = y_peak[train_index], y_peak[test_index]

    KRR = KernelRidge(gamma = 0.0005, kernel = 'rbf', alpha = 0.01)
    KRR.fit(x_train, y_train)

    yhat = KRR.predict(x_peak)

    yhatList.append(yhat.reshape(-1,))
```

Plot the resulting ensemble of models along with the original data.

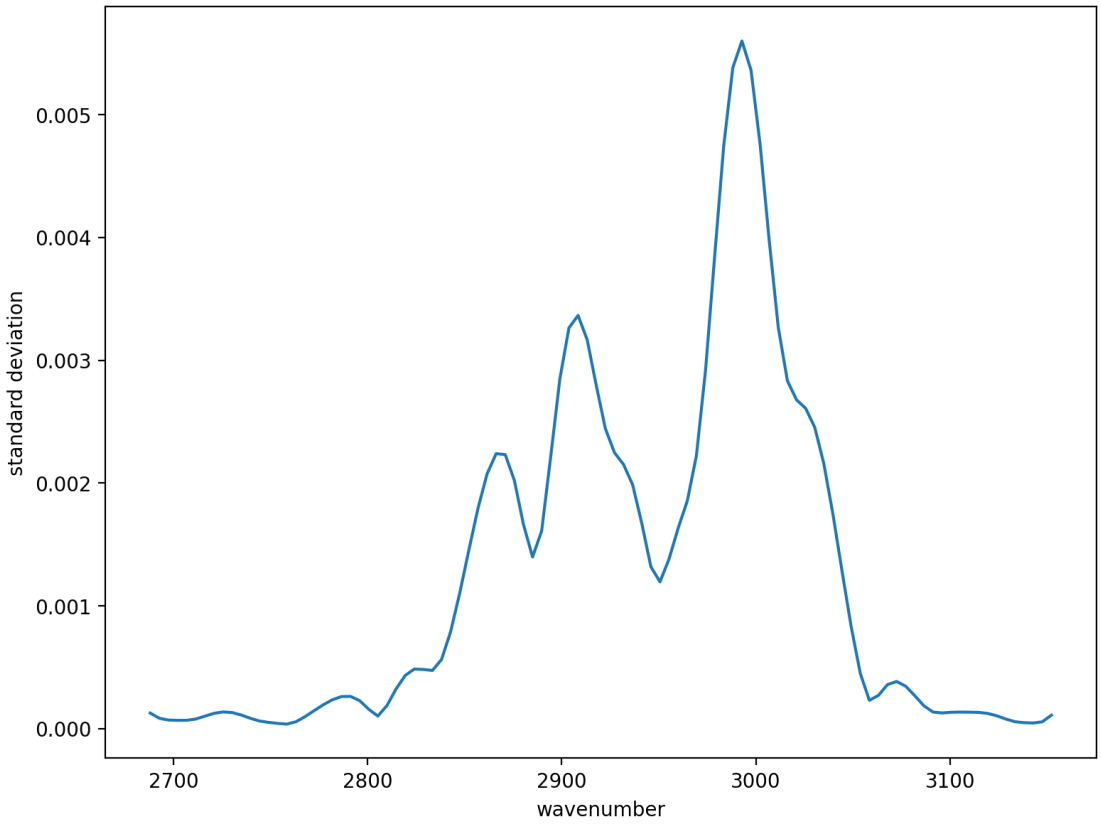
The plot should consists of 6 different lines (1 from the original data and 5 from each of the slightly different KRR models).

In [19]:
```
fig, ax = plt.subplots(figsize = (9, 7), dpi = 200)

ax.plot(x_peak, y_peak, 'o', label = 'Actual Data')
for i in range(5):
    ax.plot(x_peak, yhatList[i], '--', label = 'Prediction {}'.format(i + 1))
ax.set_xlabel('wavenumber')
ax.set_ylabel('absorbance')
ax.legend()
plt.show()
```



Plot the standard deviation of the 5 KRR model predictions as a function of wavenumber.

In [20]:
```
yhatList = np.array(yhatList)
std = yhatList.std(axis = 0)

fig, ax = plt.subplots(figsize = (9, 7), dpi = 200)
ax.plot(x_peak, std)
ax.set_xlabel('wavenumber')
ax.set_ylabel('standard deviation')
plt.show()
```



Is the predicted error homoscedastic? Briefly explain.

No, it's not.