Wine Data Set - A Case Study using Logistic Regression and PCA

These data are the results of a chemical analysis of wines grown in the same region in Italy but derived from three different cultivars. The analysis determined the quantities of 13 constituents found in each of the three types of wines.

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Wine Data Set

Download: Data Folder, Data Set Description

Abstract: Using chemical analysis determine the origin of wines

Data Set Characteristics:	Multivariate	**Number of Instances:**	178	**Area:**	Physical
Attribute Characteristics:	Integer, Real	**Number of Attributes:**	13	**Date Donated**	1991-07-01
Associated Tasks:	Classification	**Missing Values?**	No	**Number of Web Hits:**	849522

The attributes are
1) Alcohol
2) Malic acid
3) Ash
4) Alcalinity of ash
5) Magnesium
6) Total phenols
7) Flavanoids
8) Nonflavanoid phenols
9) Proanthocyanins
10)Color intensity
11)Hue
12)OD280/OD315 of diluted wines
13)Proline

In a classification context, this is a well posed problem with "well behaved" class structures. Since we can't visualise the results with 13 attributes, we need to apply dimensionality reduction techniques.

StandardScaler is used to normalize the data. Feature Scaling is done for the algorithm to converge faster.

before

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	13.690	3.260	2.540	20.000	107.000	1.830	0.560	0.500	0.800	5.880	0.960	1.820	680.000
1	12.690	1.530	2.260	20.700	80.000	1.380	1.460	0.580	1.620	3.050	0.960	2.060	495.000
2	11.620	1.990	2.280	18.000	98.000	3.020	2.260	0.170	1.350	3.250	1.160	2.960	345.000
3	13.400	3.910	2.480	23.000	102.000	1.800	0.750	0.430	1.410	7.300	0.700	1.560	750.000
4	13.500	1.810	2.610	20.000	96.000	2.530	2.610	0.280	1.660	3.520	1.120	3.820	845.000
5	13.730	1.500	2.700	22.500	101.000	3.000	3.250	0.290	2.380	5.700	1.190	2.710	1285.000
6	12.290	2.830	2.220	18.000	88.000	2.450	2.250	0.250	1.990	2.150	1.150	3.300	290.000
7	12.600	1.340	1.900	18.500	88.000	1.450	1.360	0.290	1.350	2.450	1.040	2.770	562.000
8	11.410	0.740	2.500	21.000	88.000	2.480	2.010	0.420	1.440	3.080	1.100	2.310	434.000
9	13.640	3.100	2.560	15.200	116.000	2.700	3.030	0.170	1.660	5.100	0.960	3.360	845.000
10	12.600	2.460	2.200	18.500	94.000	1.620	0.660	0.630	0.940	7.100	0.730	1.580	695.000
11	11.960	1.090	2.300	21.000	101.000	3.380	2.140	0.130	1.650	3.210	0.990	3.130	886.000

after

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0.877	0.798	0.644	0.130	0.489	-0.703	-1.428	1.072	-1.368	0.352	0.029	-1.064	-0.206
1	-0.367	-0.758	-0.398	0.334	-1.413	-1.442	-0.503	1.701	0.024	-0.841	0.029	-0.731	-0.817
2	-1.697	-0.344	-0.323	-0.453	-0.145	1.249	0.320	-1.521	-0.435	-0.757	0.902	0.519	-1.313
3	0.516	1.383	0.421	1.004	0.136	-0.752	-1.233	0.522	-0.333	0.951	-1.106	-1.425	0.025
4	0.640	-0.506	0.905	0.130	-0.286	0.445	0.680	-0.656	0.092	-0.643	0.727	1.713	0.339
5	0.926	-0.785	1.240	0.859	0.066	1.216	1.338	-0.578	1.314	0.276	1.033	0.172	1.793
6	-0.864	0.412	-0.547	-0.453	-0.850	0.314	0.309	-0.892	0.652	-1.221	0.858	0.991	-1.494
7	-0.478	-0.929	-1.737	-0.308	-0.850	-1.327	-0.606	-0.578	-0.435	-1.094	0.378	0.255	-0.596
8	-1.958	-1.469	0.495	0.421	-0.850	0.363	0.063	0.444	-0.282	-0.828	0.640	-0.384	-1.019
9	0.815	0.654	0.719	-1.270	1.122	0.724	1.111	-1.521	0.092	0.023	0.029	1.074	0.339
10	-0.478	0.079	-0.621	-0.308	-0.427	-1.048	-1.326	2.094	-1.131	0.866	-0.975	-1.397	-0.156
11	-1.274	-1.154	-0.249	0.421	0.066	1.840	0.196	-1.835	0.075	-0.774	0.160	0.755	0.475
12	-0.914	1.356	-0.621	-0.308	0.841	-1.442	-1.202	-0.578	-0.791	1.334	-1.324	-0.814	0.372
13	1.635	-0.407	1.314	0.130	1.404	0.888	1.225	-0.263	0.618	0.487	0.509	0.089	1.776

We have used **PCA (Principal Component Analysis)** for dimensionality reduction.

	0	1	2	3	4	5	6	7	8	9	10	11	12
0	0.877	0.798	0.644	0.130	0.489	-0.703	-1.428	1.072	-1.368	0.352	0.029	-1.064	-0.206
1	-0.367	-0.758	-0.398	0.334	-1.413	-1.442	-0.503	1.701	0.024	-0.841	0.029	-0.731	-0.817
2	-1.697	-0.344	-0.323	-0.453	-0.145	1.249	0.320	-1.521	-0.435	-0.757	0.902	0.519	-1.313
3	0.516	1.383	0.421	1.004	0.136	-0.752	-1.233	0.522	-0.333	0.951	-1.106	-1.425	0.025
4	0.640	-0.506	0.905	0.130	-0.286	0.445	0.680	-0.656	0.092	-0.643	0.727	1.713	0.339
5	0.926	-0.785	1.240	0.859	0.066	1.216	1.338	-0.578	1.314	0.276	1.033	0.172	1.793
6	-0.864	0.412	-0.547	-0.453	-0.850	0.314	0.309	-0.892	0.652	-1.221	0.858	0.991	-1.494
7	-0.478	-0.929	-1.737	-0.308	-0.850	-1.327	-0.606	-0.578	-0.435	-1.094	0.378	0.255	-0.596
8	-1.958	-1.469	0.495	0.421	-0.850	0.363	0.063	0.444	-0.282	-0.828	0.640	-0.384	-1.019
9	0.815	0.654	0.719	-1.270	1.122	0.724	1.111	-1.521	0.092	0.023	0.029	1.074	0.339
10	-0.478	0.079	-0.621	-0.308	-0.427	-1.048	-1.326	2.094	-1.131	0.866	-0.975	-1.397	-0.156
11	-1.274	-1.154	-0.249	0.421	0.066	1.840	0.196	-1.835	0.075	-0.774	0.160	0.755	0.475
12	-0.914	1.356	-0.621	-0.308	0.841	-1.442	-1.202	-0.578	-0.791	1.334	-1.324	-0.814	0.372
13	1.635	-0.407	1.314	0.130	1.404	0.888	1.225	-0.263	0.618	0.487	0.509	0.089	1.776
14	-0.130	0.555	0.123	0.130	0.277	-1.573	-0.750	-0.971	-1.317	0.150	-0.931	-1.620	-0.701
15	0.628	1.095	-0.658	-0.016	-0.850	-1.048	-1.511	1.701	-1.232	0.276	-0.626	-1.064	-0.536
16	0.715	-0.596	-0.212	-0.978	1.193	1.462	1.379	-0.185	1.246	0.457	-0.015	1.102	0.174
17	1.685	-0.623	1.240	1.587	-0.145	0.888	-0.657	1.308	1.857	3.354	-1.673	-0.870	-0.272
18	0.902	-0.461	-0.026	-0.861	0.066	0.576	0.957	-0.735	0.142	-0.525	0.684	1.963	0.967
19	-0.951	-0.974	-1.589	-0.162	-0.568	0.166	0.093	0.208	0.804	-0.989	-0.407	0.602	-1.422

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When we apply PCA, we get two principal components with maximum variance. Only the attributes with larger variance will contribute better for the results. This is understood by observing the **explained variance matrix.**

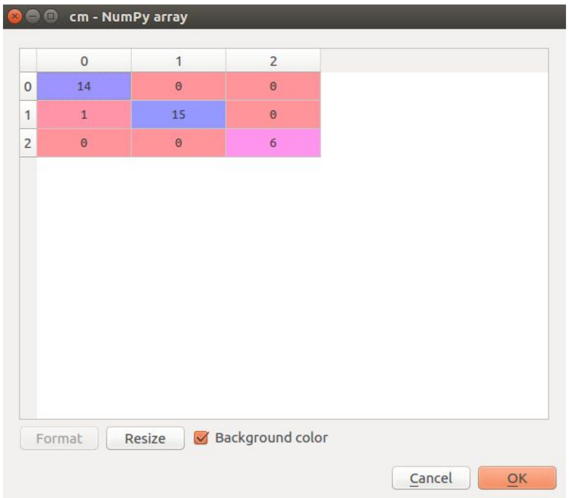
explained_variance - NumPy array

	0
0	0.369
1	0.193
2	0.108
3	0.074
4	0.062
5	0.049
6	0.041
7	0.025
8	0.023
9	0.019
10	0.017
11	0.013
12	0.007

The **PCA algorithm reduces the 13 attribute dataset into 2 principal components** as shown below.

	0	1
0	-2.179	-1.072
1	-1.808	1.578
2	1.098	2.221
3	-2.556	-1.662
4	1.857	0.242
5	2.583	-1.377
6	0.873	2.256
7	-0.418	2.354
8	-0.305	2.277
9	2.141	-1.101
10	-2.981	-0.247
11	1.962	1.254
12	-2.162	-0.976
13	2.220	-2.395
14	-2.302	-0.206
15	-3.010	-0.279
16	2.634	-0.868
17	-1.092	-3.539
18	2.626	-0.003
19	0.198	2.292

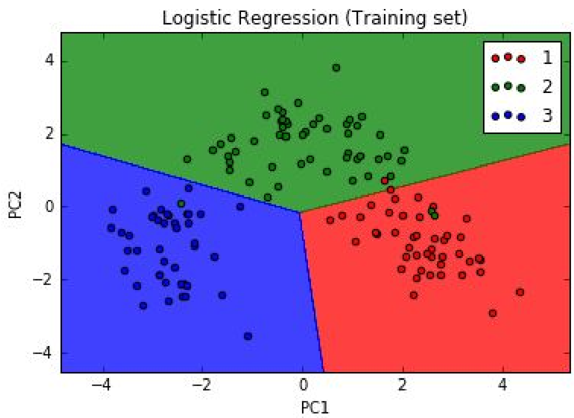
The **confusion matrix** is constructed to find out the accuracy of prediction. The diagonal elements are the correctly predicted outputs. The other cell elements are the incorrectly predicted outputs.

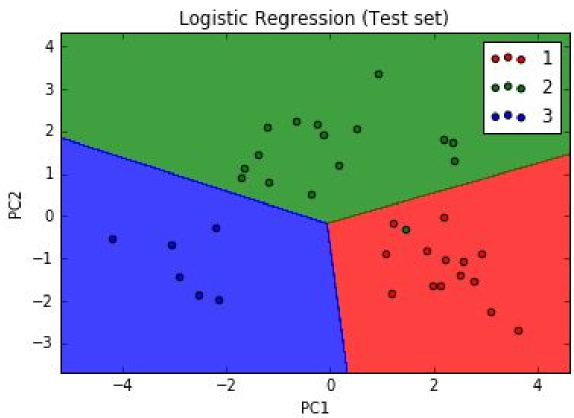


	0	1	2
0	14	0	0
1	1	15	0
2	0	0	6

We are using **Matplotlib.pyplot** python library to visualise the results. We are using a mesh grid to plot the results. The training set and test set data is visualised. There are 3 prediction regions.

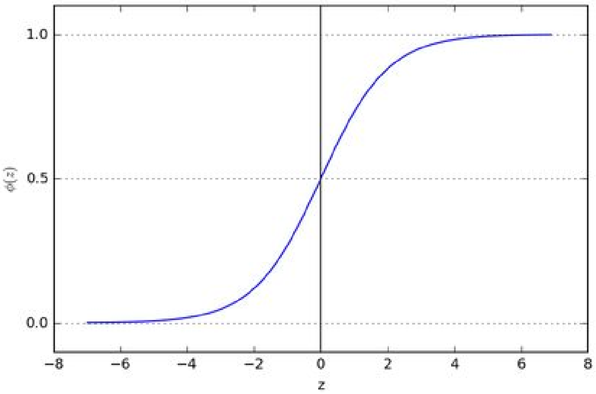
The green dot in blue region is an **outlier**.





Logistic Regression is a classification algorithm, which uses sigmoid function.

$$P(y = 1 \mid x) = \phi(z) = \frac{1}{1 + e^{-z}}$$



The model predicts with 97.22 % accuracy.

Relevant Papers:
(1)
S. Aeberhard, D. Coomans and O. de Vel,
Comparison of Classifiers in High Dimensional Settings,
Tech. Rep. no. 92-02, (1992), Dept. of Computer Science and Dept. of
Mathematics and Statistics, James Cook University of North Queensland.
(Also submitted to Technometrics).

The data was used with many others for comparing various
classifiers. The classes are separable, though only RDA
has achieved 100% correct classification.
(RDA : 100%, QDA 99.4%, LDA 98.9%, 1NN 96.1% (z-transformed data))
(All results using the leave-one-out technique)

(2)
S. Aeberhard, D. Coomans and O. de Vel,
"THE CLASSIFICATION PERFORMANCE OF RDA"
Tech. Rep. no. 92-01, (1992), Dept. of Computer Science and Dept. of
Mathematics and Statistics, James Cook University of North Queensland.
(Also submitted to Journal of Chemometrics).

Here, the data was used to illustrate the superior performance of
the use of a new appreciation function with RDA.