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1 Practical 2

2 Task 1: The Data

We use the mouse protein expression dataset: https://archive.ics.uci.edu/ml/datasets/Mice+Protein+Expression Please use the code provided below for loading the dataset. Let's start with a bit of exploration.

2.0.1 Tasks 1.1: Dataset Exploration

- How many samples / features are provided?
- How many labels does the dataset have?
- What is the value range of the individuals predictors?
- Visualize the 10 first samples of the dataset in a form that highlights their differences.
- Visualize the variance of each predictor.

[1]:
```
import pandas as pd
import numpy as np
from matplotlib import pyplot as plt

file = 'data/Data_Cortex_Nuclear.csv'
df = pd.read_csv(file)

N = 10  # use only every tenth sample (row)
X_all = df.iloc[::N,1:65].to_numpy()
t_all = (df['Behavior'] == 'S/C').to_numpy()[::N]

idx = ~np.any(np.isnan(X_all), axis=1) #check which rows are without missings
X_all = X_all[idx]
t_all = t_all[idx]
```

[2]:
```
df.describe(include = [np.number])
```

[2]:
```
          DYRK1A_N      ITSN1_N       BDNF_N        NR1_N       NR2A_N  \
count  1077.000000  1077.000000  1077.000000  1077.000000  1077.000000
mean      0.425810     0.617102     0.319088     2.297269     3.843934
std       0.249362     0.251640     0.049383     0.347293     0.933100
min       0.145327     0.245359     0.115181     1.330831     1.737540
25%       0.288121     0.473361     0.287444     2.057411     3.155678
```

50%	0.366378	0.565782	0.316564	2.296546	3.760855
75%	0.487711	0.698032	0.348197	2.528481	4.440011
max	2.516367	2.602662	0.497160	3.757641	8.482553

	pAKT_N	pBRAF_N	pCAMKII_N	pCREB_N	pELK_N	…	\
count	1077.000000	1077.000000	1077.000000	1077.000000	1077.000000	…	
mean	0.233168	0.181846	3.537109	0.212574	1.428682	…	
std	0.041634	0.027042	1.295169	0.032587	0.466904	…	
min	0.063236	0.064043	1.343998	0.112812	0.429032	…	
25%	0.205755	0.164595	2.479834	0.190823	1.203665	…	
50%	0.231177	0.182302	3.326520	0.210594	1.355846	…	
75%	0.257261	0.197418	4.481940	0.234595	1.561316	…	
max	0.539050	0.317066	7.464070	0.306247	6.113347	…	

	SHH_N	BAD_N	BCL2_N	pS6_N	pCFOS_N	\
count	1080.000000	867.000000	795.000000	1080.000000	1005.000000	
mean	0.226676	0.157914	0.134762	0.121521	0.131053	
std	0.028989	0.029537	0.027417	0.014276	0.023863	
min	0.155869	0.088305	0.080657	0.067254	0.085419	
25%	0.206395	0.136424	0.115554	0.110839	0.113506	
50%	0.224000	0.152313	0.129468	0.121626	0.126523	
75%	0.241655	0.174017	0.148235	0.131955	0.143652	
max	0.358289	0.282016	0.261506	0.158748	0.256529	

	SYP_N	H3AcK18_N	EGR1_N	H3MeK4_N	CaNA_N
count	1080.000000	900.000000	870.000000	810.000000	1080.000000
mean	0.446073	0.169609	0.183135	0.205440	1.337784
std	0.066432	0.059402	0.040406	0.055514	0.317126
min	0.258626	0.079691	0.105537	0.101787	0.586479
25%	0.398082	0.125848	0.155121	0.165143	1.081423
50%	0.448459	0.158240	0.174935	0.193994	1.317441
75%	0.490773	0.197876	0.204542	0.235215	1.585824
max	0.759588	0.479763	0.360692	0.413903	2.129791

[8 rows x 77 columns]

[3]:
```
df.describe(include = [object])
```

[3]:

	MouseID	Genotype	Treatment	Behavior	class
count	1080	1080	1080	1080	1080
unique	1080	2	2	2	8
top	18899_2	Control	Memantine	S/C	c-SC-m
freq	1	570	570	555	150

The dataset contains 77 numerical columns, which may be used as features, as well as 1080 observations (or ‘samples’). It is to be noted, that it is a longitudinal dataset and therefore contains repeated measures on the individual subjects. Correlation between the observations is present. 8

different labels are contained, as indicated by the facotr-variable 'class'.

In the following a random subset of the data is used with 105 samples and 64 features, where no missing values are present. The 8 labels are coarse-grained into two classes decribing the behaviour of the subject. This is the target variable.

Nr. of samples/features & labels

[4]:
```
print('Nr of samples: ' + str(X_all.shape[0]))
print('Nr of features: ' + str(X_all.shape[1]))
print('')

nr_labels = len(df['class'].unique())
print('Nr. of labels: ' + str(nr_labels))
print('')
print('Label names: ')
print(df['class'].unique())
```

```
Nr of samples: 105
Nr of features: 64

Nr. of labels: 8

Label names:
['c-CS-m' 'c-SC-m' 'c-CS-s' 'c-SC-s' 't-CS-m' 't-SC-m' 't-CS-s' 't-SC-s']
```

Task 1.2: Data Preprocessing:
- Write a function `split_data(X, y, frac, seed)` that first shuffles your training data and then splits it into a training and a test set. `frac` determines the relative size of the test dataset, `seed` makes sure we get reproducible results.
- Write a function `preprocess(X)` which zero-centers your data and sets variance to one (per-feature).

[5]:
```
def split_data(X, y, frac=0.3, seed=None):
    if seed is not None:
        np.random.seed(seed)

    # shuffle vectors
    idx = list(range(len(y)))
    idx_shuffled = np.random.permutation(idx)
    y_shuffled = y[idx_shuffled]
    X_shuffled = X[idx_shuffled]

    # slice vectors
    idx_cutoff = round((1-frac)*len(y)) #seperates training from test (in this␣
↪order)
    X_train = X_shuffled[:idx_cutoff, :]
    X_test = X_shuffled[idx_cutoff:, :]
    y_train = y_shuffled[:idx_cutoff]
```

```python
    y_test = y_shuffled[idx_cutoff:]
    return X_train, X_test, y_train, y_test

def preprocess(X):
    X_norm = (X - X.mean(axis = 0)) / X.std(axis = 0)
    return X_norm

def calculate_accuracy(t_pred, t_true):
    accuracy_list = [1 if pred == null else 0 for pred, null in zip(t_pred, t_true)]
    accuracy = sum(accuracy_list)/len(accuracy_list)
    return accuracy
```

[6]:
```python
X_train, X_test, t_train, t_test = split_data(X_all, t_all)
X_train = preprocess(X_train)
X_test = preprocess(X_test)
```

[7]:
```python
pd.DataFrame(X_train).describe().round(3)
```

[7]:

	0	1	2	3	4	5	6	7	8	\
count	74.000	74.000	74.000	74.000	74.000	74.000	74.000	74.000	74.000	
mean	-0.000	-0.000	-0.000	0.000	-0.000	0.000	-0.000	-0.000	-0.000	
std	1.007	1.007	1.007	1.007	1.007	1.007	1.007	1.007	1.007	
min	-1.143	-1.596	-2.515	-2.368	-2.130	-1.709	-2.265	-1.684	-2.718	
25%	-0.600	-0.720	-0.577	-0.726	-0.515	-0.751	-0.658	-0.800	-0.577	
50%	-0.268	-0.157	-0.070	0.221	-0.017	-0.111	-0.081	-0.175	0.026	
75%	0.275	0.404	0.713	0.670	0.505	0.562	0.487	0.751	0.607	
max	6.123	4.398	2.534	2.449	2.565	2.513	2.780	2.332	2.605	

	9	…	54	55	56	57	58	59	60	\
count	74.000	…	74.000	74.000	74.000	74.000	74.000	74.000	74.000	
mean	0.000	…	0.000	-0.000	0.000	-0.000	0.000	0.000	0.000	
std	1.007	…	1.007	1.007	1.007	1.007	1.007	1.007	1.007	
min	-1.558	…	-2.403	-2.682	-1.231	-2.518	-2.773	-2.156	-2.852	
25%	-0.513	…	-0.498	-0.548	-0.593	-0.615	-0.648	-0.921	-0.491	
50%	-0.123	…	-0.057	0.114	-0.280	-0.073	-0.046	0.108	-0.033	
75%	0.424	…	0.645	0.639	0.399	0.607	0.788	0.732	0.580	
max	5.920	…	2.579	2.888	4.835	2.843	2.232	2.733	2.513	

	61	62	63
count	74.000	74.000	74.000
mean	-0.000	-0.000	-0.000
std	1.007	1.007	1.007
min	-2.077	-2.270	-2.999
25%	-0.746	-0.602	-0.517
50%	-0.022	0.020	0.094
75%	0.685	0.606	0.760

```
max      2.042   3.198   1.895

[8 rows x 64 columns]
```

[8]:
```
X_train.shape
```

[8]:
```
(74, 64)
```

[9]:
```
t_train.shape
```

[9]:
```
(74,)
```

[10]:
```
X_test.shape
```

[10]:
```
(31, 64)
```

[11]:
```
t_test.shape
```

[11]:
```
(31,)
```

3 Task 2: LDA

First, use Linear Discriminant Analysis to separate the classes. As discussed in the Bishop in pg. 186-189, we can find a weight vector $\vec{w}$ that performs a projection of the i-th input data point $\vec{x}_i$

$p = \vec{w}^T \vec{x}_i$

that optimally separates the classes.

Use the analytic solution to compute the optimal weights $\vec{w}$ from the training set data.

Task 2.1

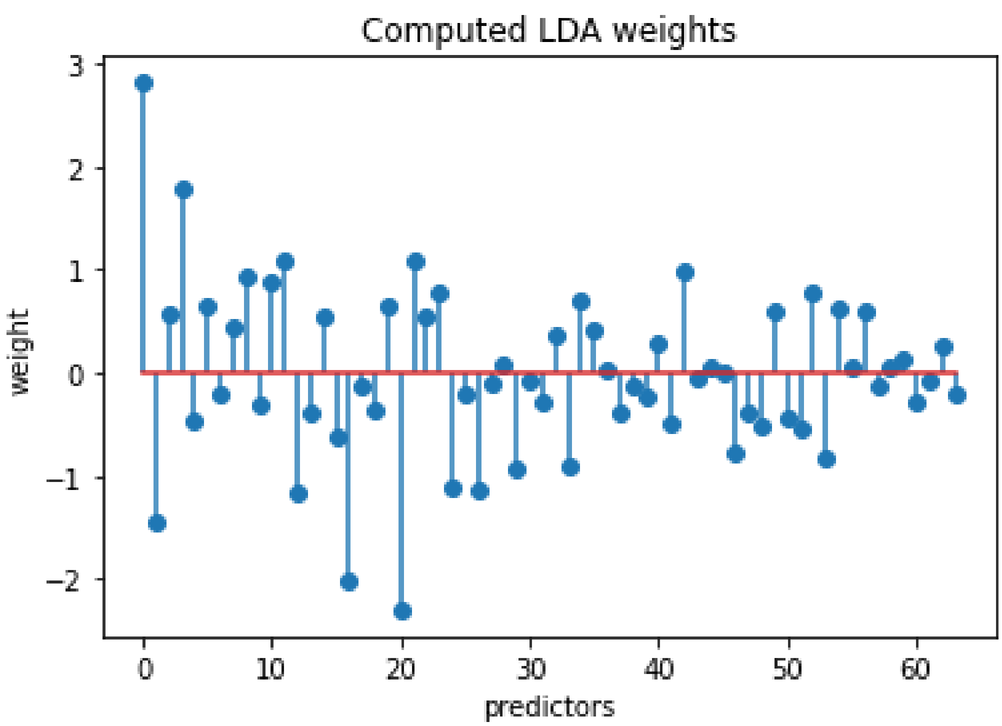
1. Implement a function `compute_lda_weights(x, y)` manually, which carries out LDA using the data `x`,`y`.
2. Apply this function on your training data.
3. Visualize the obtained weight vector $\vec{w}$ using a `plt.stemplot`.

[12]:
```
def compute_lda_weights(x, y):

    # seperate predictors into class 1 and class 0 obs. by boolean indexing
    c1_obs = x[y]
    c0_obs = x[~y]
    # compute columnwise (array-axis 0) class means
    c1_mean_vec = np.mean(c1_obs, axis = 0)
    c0_mean_vec = np.mean(c0_obs, axis = 0)
    m_diff = c1_mean_vec - c0_mean_vec

    # within-class covariance matrices
```

```
    c1_obs_centered = np.transpose(c1_obs - c1_mean_vec) #transformation needed␣
↪to match dimensions
    c1_cov_mat = np.matmul(c1_obs_centered, np.transpose(c1_obs_centered))
    c0_obs_centered = np.transpose(c0_obs - c0_mean_vec)
    c0_cov_mat = np.matmul(c0_obs_centered, np.transpose(c0_obs_centered))

    Sw = c1_cov_mat + c0_cov_mat
    Sw_inv = np.linalg.inv(Sw)
    weights = np.matmul(Sw_inv, c1_mean_vec - c0_mean_vec)

    return c1_mean_vec, c0_mean_vec, m_diff, weights
```

[13]:
```
m1, m0, mdiff, w_lda = compute_lda_weights(X_train, t_train)

plt.stem(w_lda.flatten(), use_line_collection=True)
plt.title('Computed LDA weights')
plt.ylabel('weight')
plt.xlabel('predictors')
```

[13]:
```
Text(0.5, 0, 'predictors')
```

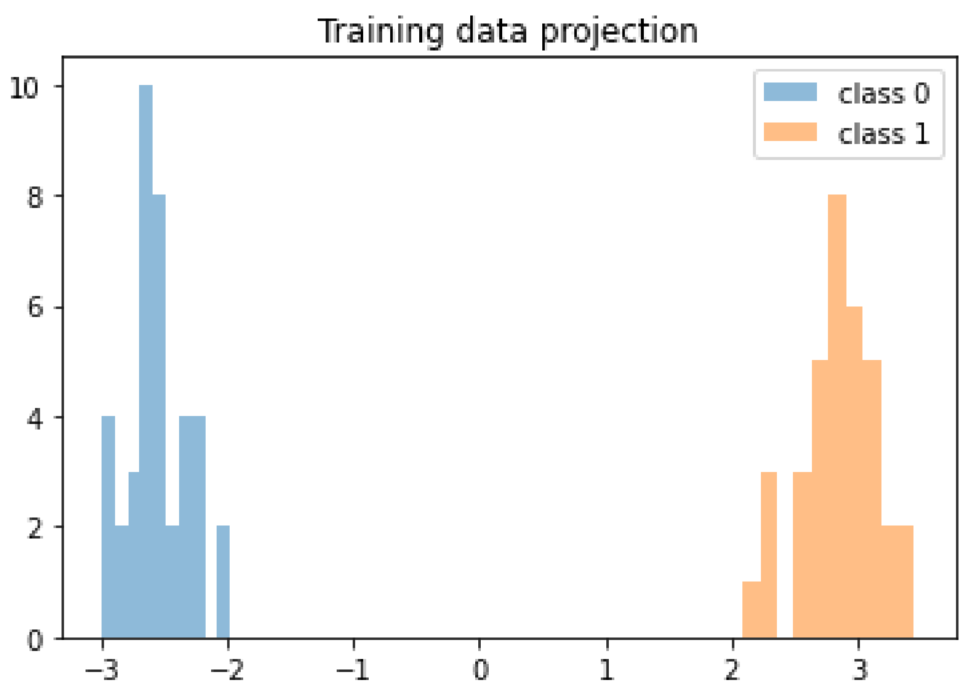


3.0.1 Task 2.3

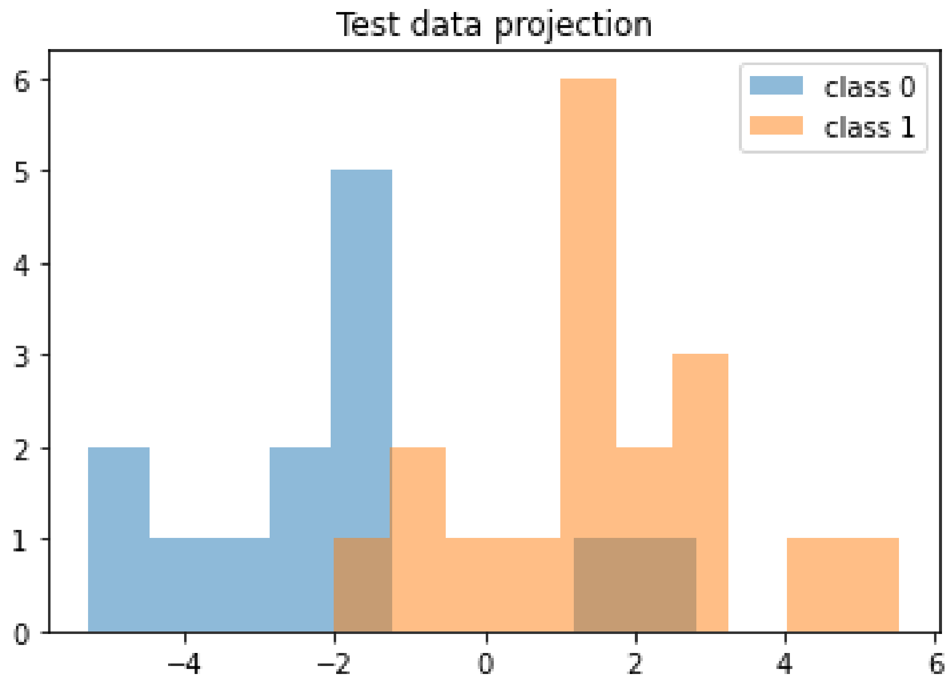
Project the training data and the test data on $\vec{w}$. Visualize the class separation using a two-color histogram. - Is the class separation good? - Is there a big difference between training and test data?

[14]:
```
X_cl0 = X_train[~t_train]
X_cl1 = X_train[t_train]
X_cl0_proj = X_cl0 @ w_lda # substract mean from predictor?
X_cl1_proj = X_cl1 @ w_lda # substract mean from predictor?

X_cl0_test = X_test[~t_test]
X_cl1_test = X_test[t_test]
X_cl0_test_proj = X_cl0_test @ w_lda # substract mean from predictor?
X_cl1_test_proj = X_cl1_test @ w_lda # substract mean from predictor?
```

[15]:
```
plt.title('Training data projection')
_ = plt.hist(X_cl0_proj,label='class 0',alpha=0.5)
_ = plt.hist(X_cl1_proj,label='class 1',alpha=0.5)
_ = plt.legend()
```



[16]:
```
plt.title('Test data projection')
_ = plt.hist(X_cl0_test_proj,label='class 0',alpha=0.5)
_ = plt.hist(X_cl1_test_proj,label='class 1',alpha=0.5)
_ = plt.legend()
```



3.0.2 Task 2.4

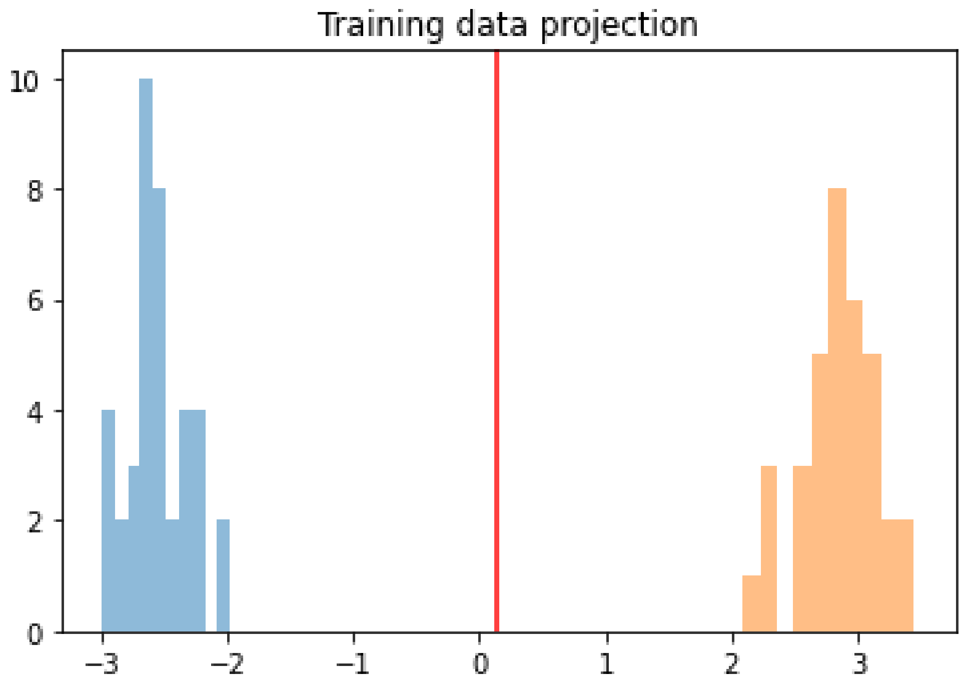
Now we make class predictions based on the projections. Read https://en.wikipedia.org/wiki/Linear_discriminant_analysis#Fisher's_linear_discriminant and compute threshold c for the projected values p based on the training data. Print the value of c and plot c into the histograms of projected values you made before!

Use c to assign class labels for training and test set. Determine the classification errors (in terms of accuracy) on both datasets and print them.

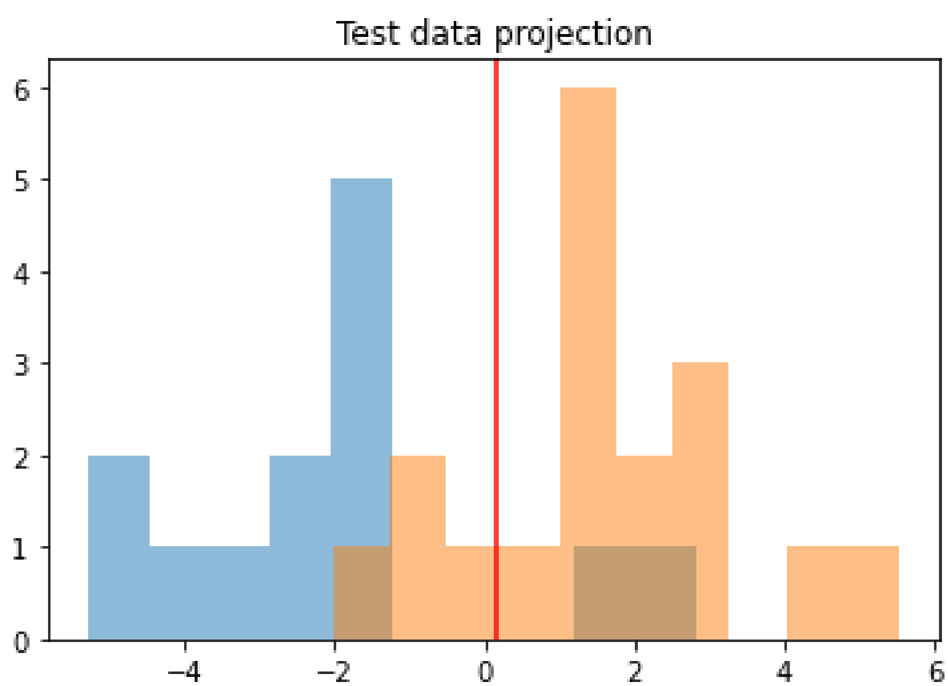
[17]:
```
c = np.matmul(w_lda, 1/2 * (m1 + m0))
c.round(4)
```

[17]: 0.1461

[18]:
```
plt.title('Training data projection')
_ = plt.hist(X_cl0_proj,label='class 0',alpha=0.5)
_ = plt.hist(X_cl1_proj,label='class 1',alpha=0.5)
_ = plt.axvline(c, color = 'red')
```



[19]:
```
plt.title('Test data projection')
_ = plt.hist(X_cl0_test_proj,label='class 0',alpha=0.5)
_ = plt.hist(X_cl1_test_proj,label='class 1',alpha=0.5)
_ = plt.axvline(c, color = 'red')
```



[20]:
```
t_pred = np.matmul(X_train, w_lda) >= c
t_pred_test = np.matmul(X_test, w_lda) >= c
```

[21]:
```
print('Training Set Cross Table')
pd.crosstab(t_pred,t_train, rownames = ['t_pred'], colnames = ['t_true'])
```

```
Training Set Cross Table
```

[21]:
```
t_true  False  True
t_pred
False      39     0
True        0    35
```

[22]:
```
print('Test set corss table')
pd.crosstab(t_pred_test,t_test, rownames = ['t_pred'], colnames = ['t_true'])
```

```
Test set corss table
```

[22]:
```
t_true  False  True
t_pred
False      11     4
True        2    14
```

[23]:
```
calculate_accuracy(t_pred_test, t_test)
```

[23]:
```
0.8064516129032258
```

3.1 Task 3: Logistic Regression

Next, we will consider classification using Logistic Regression.

For this task, we will use a different dataset:
It consists of activations from a convolutional neural network (ResNet18) for images of cats and dogs. The dataset contains 2,000 samples (i.e. CNN activations) and 256 features (i.e. the CNN activations have 256 dimensions). A target value of 0 indicates a cat, 1 a dog.

Below, you find all imports that are necessary.

[24]:
```
import numpy as np
from sklearn.linear_model import LogisticRegression
import pickle

X_all, t_all = pickle.load(open('data/cnn_features.pickle', 'rb'))
X_train, X_test, t_train, t_test = split_data(X_all, t_all)
X_train = preprocess(X_train)
X_test = preprocess(X_test)
```

[25]:
```
X_train.shape
```

[25]: (1400, 256)

[26]:
```
X_test.shape
```

[26]: (600, 256)

[27]:
```
t_train.shape
```

[27]: (1400,)

[28]:
```
t_test.shape
```

[28]: (600,)

Task 3.0: Normalize the data

Make sure the data has has zero mean and variance 1 per feature.

[29]:
```
pd.DataFrame(X_train).describe().round(3)
```

[29]:
```
              0         1         2         3         4         5         6  \
count  1400.000  1400.000  1400.000  1400.000  1400.000  1400.000  1400.000
mean      0.000     0.000     0.000     0.000     0.000     0.000     0.000
std       1.000     1.000     1.000     1.000     1.000     1.000     1.000
min      -2.792    -3.289    -3.111    -3.132    -3.133    -3.467    -3.880
25%      -0.696    -0.678    -0.689    -0.716    -0.671    -0.673    -0.644
50%      -0.058    -0.028    -0.008     0.056    -0.015     0.019     0.008
75%       0.653     0.594     0.702     0.694     0.656     0.652     0.611
max       4.116     4.535     3.172     3.022     3.190     3.388     3.612

              7         8         9  …       246       247       248  \
count  1400.000  1400.000  1400.000  …  1400.000  1400.000  1400.000
mean     -0.000    -0.000     0.000  …     0.000     0.000     0.000
std       1.000     1.000     1.000  …     1.000     1.000     1.000
min      -3.120    -3.058    -2.920  …    -3.678    -3.516    -2.961
25%      -0.667    -0.665    -0.684  …    -0.676    -0.677    -0.704
50%       0.034    -0.064    -0.023  …     0.017     0.011    -0.065
75%       0.657     0.659     0.675  …     0.668     0.676     0.650
max       3.433     3.266     2.915  …     3.443     2.749     4.487

            249       250       251       252       253       254       255
count  1400.000  1400.000  1400.000  1400.000  1400.000  1400.000  1400.000
mean     -0.000     0.000    -0.000     0.000     0.000    -0.000     0.000
std       1.000     1.000     1.000     1.000     1.000     1.000     1.000
min      -3.277    -3.845    -3.994    -2.721    -3.870    -3.251    -3.248
25%      -0.661    -0.638    -0.627    -0.739    -0.637    -0.680    -0.674
```

```
50%        0.026     0.055     0.041    -0.029     0.011     0.000    -0.015
75%        0.743     0.718     0.670     0.688     0.643     0.717     0.705
max        3.471     2.363     3.437     3.337     3.007     3.239     3.238

[8 rows x 256 columns]
```

[30]:
```
pd.Series(t_all).unique()
```

[30]:
```
array([1, 0])
```

Task 3.1: Iterative Reweighted Least Squares

1. Implement the IRLS algorithm and output at each iteration the current training accuracy. Remember the weight are updated according to:

$$w' = w - (\Phi^T R \Phi)^{-1} \Phi^T (y - t)$$

Where y is the prediction, t the ground truth target, R the weighting matrix and Φ the design matrix.
Hints:

(a) There is a bias term in logistic regression

(b) Use a small value for weight init to avoid numerical problems.

2. Apply the IRLS algorithm on data and compute the test accuracy.
3. Compare the results of your implementation to the sklearn implementation of `LogisticRegression(penalty='none')`. Do you get the same result?

[31]:
```
def sigma(x):
        return  (1 / (1 + np.exp(-x)))

def calc_eta(weights, x):
        return(weights.T @ x)



def IRLS(X, t, threshold = 0.01):

    def update_weights(weights, y, R, t=t, X=X):
        XRX_inv = np.linalg.inv(X.T @ R @ X)
        result = weights - (XRX_inv @ X.T @ (y-t))
        return result, weights

    def update_predictors(weights, X=X):
        y = np.array([sigma(calc_eta(weights, x)) for x in X])
        R = np.diag((y * (1-y)).ravel())
        return y, R

    # initialize weights
```

```python
    nr_samples = X.shape[0]
    nr_features = X.shape[1]
    weights = np.zeros((nr_features)) + 0.1

    # calculate predictors and weights repeatedly
    for i in range(20):
        y, R = update_predictors(weights)
        weights, old_weights = update_weights(weights, y, R)
        acc = calculate_accuracy(y.round(), t)
        print("round " + str(i) + ' - training set accuracy: ' + str(acc))

        #check convergence
        changes = np.absolute(weights - old_weights)
        if all(np.less_equal(changes, threshold)):
            print('Convergence')
            break


    return weights
```

[32]:
```python
w_irls = IRLS(X_train, t_train, threshold = .01)
```

```
round 0 - training set accuracy: 0.6142857142857143
round 1 - training set accuracy: 0.8978571428571429
round 2 - training set accuracy: 0.9635714285714285
round 3 - training set accuracy: 0.9721428571428572
round 4 - training set accuracy: 0.9792857142857143
round 5 - training set accuracy: 0.9935714285714285
round 6 - training set accuracy: 1.0
round 7 - training set accuracy: 1.0
round 8 - training set accuracy: 1.0
round 9 - training set accuracy: 1.0
round 10 - training set accuracy: 1.0
round 11 - training set accuracy: 1.0
round 12 - training set accuracy: 1.0
round 13 - training set accuracy: 1.0
round 14 - training set accuracy: 1.0
round 15 - training set accuracy: 1.0
round 16 - training set accuracy: 1.0
round 17 - training set accuracy: 1.0
round 18 - training set accuracy: 1.0
round 19 - training set accuracy: 1.0
```

[33]:
```python
y = np.array([sigma(calc_eta(w_irls, x)) for x in X_test])
print('Test Accuracy')
print(calculate_accuracy(y.round(), t_test))
```

```
Test Accuracy
0.85
```

3.1.1 Check with sklearn

[34]:
```python
from sklearn.linear_model import LogisticRegression

logreg = LogisticRegression(penalty = 'none')
logreg.fit(X_train, t_train.ravel())

print('Training accuracy')
t_pred = logreg.predict(X_train)
print(calculate_accuracy(t_pred, t_train))

print('Test accuracy')
t_pred = logreg.predict(X_test)
score_noreg = calculate_accuracy(t_pred, t_test)
print(score_noreg)
```

```
Training accuracy
1.0
Test accuracy
0.8783333333333333
```

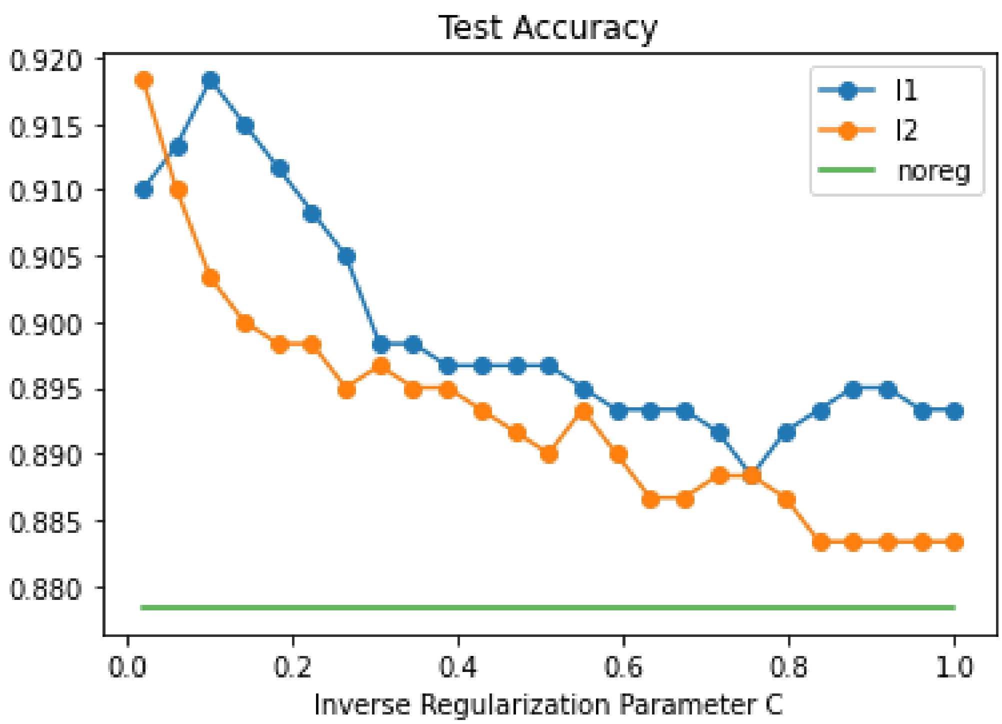
Task 3.2: Logistic Regression with Regularization

1. Set sklearn's penalty parameter to `l1` and `l2`. Use the range `np.linspace(0.02, 1, 25)` for the parameter `C`, which controls the strength of regularization. Where is the regularization strongest, for small or big `C`?
   Hint: For `l1` regularization you can use the `saga` solver.
2. Plot strength of regularization over accuracy. Does regularization improve the scores?
3. Visualize the coefficients (or just a subset of all coefficient for a better overview) of the regularized settings and the unregularized setting. What do you observe?
4. Compare the coefficients to the LDA weights.

[35]:
```python
from matplotlib import pyplot as plt
import random
```

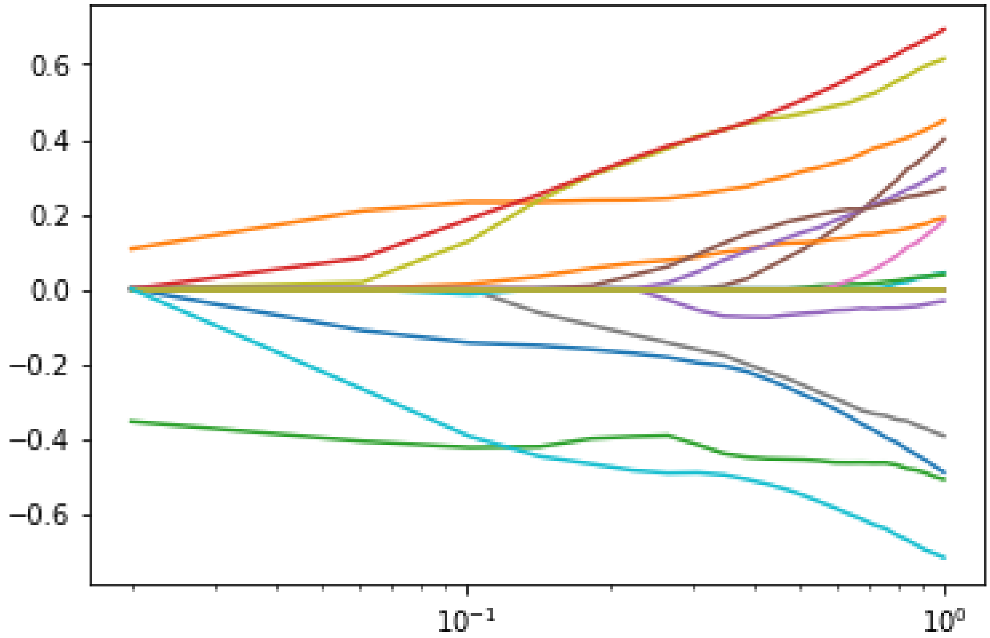
[36]:
```python
C = np.linspace(.02, 1, 25)

logreg_l2 = [LogisticRegression(penalty = 'l2', C = c).fit(X_train, t_train.
 ↪ravel()) for c in C]
t_pred_l2 = [i.predict(X_test) for i in logreg_l2]
scores_l2 = [calculate_accuracy(t_pred, t_test) for t_pred in t_pred_l2]

logreg_l1 = [LogisticRegression(penalty = 'l1', C = c, solver = 'liblinear').
 ↪fit(X_train, t_train.ravel()) for c in C]
t_pred_l1 = [i.predict(X_test) for i in logreg_l1]
scores_l1 = [calculate_accuracy(t_pred, t_test) for t_pred in t_pred_l1]
```

[37]:
```
regplot = [None, None, None]
l1_plot, = plt.plot(np.linspace(0.02, 1, 25), scores_l1, '-o')
l1_plot.set_label('l1')
l2_plot, = plt.plot(np.linspace(0.02, 1, 25), scores_l2, '-o')
l2_plot.set_label('l2')
noreg_plot, = plt.plot(np.linspace(0.02, 1, 25), [score_noreg]*25, '-')
noreg_plot.set_label('noreg')
plt.xlabel('Inverse Regularization Parameter C')
plt.legend()
plt.title('Test Accuracy')
plt.show()
```



[38]:
```
coefs_l1 = np.array([np.array(i.coef_).ravel() for i in logreg_l1])
coefs_l2 = np.array([np.array(i.coef_).ravel() for i in logreg_l2])
```

[39]:
```
# Plot of coefficients vs. alphas
#plt.figure(figsize = (16,10))
for i in random.sample(range(coefs_l1.shape[1]), 20):
        plt.plot(C, coefs_l1.T[i])
plt.xscale('log')
```



[40]:
```
# Plot of coefficients vs. alphas
#plt.figure(figsize = (16,10))
for i in random.sample(range(coefs_l2.shape[1]), 20):
        plt.plot(C, coefs_l2.T[i])
plt.xscale('log')
```