practical1_FriederikeBecker_StefanPfeiffer_TimonVogt

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1 Machine Learning - Practical I

Names: Friederike Becker, Stefan Pfeiffer, Timon Vogt

This notebook provides you with the assignments and the overall code structure you need to complete the assignment. There are also questions that you need to answer in text form. Please use full sentences and reasonably correct spelling/grammar.

Regarding submission & grading:

- Work in groups of two or three and hand in your solution as a group.
- Solutions need to be uploaded to StudIP until the submission date indicated in the course plan. Please upload a copy of this notebook and a PDF version of it after you ran it.
- Solutions need to be presented to tutors in tutorial. Presentation dates are listed in the course plan. Every group member needs to be able to explain everything.
- You have to solve N-1 exercise of each practical to get admission to the exam.
- For plots you create yourself, all axes must be labeled.
- Do not change the function interfaces.

```
[1]: # %matplotlib notebook
    %matplotlib inline

import pandas as pd
    import seaborn as sns
    import matplotlib.pyplot as plt
    import numpy as np
    from scipy.io import loadmat
    from scipy import stats
    import copy
    import pylab
    from sklearn import linear_model
    from sklearn.metrics import mean_squared_error, r2_score
```

```
/home/nbuser/anaconda3_420/lib/python3.5/site-
packages/matplotlib/font_manager.py:281: UserWarning: Matplotlib is building the
font cache using fc-list. This may take a moment.
'Matplotlib is building the font cache using fc-list.'
```

1.1 The dataset

The dataset consists of over 20.000 materials and lists their physical features. From these features, we want to learn how to predict the critical temperature, i.e. the temperature we need to cool the material to so it becomes superconductive. First load and familiarize yourself with the data set a bit.

```
[2]: data=pd.read_csv('superconduct_train.csv')
print(data.shape)
```

(21263, 82)

```
data.head()
[3]:
       number_of_elements
                             mean_atomic_mass
                                                 wtd_mean_atomic_mass
    0
                                     88.944468
                                                             57.862692
                          5
    1
                                     92.729214
                                                             58.518416
    2
                          4
                                     88.944468
                                                             57.885242
    3
                          4
                                     88.944468
                                                             57.873967
    4
                                     88.944468
                                                             57.840143
       gmean_atomic_mass
                            wtd_gmean_atomic_mass
                                                     entropy_atomic_mass
    0
                66.361592
                                         36.116612
                                                                  1.181795
    1
                73.132787
                                         36.396602
                                                                  1.449309
    2
                66.361592
                                         36.122509
                                                                  1.181795
    3
                66.361592
                                         36.119560
                                                                  1.181795
    4
                66.361592
                                         36.110716
                                                                  1.181795
       wtd_entropy_atomic_mass
                                   range_atomic_mass
                                                        wtd_range_atomic_mass
    0
                        1.062396
                                           122.90607
                                                                     31.794921
                        1.057755
                                           122.90607
                                                                     36.161939
    1
    2
                                           122.90607
                        0.975980
                                                                     35.741099
    3
                                           122.90607
                        1.022291
                                                                     33.768010
                                           122.90607
                                                                     27.848743
    4
                        1.129224
                                          wtd_mean_Valence
                                                              gmean_Valence
       std_atomic_mass
                               . . .
    0
              51.968828
                                                   2.257143
                                                                    2.213364
    1
              47.094633
                                                   2.257143
                                                                    1.888175
    2
                                                   2.271429
                                                                    2.213364
              51.968828
    3
              51.968828
                                                   2.264286
                                                                    2.213364
                               . . .
    4
              51.968828
                                                   2.242857
                                                                    2.213364
       wtd_gmean_Valence
                            entropy_Valence
                                               wtd_entropy_Valence
                                                                      range_Valence
    0
                 2.219783
                                    1.368922
                                                           1.066221
                                                                                   1
                                    1.557113
                                                           1.047221
                                                                                   2
    1
                 2.210679
    2
                 2.232679
                                    1.368922
                                                           1.029175
                                                                                   1
    3
                 2.226222
                                    1.368922
                                                           1.048834
                                                                                   1
    4
                 2.206963
                                    1.368922
                                                           1.096052
                                                                                   1
```

```
wtd_range_Valence std_Valence wtd_std_Valence critical_temp
            1.085714
                         0.433013
                                                               29.0
0
                                           0.437059
            1.128571
                                                               26.0
1
                         0.632456
                                           0.468606
            1.114286
                         0.433013
                                           0.444697
                                                               19.0
            1.100000
                         0.433013
                                           0.440952
                                                               22.0
3
            1.057143
                         0.433013
                                           0.428809
                                                               23.0
```

[5 rows x 82 columns]

Because the dataset is rather large, we prepare a small subset of the data as training set, and another subset as test set. To make the computations reproducible, we set the random seed.

```
[4]: target_clm = 'critical_temp' # the critical temperature is our target variable
    n_trainset = 200 # size of the training set
    n_testset = 500 #size of the test set

[5]: print("This is an autosave test.")
```

This is an autosave test.

```
[6]: # set random seed to make sure every test set is the same
   np.random.seed(seed=1)
   idx = np.arange(data.shape[0])
   idx_shuffled = np.random.permutation(idx) # shuffle indices to split into_
    →training and test set
   test_idx = idx_shuffled[:n_testset]
   train_idx = idx_shuffled[n_testset:n_testset+n_trainset]
   train_full_idx = idx_shuffled[n_testset:]
   X_test = data.loc[test_idx, data.columns != target_clm].values
   y_test = data.loc[test_idx, data.columns == target_clm].values
   print('Test set shapes (X and y)', X_test.shape, y_test.shape)
   X_train = data.loc[train_idx, data.columns != target_clm].values
   y_train = data.loc[train_idx, data.columns == target_clm].values
   print('Small training set shapes (X and y):',X_train.shape, y_train.shape)
   X_train_full = data.loc[train_full_idx, data.columns != target_clm].values
   y_train_full = data.loc[train_full_idx, data.columns == target_clm].values
   print('Full training set shapes (X and y):', X_train_full.shape, y_train_full.
     →shape)
```

```
Test set shapes (X and y) (500, 81) (500, 1)
Small training set shapes (X and y): (200, 81) (200, 1)
Full training set shapes (X and y): (20763, 81) (20763, 1)
```

1.2 Task 1: Plot the dataset

To explore the dataset, use X_train_full and y_train_full for two descriptive plots:

- **Histogram** of the target variable. Use plt.hist.
- Scatterplots relating the target variable to one of the feature values. For this you will need 81 scatterplots. Arrange them in one big figure with 9x9 subplots. Use plt.scatter. You may need to adjust the marker size and the alpha blending value.

```
[7]: # Histogram of the target variable

plt.hist(y_train_full, bins=50)

plt.title("Histogram of the critical temperature for superconducting behaviour

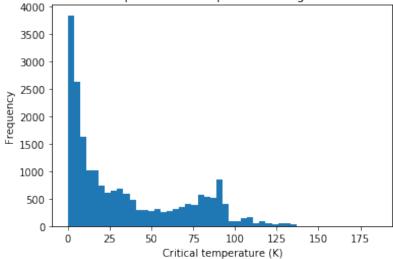
→of various materials")

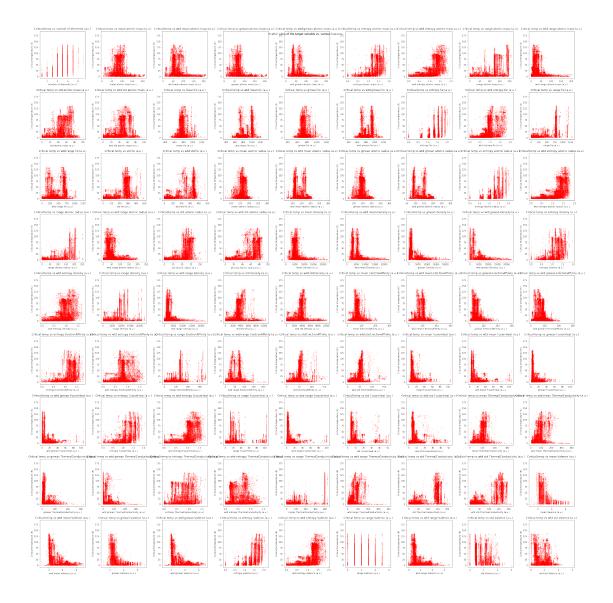
plt.xlabel("Critical temperature (K)")

plt.ylabel("Frequency")

plt.show()
```

Histogram of the critical temperature for superconducting behaviour of various materials





Which material properties may be useful for predicting superconductivity? What other observations can you make?

When evaluating this grid, one should look for plots that show a small spread in the critical temperature for all values of the material property it is plotted against. This is because a given value of the predictor would then allow us to make a precise prediction for the outcome. Here we are however observing that for all the variables in the dataset, the critical temperature takes on a large spread for at least some values of that variable/predictor. There are however some variables for which the spread of the critical temperature is smaller at some of its values - e.g. when looking at "wtd entropy atomic radius", we can see that observations with small values of this variable tend to have smaller critical temperatures (similar relations can be stated for a lot of the variables describing the atomic radius), making it a variable with at least some predictive power. All in all though, the data show that guessing ~0K as the critical superconductivity temperature is correct a lot of times.

1.3 Task 2: Implement your own OLS estimator

We want to use linear regression to predict the critical temperature. Implement the ordinary least squares estimator without regularization 'by hand':

```
w = (X^T X)^{-1} X^T y
```

To make life a bit easier, we provide a function that can be used to plot regression results. In addition it computes the mean squared error and the squared correlation between the true and predicted values.

```
[9]: | def plot_regression_results(y_test,y_pred,weights):
        '''Produces three plots to analyze the results of linear regression:
            -True vs predicted
            -Raw residual histogram
            -Weight histogram
        Inputs:
            y_test: (n_observations,) numpy array with true values
            y_pred: (n_observations,) numpy array with predicted values
            weights: (n_weights) numpy array with regression weights'''
        print('MSE: ', mean_squared_error(y_test,y_pred))
        print('r^2: ', r2_score(y_test,y_pred))
        fig,ax = plt.subplots(1,3,figsize=(9,3))
        #predicted vs true
        ax[0].scatter(y_test,y_pred)
        ax[0].set_title('True vs. Predicted')
        ax[0].set_xlabel('True %s' % (target_clm))
        ax[0].set_ylabel('Predicted %s' % (target_clm))
        #residuals
        error = np.squeeze(np.array(y_test)) - np.squeeze(np.array(y_pred))
        ax[1].hist(np.array(error),bins=30)
        ax[1].set_title('Raw residuals')
        ax[1].set_xlabel('(true-predicted)')
        #weight histogram
        ax[2].hist(weights,bins=30)
        ax[2].set_title('weight histogram')
        plt.tight_layout()
```

As an example, we here show you how to use this function with random data.

```
[10]: # weights is a vector of length 82: the first value is the intercept (beta0), ⊔

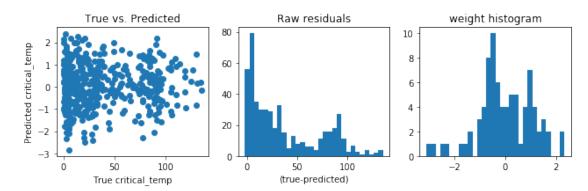
→ then 81 coefficients

weights = np.random.randn(82)

# Model predictions on the test set
```

```
y_pred_test = np.random.randn(y_test.size)
plot_regression_results(y_test, y_pred_test, weights)
```

MSE: 2640.432578444892 r^2: -1.108062856115481



Implement OLS linear regression yourself. Use X_{train} and y_{train} for estimating the weights and compute the MSE and r^2 from X_{test} . When you call our plotting function with the regession result, you should get mean squared error of 599.7.

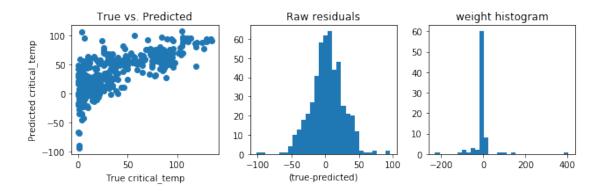
```
[11]: def OLS_regression(X_test, X_train, y_train):
           '''Computes OLS weights for linear regression without regularization on the
       \hookrightarrow training set and
              returns weights and testset predictions.
              Inputs:
                \textit{X\_test:} (n_observations, 81), numpy array with predictor values of the \sqcup
       \rightarrow test set
                X_{-}train: (n_observations, 81), numpy array with predictor values of the
       \hookrightarrow training set
                y_{\perp}train: (n_observations,) numpy array with true target values for the \Box
       \hookrightarrow training set
              Outputs:
                weights: The weight vector for the regerssion model including the offset
                y_pred: The predictions on the TEST set
              Note:
                Both the training and the test set need to be appended manually by a_{\sqcup}
       \rightarrow columns of 1s to add
                an offset term to the linear regression model.
           I \cap I \cap I
```

[12]: # Plots of the results

HIDE THIS CELL

weights, y_pred = OLS_regression(X_test, X_train, y_train)
plot_regression_results(y_test, y_pred, weights)

MSE: 599.7397625913964 r^2: 0.5211810643545935



What do you observe? Is the linear regression model good?

The weight histogram shows that most of the weights (or coefficients) are near zero, which is a possible indication that they have no strong linear influence on the critical temperature (this could also possibly be a scaling issue). However, there are still quite a few predictors that are assigned non-zero weights, indicating that they do have strong predictive power in the linear model. The plot of the true vs. predicted values shows an anomaly: our model is predicting values below zero, which is outside the possible range of values for the critical temperature. Furthmore, it makes very few predictions above 100, even though there are observations in the data with such a high value for the critical temperature. The linear model thus has problems making predictions for observations that have a high true value and especially for those that have a low true value. In a model with perfect predictive power, we would want all of our points to lie on a 45 degree line in this plot. When disregarding the points that have a predicted temperature below zero, we can see that quite a few of the points lie on or somewhere near this 45 degree line (even though this is hard to tell with alpha set to 1). However, the histogram of the raw residuals supports this assumption, showing that most residuals are very small. To sum up, the linear model is not perfect, but seems to be better than just random guessing.

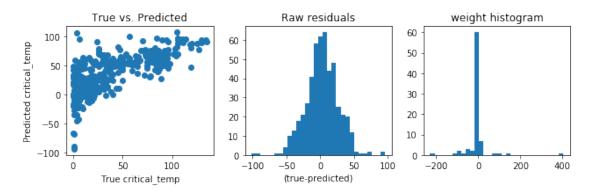
1.4 Task 3: Compare your implementation to sklearn

Now, familarize yourself with the sklearn library. In the section on linear models: https://scikit-learn.org/stable/modules/classes.html#module-sklearn.linear_model you will find sklearn.linear_model.LinearRegression, the sklearn implementation of the OLS estimator. Use this sklearn class to implement OLS linear regression. Again obtain estimates of the weights on X_train and y_train and compute the MSE and r^2 on X_test.

```
[13]: def sklearn_regression(X_test, X_train, y_train):
         → the sklearn library on the training set and
            returns weights and testset predictions.
            Inputs:
              X_{-}test: (n_observations, 81), numpy array with predictor values of the _{\!\!\!\!\perp}
      \rightarrow test set
              X_{\perp}train: (n_{\perp}observations, 81), numpy array with predictor values of the
      \rightarrow training set
              y_train: (n_observations,) numpy array with true target values for the __
      \hookrightarrow training set
            Outputs:
              weights: The weight vector for the regerssion model including the offset
              y_pred: The predictions on the TEST set
            Note:
              The sklearn library automatically takes care of adding a column for the 
      \hookrightarrow offset.
         111
```

[14]: weights, y_pred = sklearn_regression(X_test, X_train, y_train)
plot_regression_results(y_test, y_pred, weights.T)

MSE: 599.739762618123 r^2: 0.5211810643332555

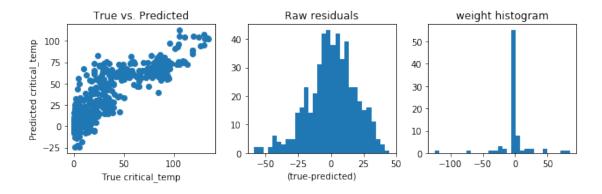


If you implemented everything correctly, the MSE is again 599.74.

Fit the model using the larger training set, X_train_full and y_train_full, and again evaluate on X_test.

[15]: weights, y_pred = sklearn_regression(X_test, X_train_full, y_train_full)
plot_regression_results(y_test, y_pred, weights.T)

MSE: 329.8607010411003 r^2: 0.7366465263178581



How does test set performance change? What else changes?

The test set performance has improved drastically. The MSE went down to 329.9 (from 599.7). Furthmore, one can see in the true vs. predicted graph that the model seems to make far less "nonsensical" predictions below 0 and that all other points also lie more closely to the ideal 45 degree line. This observation is also supported by the histogram of the raw residuals, which shows that most residuals have now moved closer to zero. The largest residuals are now around an absolute value of 50, as opposed to 100 before. The weight histogram shows that most weights are still near 0 and that the few large coefficients have also become smaller - this might be because in the small training data, there could have been a few outlier observations that drastically influenced the coefficients.

1.5 Task 4: Regularization with ridge regression

We will now explore how a penalty term on the weights can improve the prediction quality for finite data sets. Implement the analytical solution of ridge regression

$$w = (XX^T + \alpha \bar{I}_D)^{-1}X^Ty$$

as a function that can take different values of α , the regularization strength, as an input. In the lecture, this parameter was called λ , but this is a reserved keyword in Python.

```
[16]: def ridge_regression(X_test, X_train, y_train, alpha):
          '''Computes OLS weights for regularized linear regression with
      \rightarrow regularization strength alpha
             on the training set and returns weights and testset predictions.
               X_{-}test: (n_{-}observations, 81), numpy array with predictor values of the \Box
      \rightarrow test set
               X_train: (n_observations, 81), numpy array with predictor values of the
      \rightarrow training set
               y_train: (n_observations,) numpy array with true target values for the _ i
      \rightarrow training set
               alpha: scalar, regularization strength
             Outputs:
               weights: The weight vector for the regerssion model including the offset
               y\_pred: The predictions on the TEST set
             Note:
               Both the training and the test set need to be appended manually by a_{i,j}
      \rightarrow columns of 1s to add
               an offset term to the linear regression model.
                   ----- INSERT CODE -----
```

Now test a range of log-spaced α s (~10-20), which cover several orders of magnitude, e.g. from 10^-7 to 10^7.

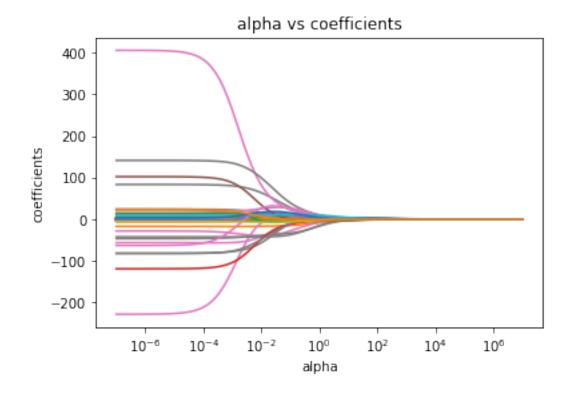
- For each α , you will get one model with one set of weights.
- For each model, compute the error on the test set.

Store both the errors and weights of all models for later use. You can use the function mean_squared_error from sklearn (imported above) to compute the MSE.

Make a single plot that shows for each coefficient how it changes with α , i.e. one line per coefficient. Also think about which scale is appropriate for your α -axis. You can set this using plt.xscale(...).

```
[18]: # Plot of coefficients vs. alphas

weights = np.array(weights_list)
for i in range(len(weights[0])):
    plt.plot(alphas, weights[:, i])
plt.xscale("log")
plt.title("alpha vs coefficients")
plt.xlabel("alpha")
plt.ylabel("coefficients")
plt.show()
```



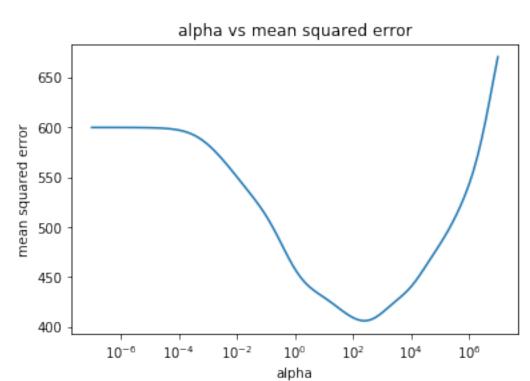
Why are the values of the weights largest on the left? Do they all change monotonically?

The values of the weights are largest on the left because the α value on the left is smallest and therefore large weight values are not as heavy penalised. Certain values do not change monotonically but go from < 0 to > 0 before converging finally to 0.

Plot how the performance (i.e. the error) changes as a function of α . As a sanity check, the MSE value for very small α s should be close to the test-set MSE of the unregularized solution, i.e. 599.

```
[19]: # Plot of MSE vs. alphas
    errors = np.array(error_list)
    plt.plot(alphas, errors)
    plt.xscale("log")
    plt.title("alpha vs mean squared error")
```

```
plt.xlabel("alpha")
plt.ylabel("mean squared error")
plt.show()
```



Which value of α gives the minimum MSE? Is it better than the unregularized model? Why should the curve reach ~600 on the left?

The minimum MSE is reached an α of around 100, where the mean squared error is around 400. Therefore it is better than the MSE of the unregularized model of around 600. The curve should reach ~600 on the left since an α of 0 is the same as the unregularized model.

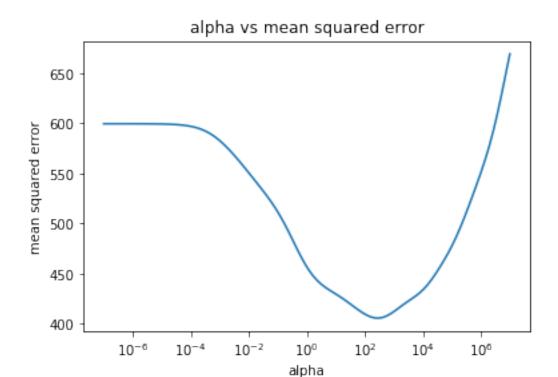
Now implement the same model using sklearn. Use the linear_model.Ridge object to do so.

```
[20]: def ridge_regression_sklearn(X_test, X_train, y_train,alpha):
    '''Computes OLS weights for regularized linear regression with
    →regularization strength alpha using the sklearn
    library on the training set and returns weights and testset predictions.

Inputs:
    X_test: (n_observations, 81), numpy array with predictor values of the
    →test set
    X_train: (n_observations, 81), numpy array with predictor values of the
    →training set
    y_train: (n_observations,) numpy array with true target values for the
    →training set
    alpha: scalar, regularization strength
```

This time, only plot how the performance changes as a function of α .

```
[21]: # Plot of MSE vs. alphas
     alphas = np.logspace(-7,7,100)
     error_list = []
     weights_list = []
     for a in alphas:
         weights, y_pred = ridge_regression_sklearn(X_test, X_train, y_train, a)
         error = mean_squared_error(y_test,y_pred)
         error_list.append(error)
         weights_list.append(weights)
     errors = np.array(error_list)
     plt.plot(alphas, errors)
     plt.xscale("log")
     plt.title("alpha vs mean squared error")
     plt.xlabel("alpha")
     plt.ylabel("mean squared error")
     plt.show()
```



Note: Don't worry if the curve is not exactly identical to the one you got above. The loss function we wrote down in the lecture has α defined a bit differently compared to sklearn. However, qualitatively it should look the same.

1.6 Task 5: Cross-validation

Until now, we always estimated the error on the test set directly. However, we typically do not want to tune hyperparameters of our inference algorithms like α on the test set, as this may lead to overfitting. Therefore, we tune them on the training set using cross-validation. As discussed in the lecture, the training data is here split in n_folds-ways, where each of the folds serves as a held-out dataset in turn and the model is always trained on the remaining data. Implement a function that performs cross-validation for the ridge regression parameter α . You can reuse functions written above.

```
[22]: def ridgeCV(X, y, n_folds, alphas):

'''Runs a n_fold-crossvalidation over the ridge regression parameter alpha.

The function should train the linear regression model for each fold on → all values of alpha.

Inputs:

X: (n_obs, n_features) numpy array - predictor

y: (n_obs,) numpy array - target

n_folds: integer - number of CV folds

alphas: (n_parameters,) - regularization strength parameters to CV over
```

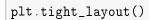
```
Outputs:
      cv_results_mse: (n_folds, len(alphas)) numpy array, MSE for each_
\hookrightarrow cross-validation fold
    Note:
      Fix the seed for reproducibility.
      111
  cv_results_mse = np.zeros((n_folds, len(alphas)))
  np.random.seed(seed=58723968)
  # ----- INSERT CODE -----
  random_state = np.random.get_state()
  np.random.shuffle(X)
  np.random.set_state(random_state)
  np.random.shuffle(y)
  X_folds = np.array_split(X, n_folds)
  y_folds = np.array_split(y, n_folds)
  for n in range(n_folds):
      training_data_x = np.concatenate(X_folds[:n] + X_folds[n+1:])
      training_data_y = np.concatenate(y_folds[:n] + y_folds[n+1:])
      for i in range(len(alphas)):
          a = alphas[i]
          _, y_pred = ridge_regression_sklearn(X_folds[n], training_data_x,_
→training_data_y, a)
          error = mean_squared_error(y_folds[n],y_pred)
          cv_results_mse[n, i] = error
  # ----- END CODE -----
  return cv_results_mse
```

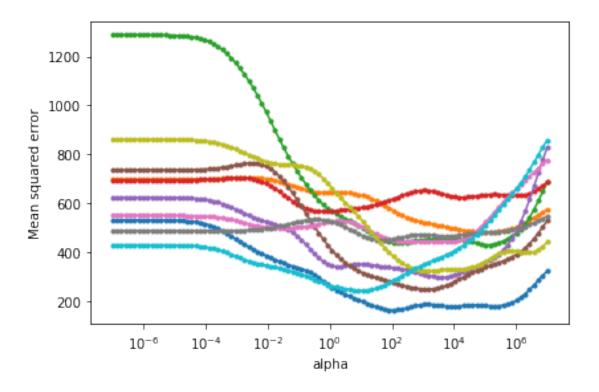
Now we run 10-fold cross-validation using the training data of a range of α s.

```
[23]: alphas = np.logspace(-7,7,100)
mse_cv = ridgeCV(X_train, y_train, n_folds=10, alphas=alphas)
```

We plot the MSE trace for each fold separately:

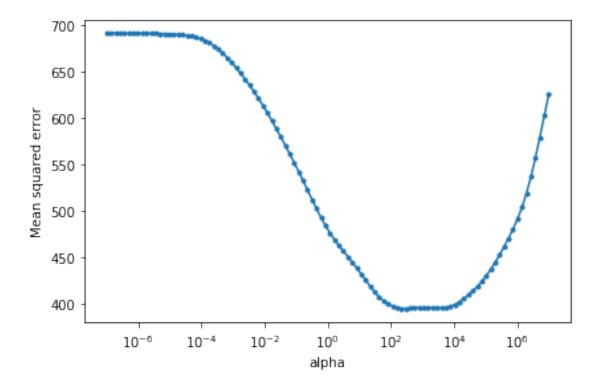
```
[24]: plt.figure(figsize=(6,4))
  plt.plot(alphas, mse_cv.T, '.-')
  plt.xscale('log')
  plt.xlabel('alpha')
  plt.ylabel('Mean squared error')
```





We also plot the average across folds:

```
[27]: plt.figure(figsize=(6,4))
  plt.plot(alphas, np.mean(mse_cv,axis=0), '.-')
  plt.xscale('log')
  plt.xlabel('alpha')
  plt.ylabel('Mean squared error')
  plt.tight_layout()
```



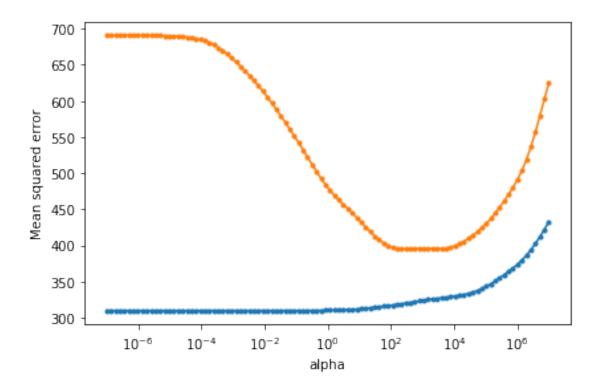
What is the optimal α ? Is it similar to the one found on the test set? Do the cross-validation MSE and the test-set MSE match well or differ strongly?

The optimal α in our CV experiment seems to be slightly above 10^3 , so slightly above 1000, whereas the MSE of the test-set was at slightly above 100, which does not seem to be drastically different, at least not when considering the wider range of α 's that were considered here.

We will now run cross-validation on the full training data. This will take a moment, depending on the speed of your computer. Afterwards, we will again plot the mean CV curves for the full data set (blue) and the small data set (orange).

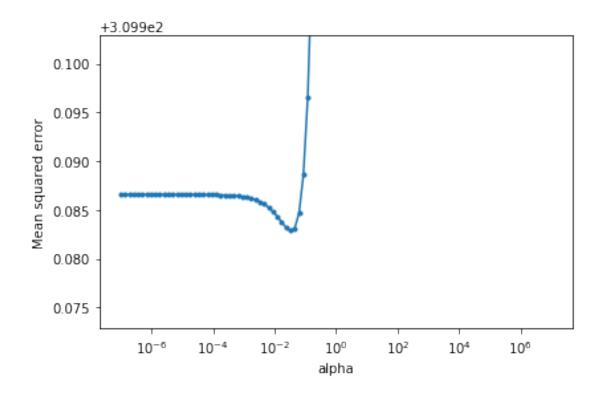
```
[28]: alphas = np.logspace(-7,7,100)
    mse_cv_full = ridgeCV(X_train_full, y_train_full, n_folds=10, alphas=alphas)

[29]: plt.figure(figsize=(6,4))
    plt.plot(alphas, np.mean(mse_cv_full,axis=0), '.-')
    plt.plot(alphas, np.mean(mse_cv,axis=0), '.-')
    plt.xscale('log')
    plt.xlabel('alpha')
    plt.ylabel('Mean squared error')
    plt.tight_layout()
```



We zoom in on the blue curve to the very right:

```
[30]: plt.figure(figsize=(6,4))
  plt.plot(alphas, np.mean(mse_cv_full,axis=0), '.-')
  plt.xscale('log')
  minValue = np.min(np.mean(mse_cv_full,axis=0))
  plt.ylim([minValue-.01, minValue+.02])
  plt.xlabel('alpha')
  plt.ylabel('Mean squared error')
  plt.tight_layout()
```



Why does the CV curve on the full data set look so different? What is the optimal value of α and why is it so much smaller than on the small training set?

On the full data, we get an optimal value of slightly below 0.1 (or 10^{-1}) for α , which is much smaller than the 1000 we got on the small training set. This could be because our first training set was very small at 200 observations and thus our model had to be regularized heavily (i.e. α large) in order to make good predictions on our current hold-out set in the cross-validation. When training a model on more data points, the model is not influenced as heavily by single observations and thus does not have to be regularized to make good predictions on the new data in the hold-out set.

[]: