APA-L2-python

September 6, 2018

1 APA Laboratori 2 - Visualitzacio

In [1]:
```
# Uncomment to upgrade packages
# !pip install pandas --upgrade
# !pip install numpy --upgrade
# !pip install scipy --upgrade
# !pip install statsmodels --upgrade
# !pip install scikit-learn --upgrade
%load_ext autoreload
```

In [2]:
```
#%matplotlib notebook
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sn
import pandas as pd
from IPython.core.interactiveshell import InteractiveShell
InteractiveShell.ast_node_interactivity = "all"
pd.set_option('precision', 3)
```

In [3]:
```
# extra imports
from numpy.linalg import eig
from numpy.random import multivariate_normal
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler
from pandas import read_csv
from pandas.plotting import scatter_matrix
from mpl_toolkits.mplot3d import Axes3D
```

In [4]:
```
np.random.seed(222)
```

1.1 Example 1: Comparison between PCA and LDA on 2D toy data

Fisher's discriminant analysis (FDA) is a method that finds a linear combination of features to project or separate two or more classes of objects

If your goal is to perform (linear) dimensionality reduction for class discrimination, you should use FDA instead of PCA; PCA is useful for signal representation (but not necessarily for discrimination)

Sigma is a 2x2 positive-definite symmetric matrix specifying the covariance matrix of two variables

```
In [5]: N= 200

        Sigma = np.array(((2,1.3),(1.3,1)))
        Sigma

Out[5]: array([[2. , 1.3],
               [1.3, 1. ]])
```

these are the eigenvalues:

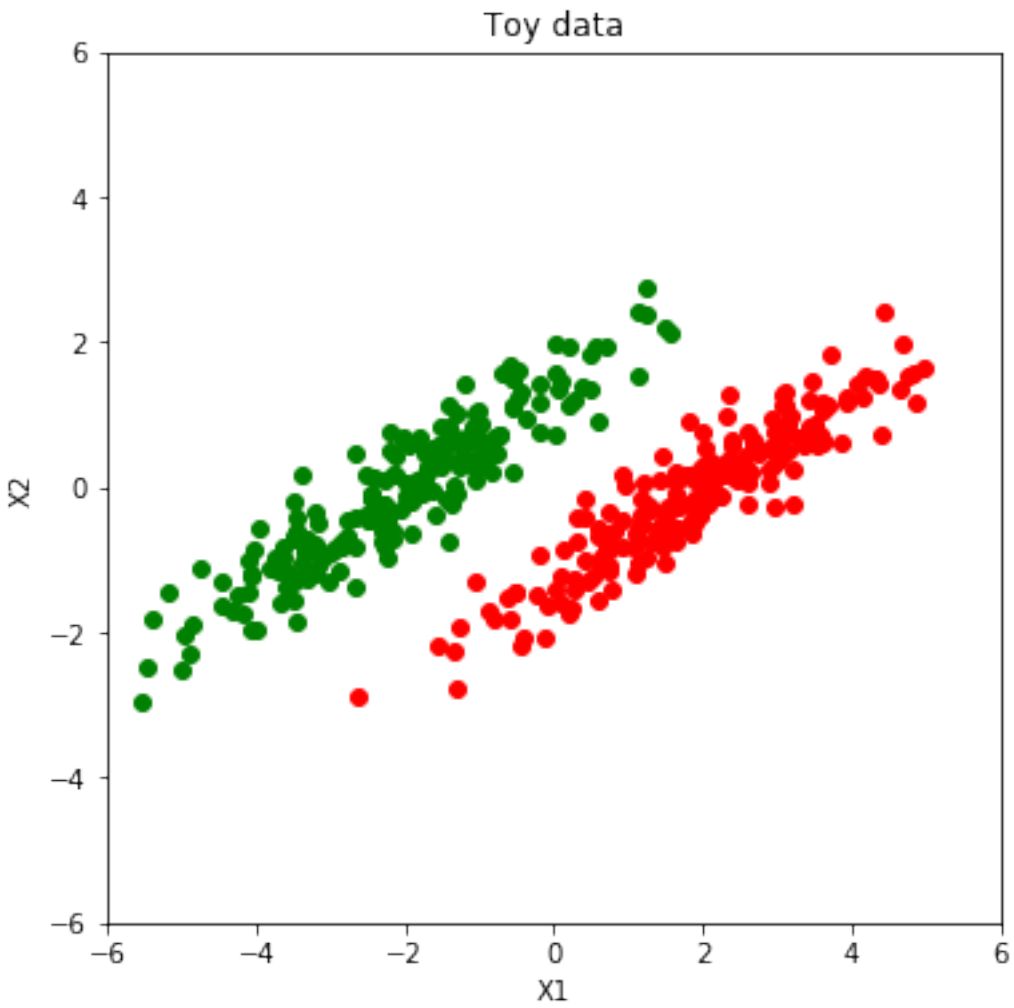
```
In [6]: eig(Sigma)[0]

Out[6]: array([2.89283883, 0.10716117])
```

Let's create class 1 ('red' class)

```
In [7]: mean_1 = np.array((2,0))

        X_red = multivariate_normal(mean_1,Sigma,N)
```

Let's create class 2 ('green' class)

```
In [8]: mean_2 = -mean_1

        X_green = multivariate_normal(mean_2,Sigma,N)

        fig, ax = plt.subplots(figsize=(6,6))
        plt.plot(X_red[:,0],X_red[:,1],'ro',X_green[:,0],X_green[:,1],'go')
        ax.set_xlim([-6,6])
        ax.set_ylim([-6,6])
        ax.set_xlabel("X1")
        ax.set_ylabel("X2")
        plt.title("Toy data");
```



Now we glue both classes one after the other and create a dataframe

```
In [9]: d= pd.DataFrame({'Target':['red']*N + ['green']*N,
                         'X1': np.hstack((X_red[:,0], X_green[:,0])),
                         'X2':np.hstack((X_red[:,1], X_green[:,1]))})
        d.describe(include='all')
```

Out[9]:

	Target	X1	X2
count	400	400.000	400.000
unique	2	NaN	NaN
top	green	NaN	NaN
freq	200	NaN	NaN
mean	NaN	-0.068	-0.051
std	NaN	2.450	1.026
min	NaN	-5.530	-2.938
25%	NaN	-1.974	-0.799
50%	NaN	0.032	0.039

```
        75%        NaN    1.900    0.670
        max        NaN    4.974    2.762
```

call to FDA (also known as LDA, because it is linear)

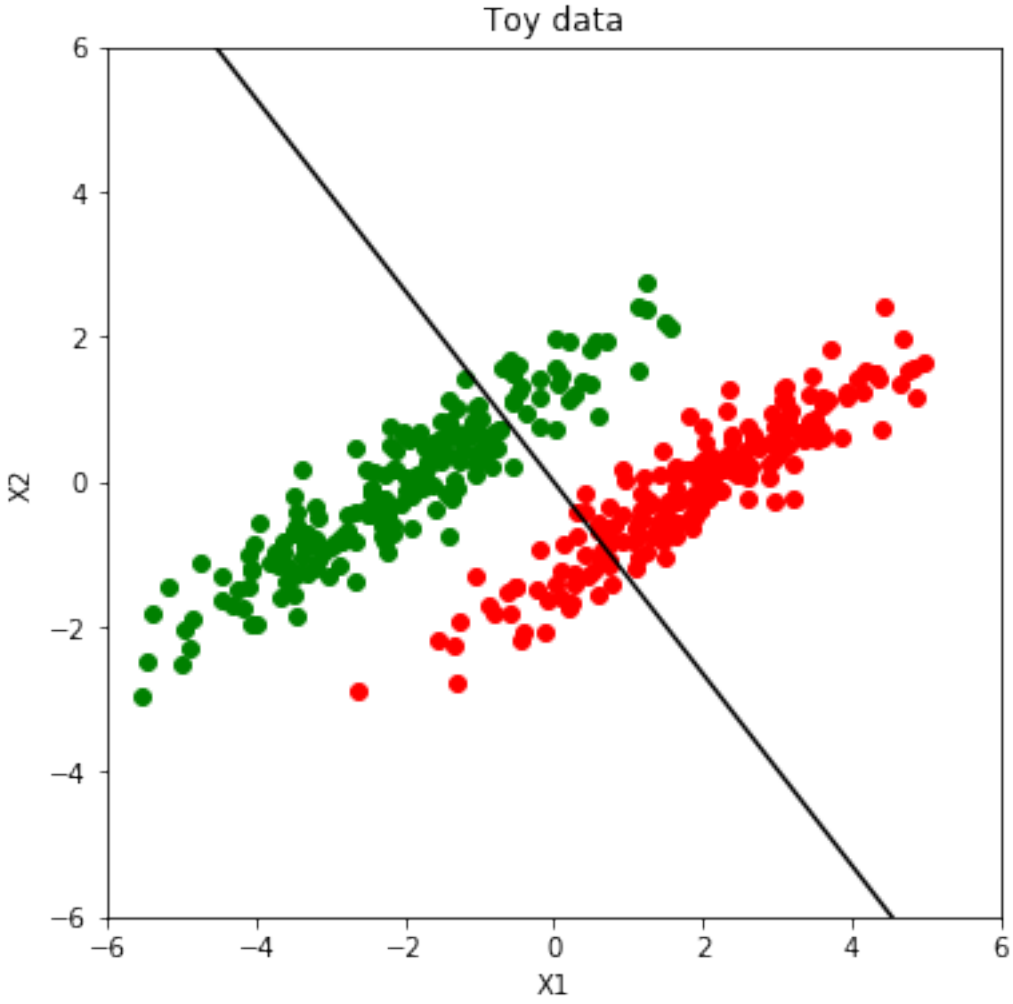
```
In [10]: myLDA = LinearDiscriminantAnalysis()

         myLDA.fit(d[['X1','X2']], d['Target'])

         print('Priors:')
         pd.DataFrame(myLDA.priors_)
         print('Means:')
         pd.DataFrame(myLDA.means_)
         print('Coefs:')
         pd.DataFrame(myLDA.coef_)

Out[10]: LinearDiscriminantAnalysis(n_components=None, priors=None, shrinkage=None,
                       solver='svd', store_covariance=False, tol=0.0001)

Priors:


Out[10]:      0
         0  0.5
         1  0.5

Means:


Out[10]:        0      1
         0 -2.034 -0.021
         1  1.898 -0.081

Coefs:


Out[10]:          0      1
         0  12.997 -17.17
```

Now we show the best projection direction on the original space. This direction maximizes the separability of the classes. For that, we first need the slope:

```
In [11]: LDAslope = myLDA.scalings_[1]/myLDA.scalings_[0]
         LDAslope

Out[11]: array([-1.32109019])
```

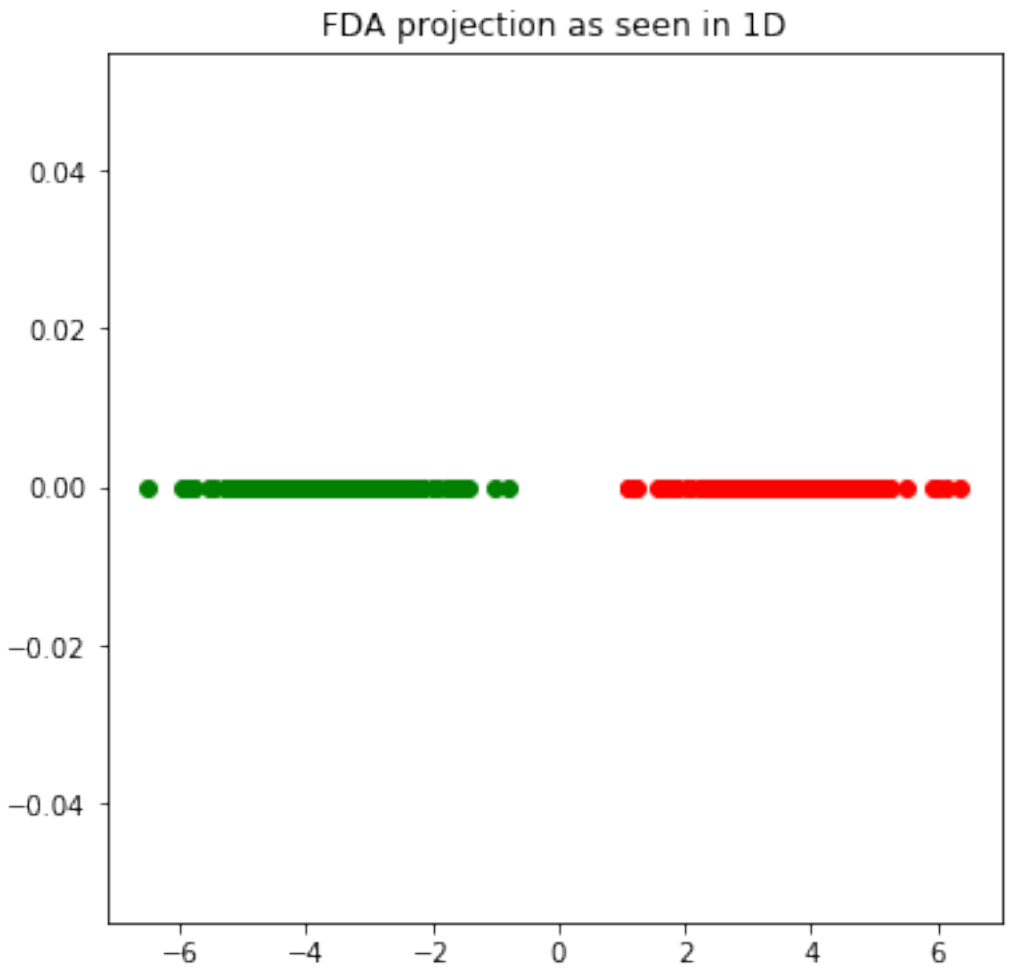
And now we can perform the visualization:

```
In [12]: fig, ax = plt.subplots(figsize=(6,6))
         plt.plot(X_red[:,0],X_red[:,1],'ro',X_green[:,0],X_green[:,1],'go')
         plt.plot(np.linspace(-6,6), LDAslope*np.linspace(-6,6),c='k')
         ax.set_xlim([-6,6])
         ax.set_ylim([-6,6])
         ax.set_xlabel("X1")
         ax.set_ylabel("X2")
         plt.title("Toy data");
```



We can also compute the projections of the two classes

```
In [13]: myLDA_proj = d['X1'] * myLDA.scalings_[0] + d['X2'] * myLDA.scalings_[1]

         fig, ax = plt.subplots(figsize=(6,6))
         plt.plot(myLDA_proj[:N], [0]*N, 'ro' , myLDA_proj[N:], [0]*N, 'go')
         plt.title('FDA projection as seen in 1D')
         ax.set_xlabel=('Discriminant');
```



To understand what is going on, do:

```
In [14]: print('Priors:')
         pd.DataFrame(myLDA.priors_)
         print('Means:')
         pd.DataFrame(myLDA.means_)
         print('Coefs:')
         pd.DataFrame(myLDA.coef_)
```

```
Priors:
```

```
Out[14]:      0
         0  0.5
         1  0.5
```

```
Means:
```

```
Out[14]:        0      1
         0 -2.034 -0.021
         1  1.898 -0.081
```

Coefs:

```
Out[14]:         0      1
         0  12.997 -17.17
```

of which ...

```
In [15]: print('Scalings:')
         pd.DataFrame(myLDA.scalings_)
```

Scalings:

```
Out[15]:        0
         0  1.800
         1 -2.378
```

... are the coefficients of the linear discriminant
So we are projecting the data into the direction that maximizes (linear) separability:
`projection(X) = X1*myLDA.scalings_[0] + X2*myLDA.scalings[1]`

Now we compute PCA:

```
In [16]: myPCA = PCA(whiten=True)
         myPCA.fit(StandardScaler().fit_transform(d[['X1','X2']]));
```

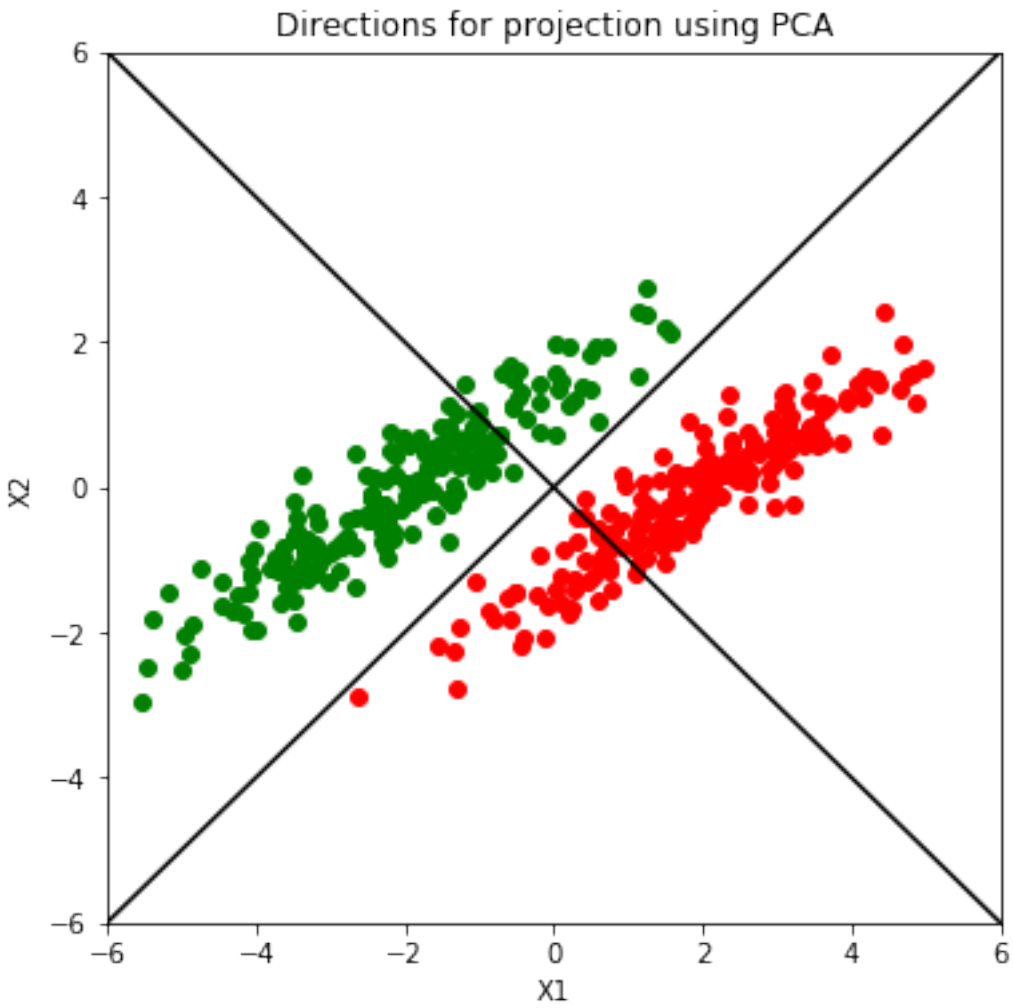
Now we need to project the data in the first principal component

```
In [17]: PCAslope1 = myPCA.components_[1,0]/myPCA.components_[0,0]
         PCAslope2 = myPCA.components_[1,1]/myPCA.components_[0,1]
         PCAslope1
         PCAslope2
```

```
Out[17]: 0.9999999999999993
```

```
Out[17]: -1.0000000000000007
```

```
In [18]: fig, ax = plt.subplots(figsize=(6,6))
         plt.plot(X_red[:,0],X_red[:,1],'ro',X_green[:,0],X_green[:,1],'go')
         plt.plot(np.linspace(-6,6), PCAslope1*np.linspace(-6,6),c='k')
         plt.plot(np.linspace(-6,6), PCAslope2*np.linspace(-6,6),c='k')
         ax.set_xlim([-6,6])
         ax.set_ylim([-6,6])
         ax.set_xlabel("X1")
         ax.set_ylabel("X2")
         plt.title("Directions for projection using PCA");
```



We can see that the FDA projection maximices separability while the PCA projection maximices variability

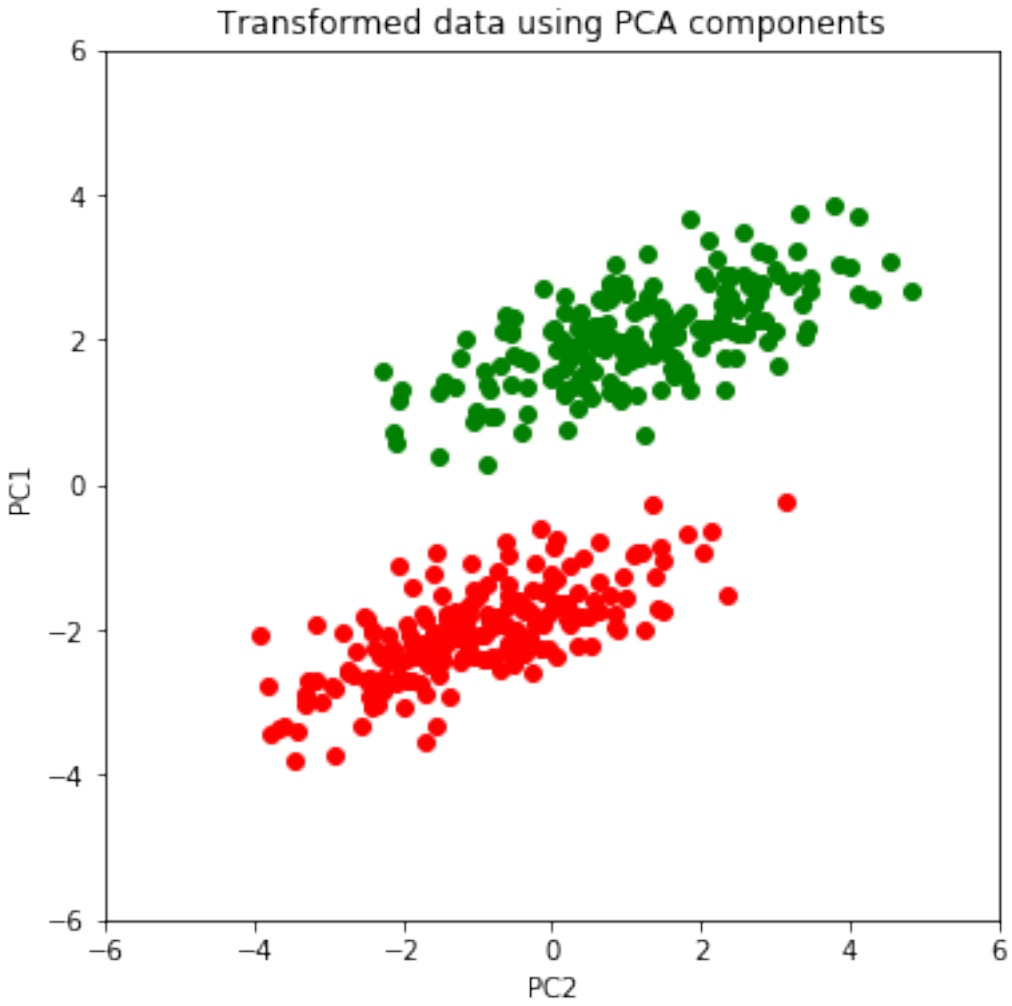
The rotation matrix allows to transform the data to an ortogonal space

```
In [19]: pd.DataFrame(myPCA.components_)

Out[19]:        0      1
         0 -0.707 -0.707
         1 -0.707  0.707
```

If we apply the rotation matrix to the data we obtain a new dataset where most of the variance is held by the first components

```
In [20]: tr_data = myPCA.transform(d[['X1','X2']])

         fig, ax = plt.subplots(figsize=(6,6))
         plt.plot(tr_data[:N,0],tr_data[:N,1],'ro',
```

```
        tr_data[N:,0],tr_data[N:,1],'go')
ax.set_xlim([-6,6])
ax.set_ylim([-6,6])
ax.set_xlabel("PC2")
ax.set_ylabel("PC1")
plt.title("Transformed data using PCA components");
```



1.2 Example 2: Visualizing crabs with FDA

Campbell studied rock crabs of the genus "Leptograpsus" in 1974. One species, Leptograpsus variegatus, had been split into two new species, previously grouped by colour (orange and blue). Preserved specimens lose their colour, so it was hoped that morphological differences would enable museum material to be classified.

Data is available on 50 specimens of each sex of each species (so 200 in total), collected on sight at Fremantle, Western Australia. Each specimen has measurements on: the width of the frontal lobe (FL), the rear width (RW), the length along the carapace midline (CL), the maximum width

(CW) of the carapace, and the body depth (BD) in mm, in addition to colour (that is, species) and sex.

```
In [21]: crabs_data= read_csv("crabs.csv", header=0)
         crabs_data.describe(include='all')
         crabs_data.head()
```

Out[21]:

	sp	sex	index	FL	RW	CL	CW	BD
count	200	200	200.000	200.000	200.000	200.000	200.000	200.000
unique	2	2	NaN	NaN	NaN	NaN	NaN	NaN
top	B	M	NaN	NaN	NaN	NaN	NaN	NaN
freq	100	100	NaN	NaN	NaN	NaN	NaN	NaN
mean	NaN	NaN	25.500	15.583	12.738	32.105	36.415	14.030
std	NaN	NaN	14.467	3.495	2.573	7.119	7.872	3.425
min	NaN	NaN	1.000	7.200	6.500	14.700	17.100	6.100
25%	NaN	NaN	13.000	12.900	11.000	27.275	31.500	11.400
50%	NaN	NaN	25.500	15.550	12.800	32.100	36.800	13.900
75%	NaN	NaN	38.000	18.050	14.300	37.225	42.000	16.600
max	NaN	NaN	50.000	23.100	20.200	47.600	54.600	21.600

Out[21]:

	sp	sex	index	FL	RW	CL	CW	BD
0	B	M	1	8.1	6.7	16.1	19.0	7.0
1	B	M	2	8.8	7.7	18.1	20.8	7.4
2	B	M	3	9.2	7.8	19.0	22.4	7.7
3	B	M	4	9.6	7.9	20.1	23.1	8.2
4	B	M	5	9.8	8.0	20.3	23.0	8.2

The goal is to separate the 200 crabs into four classes, given by the 2x2 configurations for sex (Male/Female) and species (Blue/Orange)

```
In [22]: crabs_data['Class'] =  crabs_data.sp + crabs_data.sex
```

Now 'BF' stands now for 'Blue Female', and so on

```
In [23]: crabs_data.groupby('Class').size()
```

```
Out[23]: Class
         BF    50
         BM    50
         OF    50
         OM    50
         dtype: int64
```

using the rest of the variables as predictors (except 'index', which is only an index)

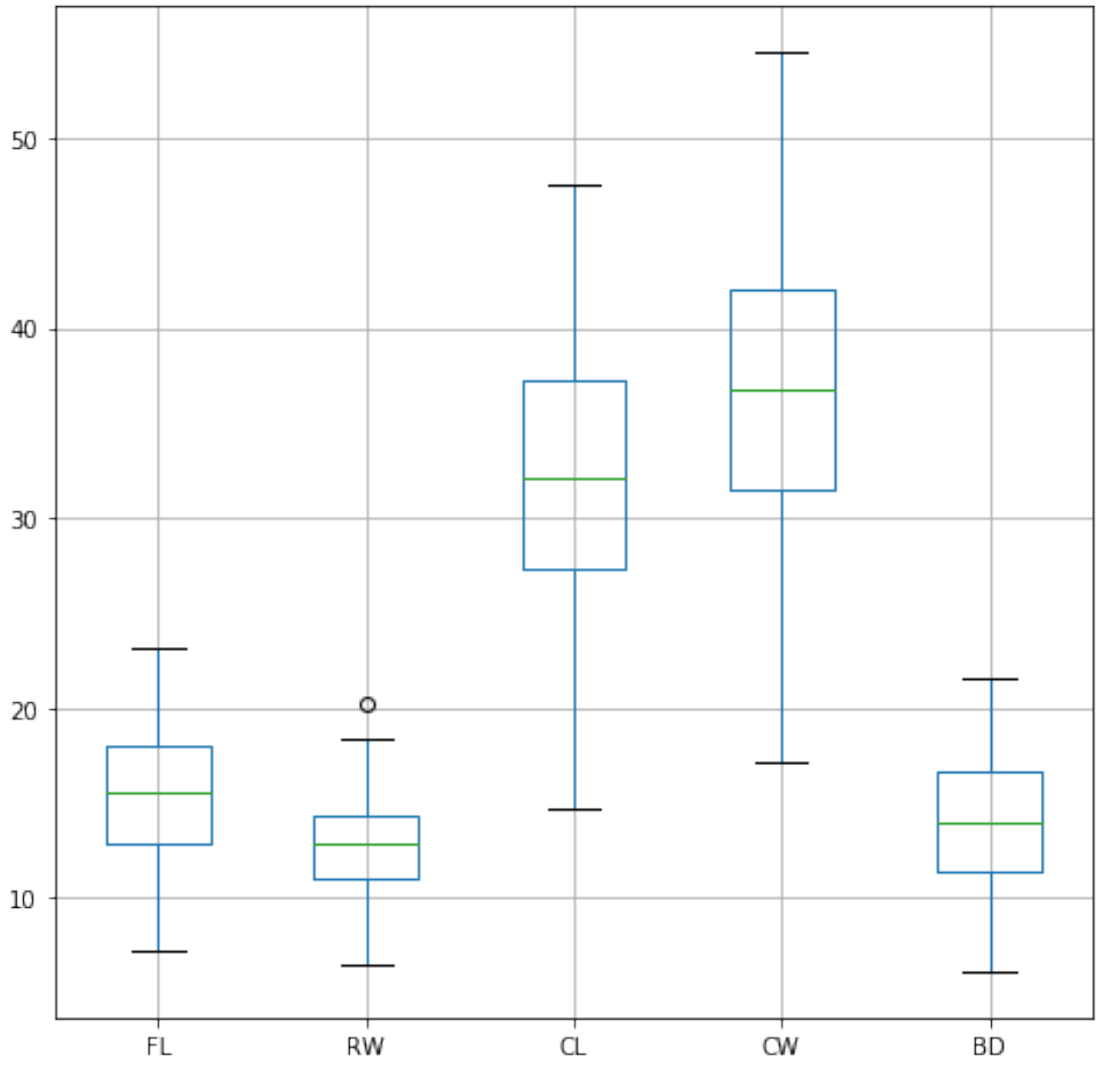
```
In [24]: crabs_sel = crabs_data[['FL', 'RW','CL','CW','BD']]
         crabs_sel.describe()
```

Out[24]:

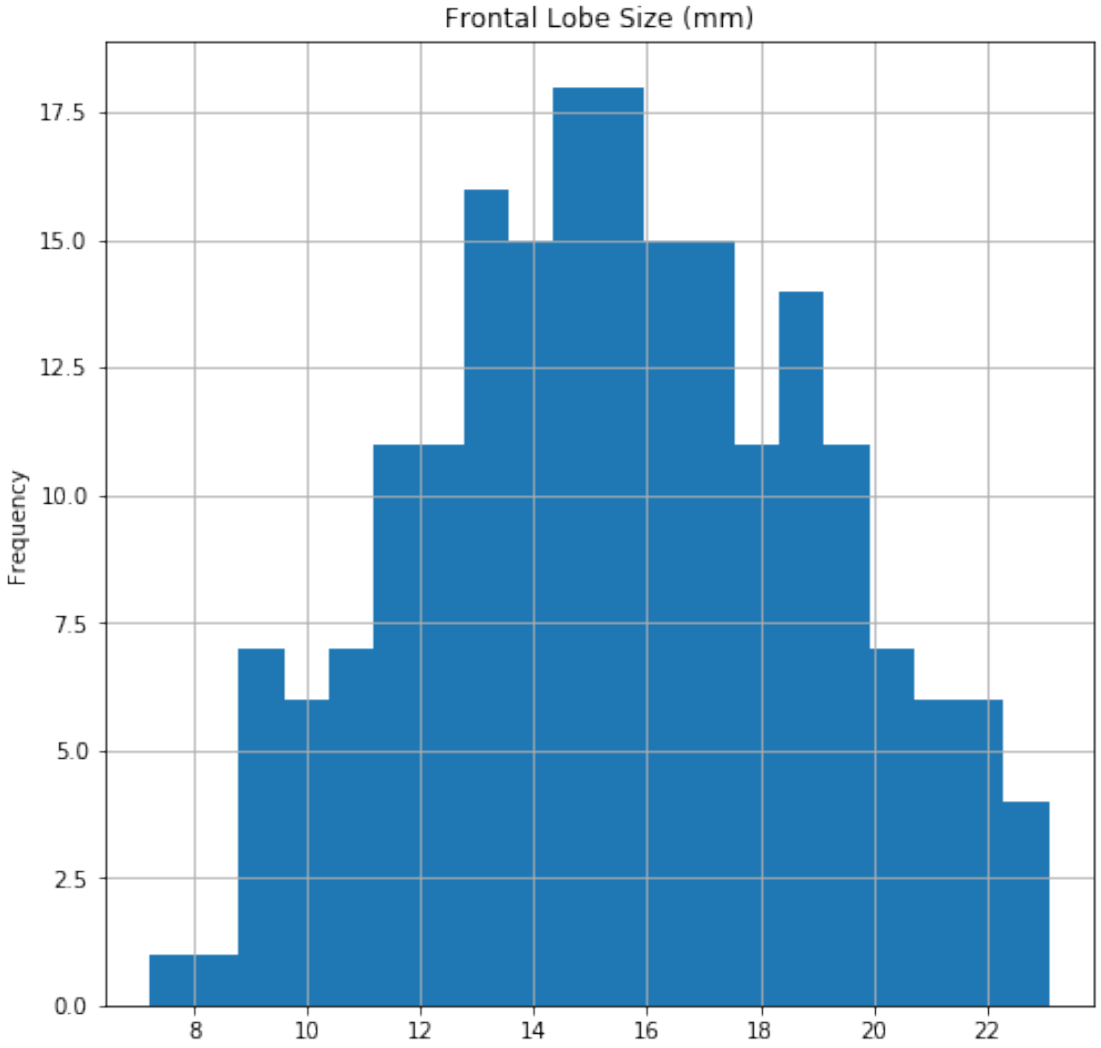
	FL	RW	CL	CW	BD
count	200.000	200.000	200.000	200.000	200.000
mean	15.583	12.738	32.105	36.415	14.030
std	3.495	2.573	7.119	7.872	3.425
min	7.200	6.500	14.700	17.100	6.100
25%	12.900	11.000	27.275	31.500	11.400
50%	15.550	12.800	32.100	36.800	13.900
75%	18.050	14.300	37.225	42.000	16.600
max	23.100	20.200	47.600	54.600	21.600

Various preliminary plots (notice all 5 predictors are continuous)

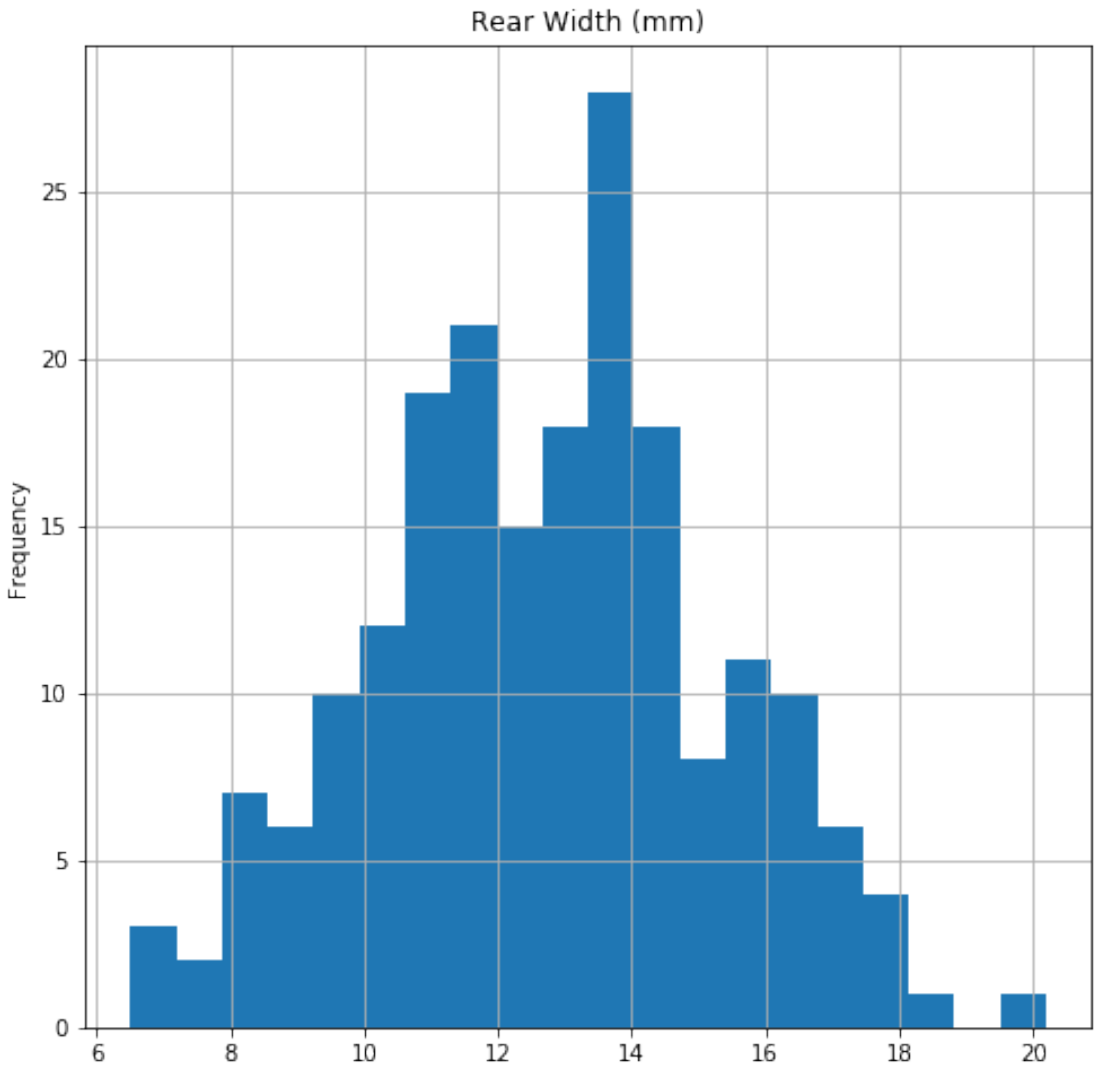
In [25]:
```
fig, ax = plt.subplots(figsize=(8,8))
crabs_sel.boxplot();
```



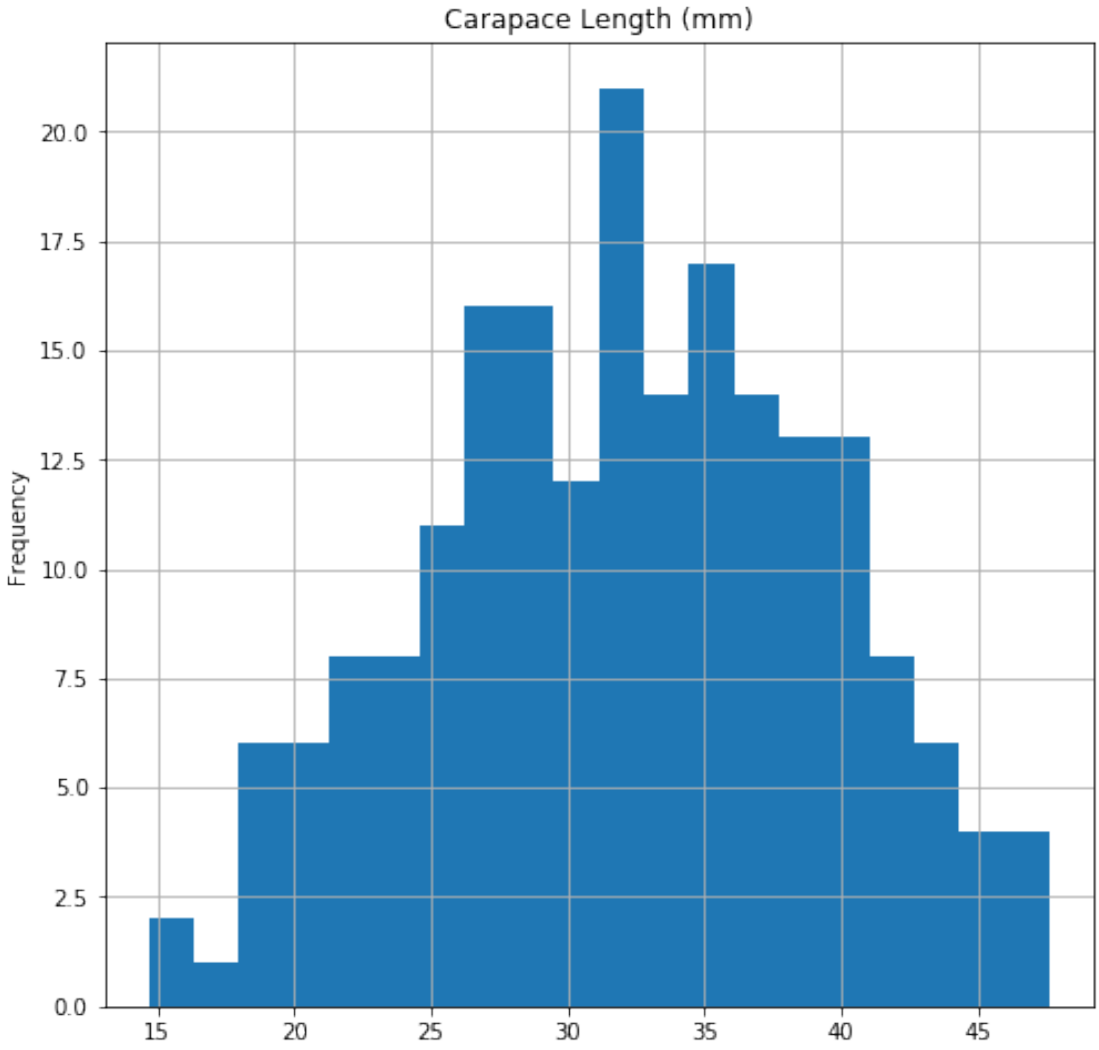
In [26]:
```
fig, ax = plt.subplots(figsize=(8,8))
plt.title('Frontal Lobe Size (mm)')
ax.set_ylabel('Frequency')
crabs_sel.FL.hist(bins=20);
```



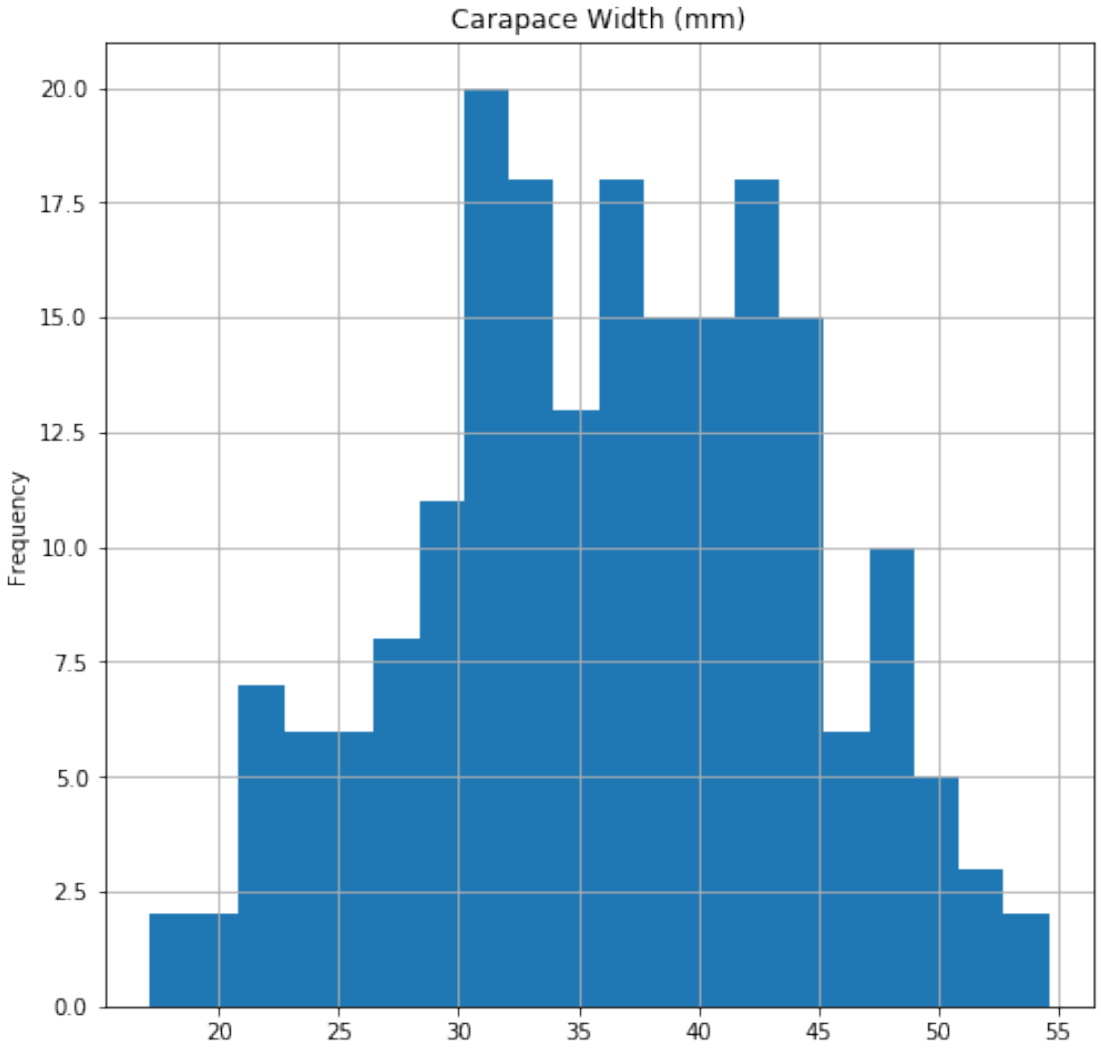
In [27]:
```
fig, ax = plt.subplots(figsize=(8,8))
plt.title('Rear Width (mm)')
ax.set_ylabel('Frequency')
crabs_sel.RW.hist(bins=20);
```



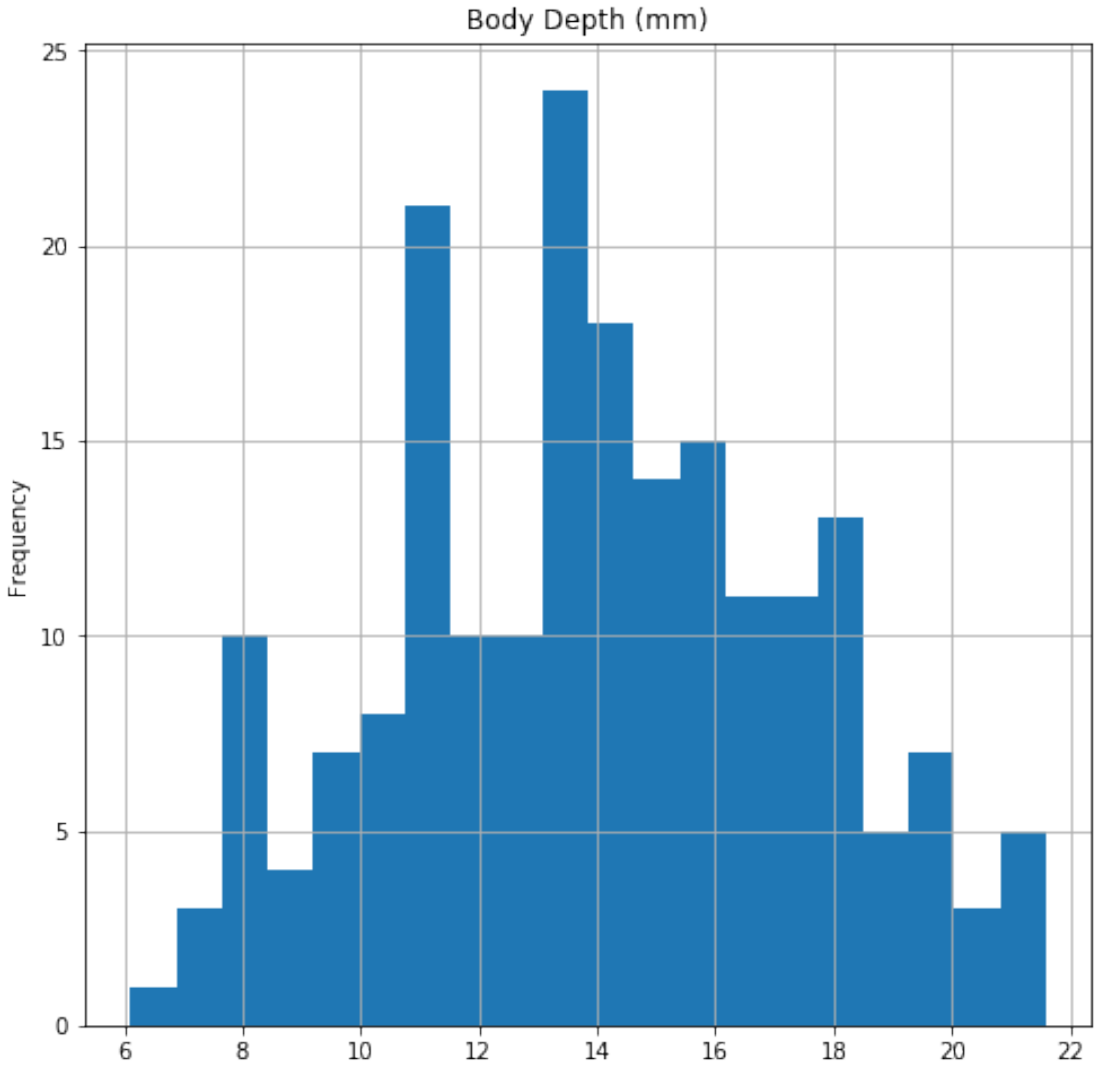

```
In [28]: fig, ax = plt.subplots(figsize=(8,8))
         plt.title('Carapace Length (mm)')
         ax.set_ylabel('Frequency')
         crabs_sel.CL.hist(bins=20);
```




```
In [29]: fig, ax = plt.subplots(figsize=(8,8))
         plt.title('Carapace Width (mm)')
         ax.set_ylabel('Frequency')
         crabs_sel.CW.hist(bins=20);
```




```
In [30]: fig, ax = plt.subplots(figsize=(8,8))
         plt.title('Body Depth (mm)')
         ax.set_ylabel('Frequency')
         crabs_sel.BD.hist(bins=20);
```



Now let's visualize data using FDA

```
In [31]: lda_model = LinearDiscriminantAnalysis()

         crabs_trans = pd.DataFrame(lda_model.fit_transform(crabs_sel, crabs_data.Class))
         crabs_trans.columns=['LD1', 'LD2', 'LD3']

         print('Priors:')
         pd.DataFrame(lda_model.priors_)
         print('Means:')
         pd.DataFrame(lda_model.means_)
         print('Coefs:')
         pd.DataFrame(lda_model.coef_)
         print('Explained Variance Ratio')
         pd.DataFrame(lda_model.explained_variance_ratio_ )
```

```
Priors:
```

Out[31]:
	0
0	0.25
1	0.25
2	0.25
3	0.25

```
Means:
```

Out[31]:
	0	1	2	3	4
0	13.270	12.138	28.102	32.624	11.816
1	14.842	11.718	32.014	36.810	13.350
2	17.594	14.836	34.618	39.036	15.632
3	16.626	12.262	33.688	37.188	15.324

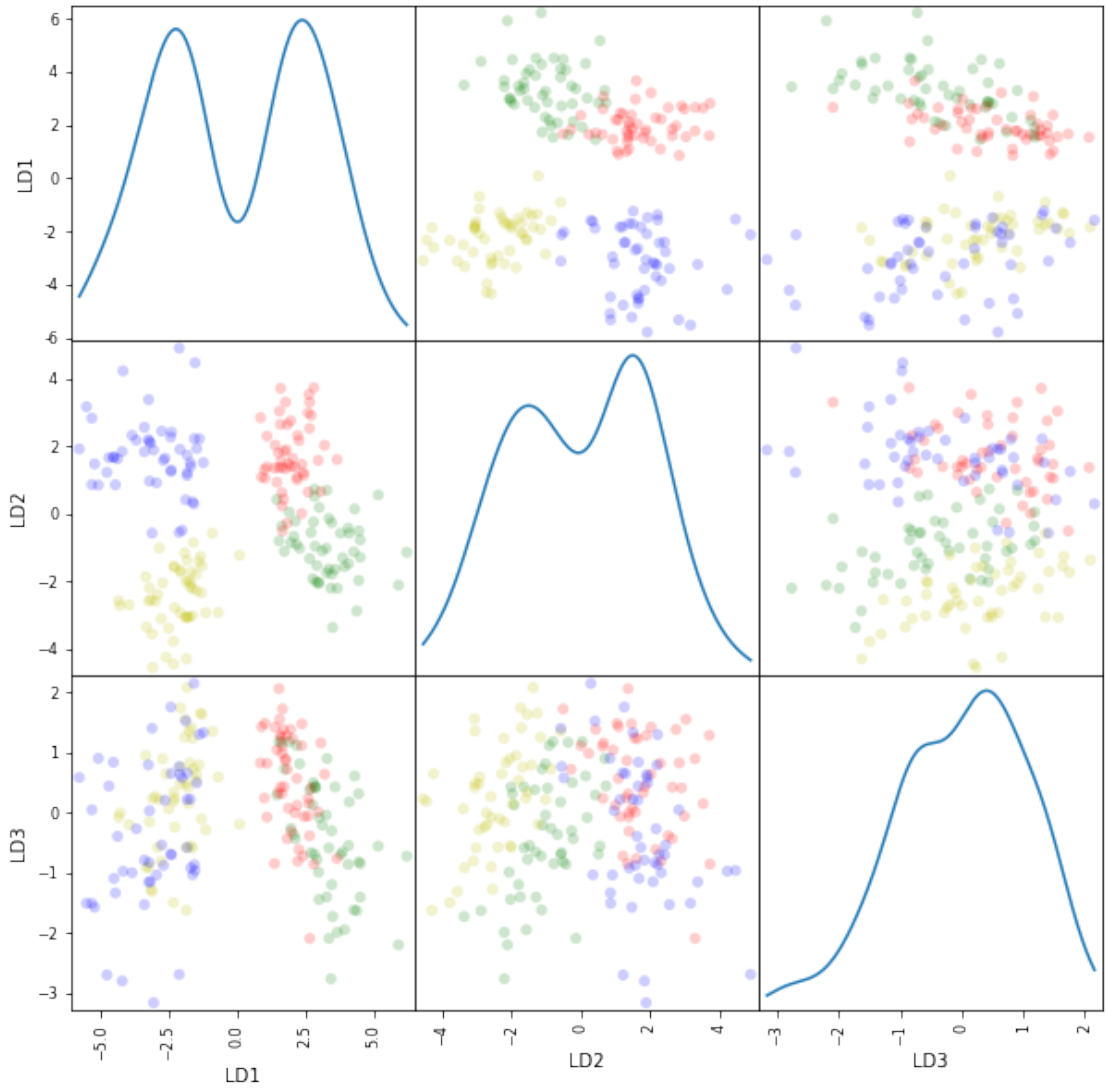
```
Coefs:
```

Out[31]:
	0	1	2	3	4
0	-3.556	1.623	-1.912	3.777	-2.930
1	-4.659	-3.829	0.192	4.673	-4.538
2	5.734	4.448	-1.547	-3.367	2.874
3	2.482	-2.243	3.267	-5.083	4.594

```
Explained Variance Ratio
```

Out[31]:
	0
0	0.686
1	0.300
2	0.014

In [32]:
```
colors_crabs = {'BF':'r', 'BM':'g', 'OF':'b', 'OM':'y'}

scatter_matrix(crabs_trans,
               alpha=0.2,
               figsize=(10, 10),
               diagonal='kde',
               marker='o',
               c=crabs_data.Class.apply(lambda x: colors_crabs[x]));
```



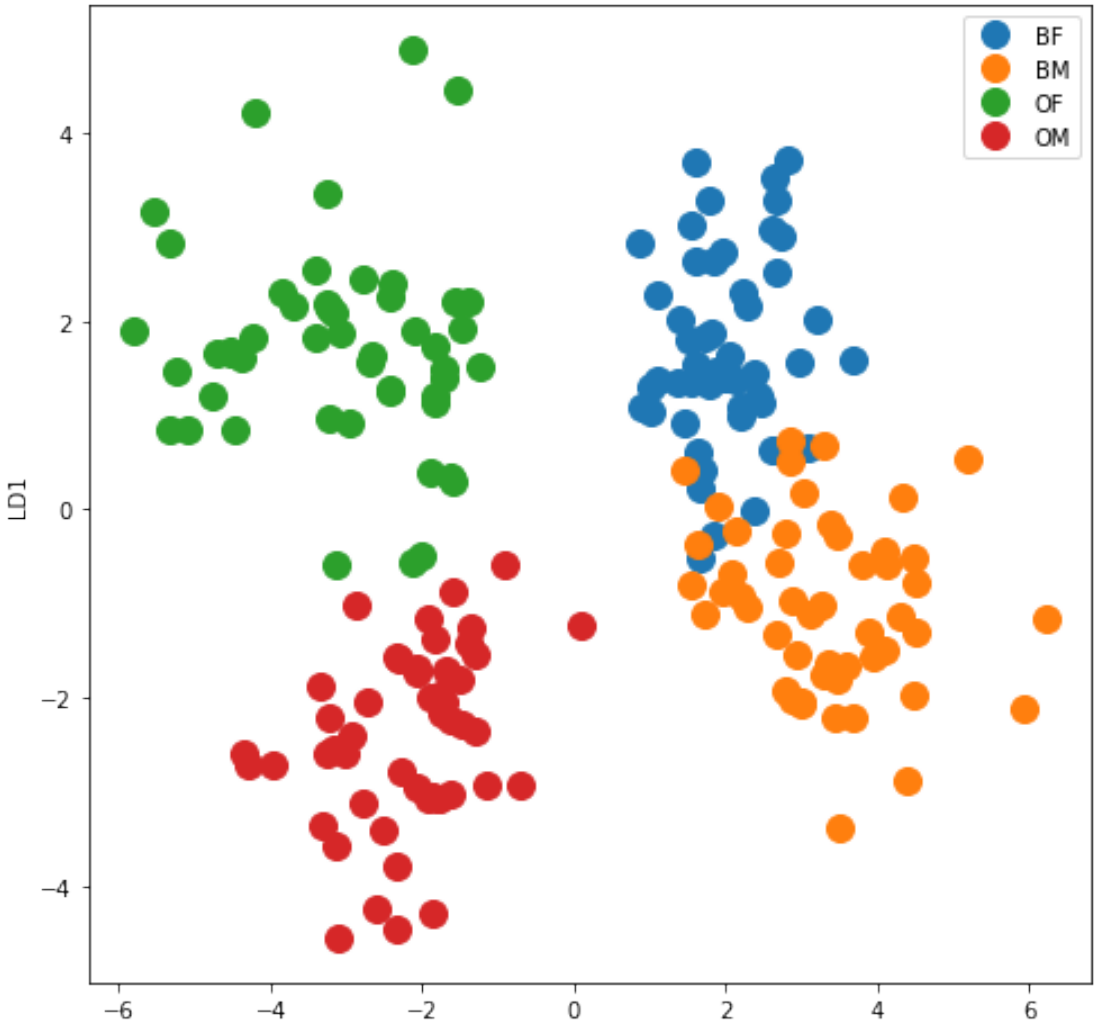
As there are four classes (called 'groups' in LDA), we get three linear discriminants (LDs) for projection (always the number of classes minus 1)

We are performing dimensionality reduction 5D --> 3D, and plotting the projected data into the first two LDs (the 2 most important dimensions)

We do our own plotting method, with color and legend:

```
In [33]: crabs_trans['Class'] = crabs_data.Class
         groups = crabs_trans.groupby('Class')

         fig, ax = plt.subplots(figsize=(8,8))
         for name, group in groups:
             ax.plot(group.LD1,
                     group.LD2,
                     marker='o',
```

```
                linestyle='',
                ms=12,
                label=name)
ax.legend()
ax.set_ylabel('LD2')
ax.set_ylabel('LD1');
```



The result is quite satisfactory, right? We can see that the 5 continuous predictors do indeed represent 4 different crabs.

We can also see that crabs of the Blue "variety" are less different (regarding males and females) than those in the Orange variety

```
In [34]: crabs_trans.describe()
```

```
Out[34]:              LD1          LD2          LD3
         count  2.000e+02    2.000e+02    2.000e+02
```

```
mean   6.102e-15  8.633e-15 -6.173e-15
std    2.896e+00  2.053e+00  1.068e+00
min   -5.795e+00 -4.557e+00 -3.168e+00
25%   -2.356e+00 -1.691e+00 -7.675e-01
50%    4.740e-01  1.571e-01  1.394e-01
75%    2.606e+00  1.623e+00  7.960e-01
max    6.228e+00  4.899e+00  2.155e+00
```

Now let's analyze the numerical output of lda() in more detail:

```
In [35]: print('Priors:')
         pd.DataFrame(lda_model.priors_)
         print('Means:')
         pd.DataFrame(lda_model.means_)
         print('Coefs:')
         pd.DataFrame(lda_model.scalings_)
         print('Explained Variance Ratio')
         pd.DataFrame(lda_model.explained_variance_ratio_ )
```

```
Priors:


Out[35]:      0
         0  0.25
         1  0.25
         2  0.25
         3  0.25

Means:


Out[35]:         0       1       2       3       4
         0  13.270  12.138  28.102  32.624  11.816
         1  14.842  11.718  32.014  36.810  13.350
         2  17.594  14.836  34.618  39.036  15.632
         3  16.626  12.262  33.688  37.188  15.324

Coefs:


Out[35]:        0      1      2
         0 -1.554  0.195 -1.667
         1 -0.625  1.539  0.456
         2 -0.188 -1.095  0.681
         3  1.516  0.644 -0.655
         4 -1.355 -0.515  1.286

Explained Variance Ratio
```

```
Out[35]:        0
         0  0.686
         1  0.300
         2  0.014
```

"Prior probabilities of groups" is self-explanatory (these are estimated from the data, but can be overriden by the 'prior' parameter)

"Group means" is also self-explanatory (these are our mu's)

"Coefficients of linear discriminants" are the scaling factors we have been using to project data. These have been normalized so that the within-groups covariance matrix is spherical (a multiple of the identity).

This means that the larger the coefficient of a predictor, the more important the predictor is for the discrimination:

```
In [36]: coefs = pd.DataFrame(lda_model.scalings_)
         coefs.columns=['LD1', 'LD2', 'LD3']
         coefs.index=['FL', 'RW','CL','CW','BD']
         coefs
```

```
Out[36]:       LD1    LD2    LD3
         FL -1.554  0.195 -1.667
         RW -0.625  1.539  0.456
         CL -0.188 -1.095  0.681
         CW  1.516  0.644 -0.655
         BD -1.355 -0.515  1.286
```

We can interpret our plot so that the horizontal axis (LD1) separates the groups mainly by using FL, CW and BD; the vertical axis (LD2) separates the groups mainly by using RW and some CL, etc

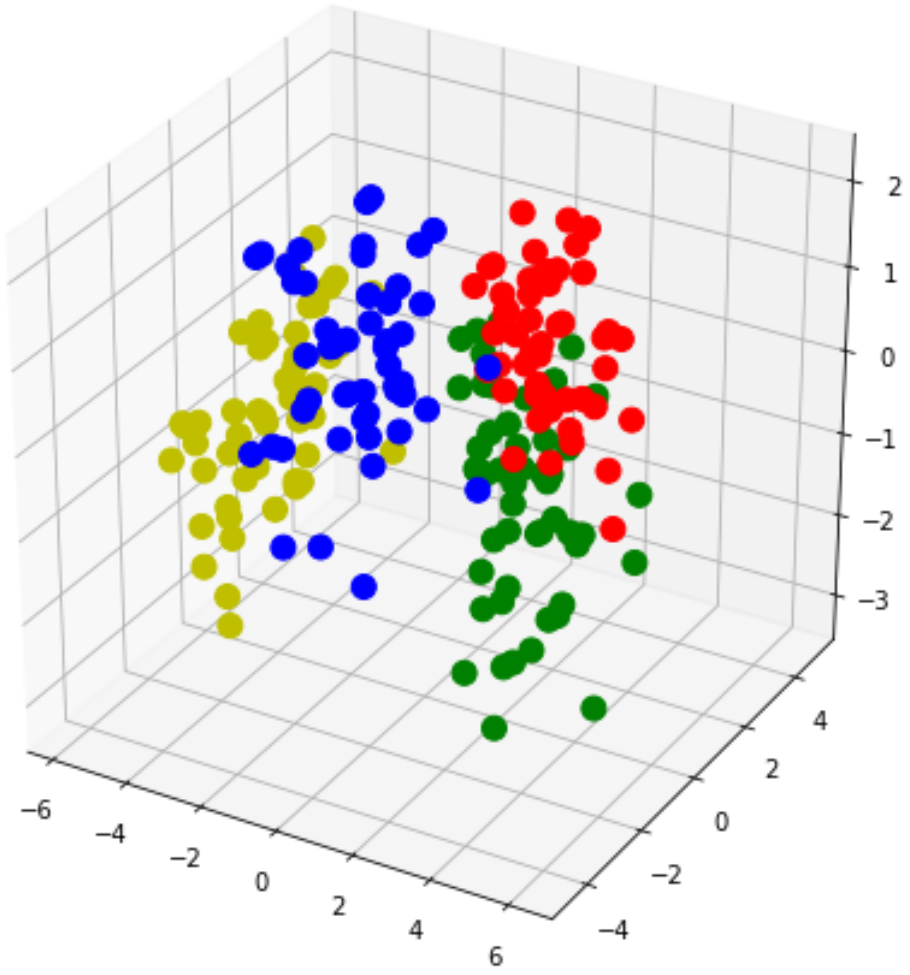
The "Proportion of trace" is the proportion of between-class variance that is explained by successive discriminants (LDs)

For instance, in our case LD1 explains 68.6% of the total between-class variance

In this case, the first two LDs account for 98.56% of total between-class variance, fairly close to 100%

This means that the third dimension adds but a little bit of discriminatory information. Let's visualize the crabs in 3D:

```
In [37]: fig = plt.figure(figsize=(8,8))
         ax = fig.add_subplot(111, projection='3d')

         plt.scatter(crabs_trans.LD1,
                     crabs_trans.LD2,
                     zs=crabs_trans.LD3,
                     depthshade=False,
                     c=crabs_trans.Class.apply(lambda x: colors_crabs[x]), s=100);
```



As the measurements are lengths, it could be sensible to take logarithms

```
In [38]: lda_logmodel = LinearDiscriminantAnalysis()

         crabs_logtrans = pd.DataFrame(lda_logmodel.fit_transform(np.log(crabs_sel), crabs_data.
         crabs_logtrans.columns=['LD1', 'LD2', 'LD3']

In [39]: print('Priors:')
         pd.DataFrame(lda_logmodel.priors_)
         print('Means:')
         pd.DataFrame(lda_logmodel.means_)
         print('Coefs:')
         pd.DataFrame(lda_logmodel.scalings_)
         print('Explained Variance Ratio')
         pd.DataFrame(lda_logmodel.explained_variance_ratio_ )
```

```
Priors:


Out[39]:       0
         0  0.25
         1  0.25
         2  0.25
         3  0.25

Means:


Out[39]:        0      1      2      3      4
         0  2.565  2.475  3.313  3.462  2.441
         1  2.673  2.444  3.438  3.578  2.561
         2  2.852  2.684  3.529  3.650  2.733
         3  2.788  2.490  3.490  3.589  2.702

Coefs:


Out[39]:         0       1       2
         0 -31.217   2.851 -25.720
         1  -9.485  24.653   6.067
         2  -9.822 -38.579  31.679
         3  65.950  21.376 -30.600
         4 -17.998  -6.002  14.541

Explained Variance Ratio


Out[39]:        0
         0  0.689
         1  0.302
         2  0.009
```

The model looks a bit better, given that he first two LDs now account for 99.09% of total between-class variance, very good indeed, so a 3D plot does not add anything visual

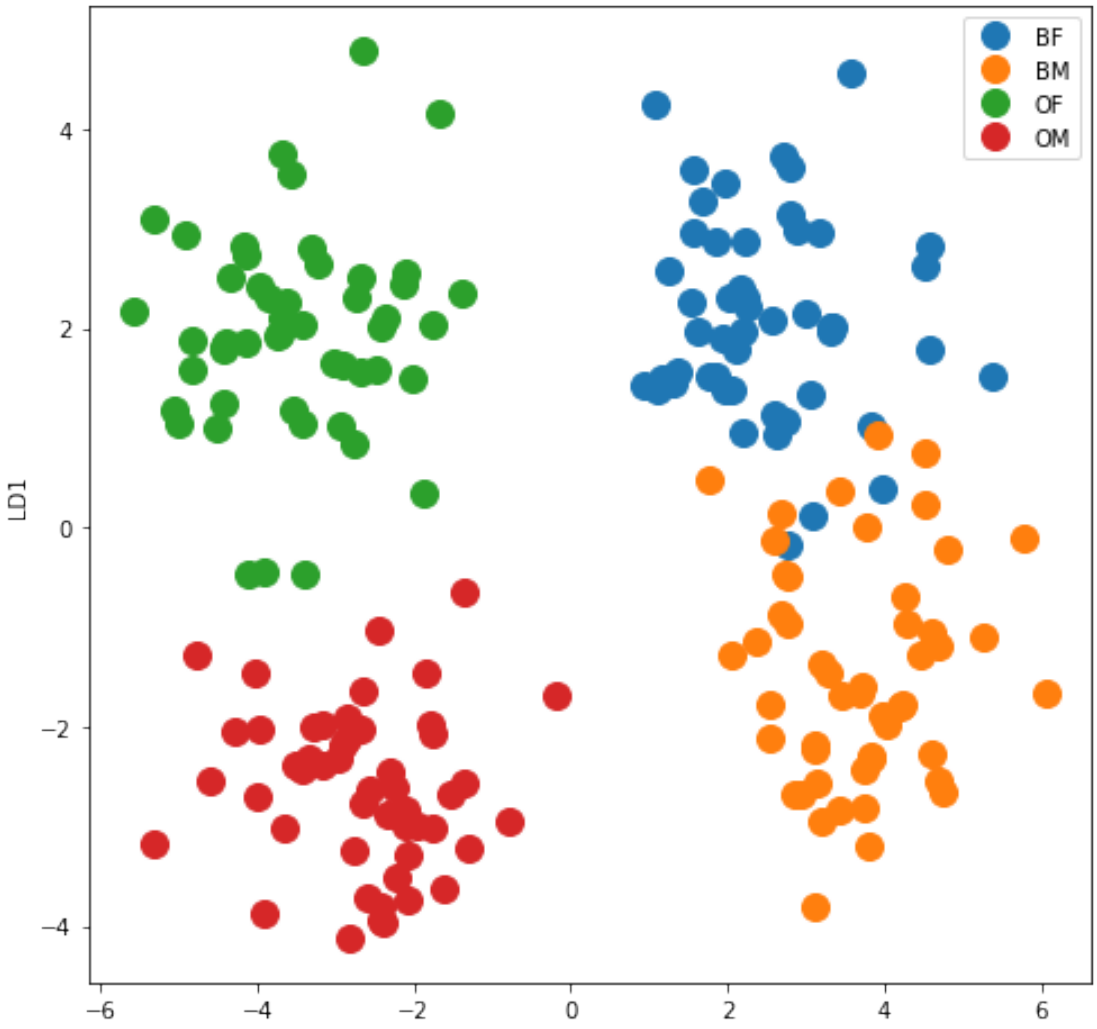
As an example, the first (log) LD is given by:

```
`LD1 = -31.2*log(FL) - 9.5*log(RW) - 9.8*log(CL) + 66*log(CW) - 18*log(BD)`
```

get the new loadings
plot the projected data in the first two LDs

```
In [40]: crabs_logtrans['Class'] = crabs_data.Class
         groups = crabs_logtrans.groupby('Class')

         fig, ax = plt.subplots(figsize=(8,8))
         for name, group in groups:
```

```
        ax.plot(group.LD1,
                group.LD2,
                marker='o',
                linestyle='',
                ms=12,
                label=name)
    ax.legend()
    ax.set_ylabel('LD2')
    ax.set_ylabel('LD1');
```



The first coordinate clearly expresses the difference between species, and the second the difference between sexes!