The Construction of an Asymmetric Biplot for Multivariate Data Sets

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Abstract

A scatterplot is a useful statistical tool for representing samples as points and variables by means of coordinate axes. A form of scatterplot that can be used for multivariate data is the biplot. In this paper, the fundamental idea behind the biplot is discussed, before its construction. An illustration using an 11-dimensional multivariate data set concerning the relationships between chemical measurements and sensory descriptors is presented.

Keywords: Biplot; Scatter plot; Calibration factor

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1 Introduction

Graphical representations are often used as a quick way to summarize and display data sets effectively. They offer an opportunity to identify patterns, groupings, outliers, and relationships, amongst others, in the data set. Although there are various graphical representations, the most commonly used representations are the two- and three-dimensional scatterplots. In these representations, the coordinate axes represent the variables of the data, while the points represent the samples. In the usual two-dimensional scatterplot, two orthogonal Cartesian axes are used to represent the variables of the data. Likewise, in the three-dimensional scatterplot, three orthogonal Cartesian axes are used to represent the data

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variables. However, data sets are often (very) large, and therefore it can be time consuming to make a visual inspection of the data using a two- or three-dimensional scatterplot. In addition, all the inter-variable relationships are not displayed in either scatterplots. For this reason, the biplot can be a useful tool for analysis.

First introduced by Gabriel (1971), the biplot is often referred to as the multivariate version of the scatterplot - as it allows for the simultaneous display of each data variable by a non-orthogonal axis on the plot (Gower & Hand, 1996). Compared to the scatterplot display, axes in the biplot display are non-orthogonal, while in the scatterplot, all two or three axes are orthogonal. Also, the number of data variables to use in the scatterplot display is limited to two or three, whereas in the biplot, there is no variable limitation. This is a unique advantage of the biplot over the scatterplot.

Generally, there are two main kinds of biplot, namely, the *symmetric biplot* and the *asymmetric biplot*. When the data set under consideration is in the form of a two-way table, the resulting biplot display is termed the symmetric biplot (Gower et al., 2011; Gower & Hand, 1996). For the asymmetric biplot, the data is in the form of a data matrix - where the columns are the variables and the rows are the samples. The roles of the columns and rows in the symmetric biplot can be interchanged without losing any information. However, this is not the case in the asymmetric biplot. In this paper, the fundamental idea behind the biplot is discussed, before it is constructed. An illustration using an 11-dimensional (multivariate) data set concerning the relationships between chemical measurements and sensory descriptors is presented.

The remainder of this paper is organized as follows. Section 2 provides the essential concepts behind the biplot, before its construction. This is followed by an application with a chemical-sensory analysis data to investigate the relationships between the sensory descriptors and the chemical quality measurements of sixteen olive oils in Section 3. Finally, some concluding remarks are presented in Section 4.

2 The biplot

In the usual three-dimensional scatterplot, three orthogonal Cartesian axes are used for reading off the values of the sample points, as well as for adding points to the plot. The fact that the (asymmetric) biplot is referred to as a *multivariate scatterplot* implies that more than two variables are represented by (non-orthogonal) axes. In the first biplot introduced by Gabriel (1971), the samples and variables of a data set were represented by vectors, but to differentiate between these two sets of vectors, Gabriel (1971) suggested that the samples of the data be represented by points. Gower & Hand (1996) went a step further by

introducing the idea of representing the variables of the data by axes, rather than vectors, while still representing the samples by points. This was done to make the biplot similar to a scatterplot.

2.1 The biplot construction

By definition, the biplot is a joint graphical display of the rows and columns of a data matrix $\mathbf{D}$ (of G rows and H columns) by means of markers $\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_G$ for its rows and markers $\mathbf{b}_1, \mathbf{b}_2, \cdots, \mathbf{b}_H$ for its columns. Here, the rows of the data matrix are the data samples, while the columns are the data variables. Each marker is chosen in such a way that the inner product $\mathbf{a}_i^T \mathbf{b}_j$ represents d_{ij}, the $(i,j)^{\text{th}}$ element of the data matrix $\mathbf{D}$ (Barnett, 1981).

The biplot is often constructed in two dimensions. This does not necessarily mean that it is limited to two dimensions, but rather, it is the most convenient biplot display. With $\mathbf{D}$ being a (very) large matrix, the rank of $\mathbf{D}$ is almost always higher than two. As a result, some approximation is done on $\mathbf{D}$ to obtain a lower rank. Methods such as Principal Component Analysis (PCA), Partial Least Squares (PLS) and Multi-Dimensional Scaling (MDS) can be used to perform this approximation.

Taking $\hat{\mathbf{D}}$ as the rank two approximation of $\mathbf{D}$, the biplot of a data matrix $\mathbf{D}$ relies on the decomposition of $\hat{\mathbf{D}}$ into the product of two matrices, $\mathbf{A}$ and $\mathbf{B}$. That is,

$$\hat{\mathbf{D}} = \mathbf{A}\mathbf{B}^T. \tag{1}$$

where $\mathbf{A}$ is the row markers matrix and $\mathbf{B}$ is the column markers matrix. Matrices $\mathbf{A}$ and $\mathbf{B}$ are defined as

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1r} \\ a_{21} & a_{22} & \cdots & a_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ a_{G1} & a_{G2} & \cdots & a_{Gr} \end{bmatrix} = \begin{bmatrix} \mathbf{a}_{(1)}^T \\ \mathbf{a}_{(2)}^T \\ \vdots \\ \mathbf{a}_{(G)}^T \end{bmatrix} \quad \text{the } (G \times r) \text{ row markers matrix,}$$

and

$$\mathbf{B} = \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1r} \\ b_{21} & b_{22} & \cdots & b_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ b_{H1} & b_{H2} & \cdots & b_{Hr} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{(1)}^T \\ \mathbf{b}_{(2)}^T \\ \vdots \\ \mathbf{b}_{(H)}^T \end{bmatrix} \quad \text{the } (H \times r) \text{ column markers matrix.}$$

Thus, the approximated rows and columns of a data matrix are represented in the biplot display. Generally, the number of columns in $\mathbf{A}$ and $\mathbf{B}$ are determined by the rank r approximation of $\mathbf{D}$. In practice, $r = 2$ is usually preferred for a convenient biplot display.

From (1), since $\mathbf{A}$ contains the information about the rows of the data, while $\mathbf{B}$ contains the information about its columns, the biplot points will be defined by the row markers ($\mathbf{A}$) of the data, whereas the biplot axes will be defined by the column markers ($\mathbf{B}$). In other words, for the biplot of a data matrix $\mathbf{D}$, G rows of $\mathbf{A}$ will serve as the biplot points, while H rows of $\mathbf{B}$ will be used in calculating the directions of the biplot axes.

Furthermore, the positions of the biplot axes give an indication of the correlations between the variables. Axes forming small angles are said to be strongly correlated - either positively or negatively. Axes are positively correlated when they lie in the same direction, while negatively correlated axes lie in opposite directions. However, axes that are close to forming right angles are said to be uncorrelated.

2.2 Calibration of biplot axes

Since the columns of $\mathbf{D}$ are represented by axes, the calibration of these axes is very important in the biplot display. This is because different calibrations are used for adding points to the biplot and for reading off values from the biplot axes. Generally, calibration is done by placing a set of tick marks on each of the biplot axes and then labelling them with any set of markers (not necessarily equally spaced) as desired, e.g., $(0, 1, 2, 3, 5, \cdots)$.

The row and column markers matrices in eqn.(1) can be rewritten as

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_{(1)}^T \\ \mathbf{a}_{(2)}^T \\ \vdots \\ \mathbf{a}_{(G)}^T \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} \mathbf{b}_{(1)}^T \\ \mathbf{b}_{(2)}^T \\ \vdots \\ \mathbf{b}_{(H)}^T \end{bmatrix},$$

with $\mathbf{a}_{(i)}^T = (a_{i1} \;\; a_{i2})$ being the (1×2) i^{th} row marker and $\mathbf{b}_{(j)}^T = (b_{j1} \;\; b_{j2})$ the (1×2) j^{th} column marker, where $i = 1, 2, \cdots, G$, $j = 1, 2, \cdots, H$ and $r = 2$. Consider the projection of $\mathbf{a}_{(i)}$ on $\mathbf{b}_{(j)}$ as shown in Figure 1.

The inner product of $\mathbf{a}_{(i)}$ on $\mathbf{b}_{(j)}$ gives the $(i,j)^{\text{th}}$ element of $\hat{\mathbf{D}}$ as $\hat{\mathbf{d}}_{ij} = \mathbf{a}_{(i)}^T \mathbf{b}_{(j)}$. From the origin $\mathbf{O}$, the length of $\mathbf{a}_{(i)}$ is given by $||\mathbf{a}_{(i)}|| = \left(\mathbf{a}_{(i)}^T \mathbf{a}_{(i)}\right)^{\frac{1}{2}}$, while the length of $\mathbf{b}_{(j)}$ is obtained by $||\mathbf{b}_{(j)}|| = \left(\mathbf{b}_{(j)}^T \mathbf{b}_{(j)}\right)^{\frac{1}{2}}$. The angle between $\mathbf{a}_{(i)}$ and $\mathbf{b}_{(j)}$ is defined by θ_{ij}. The

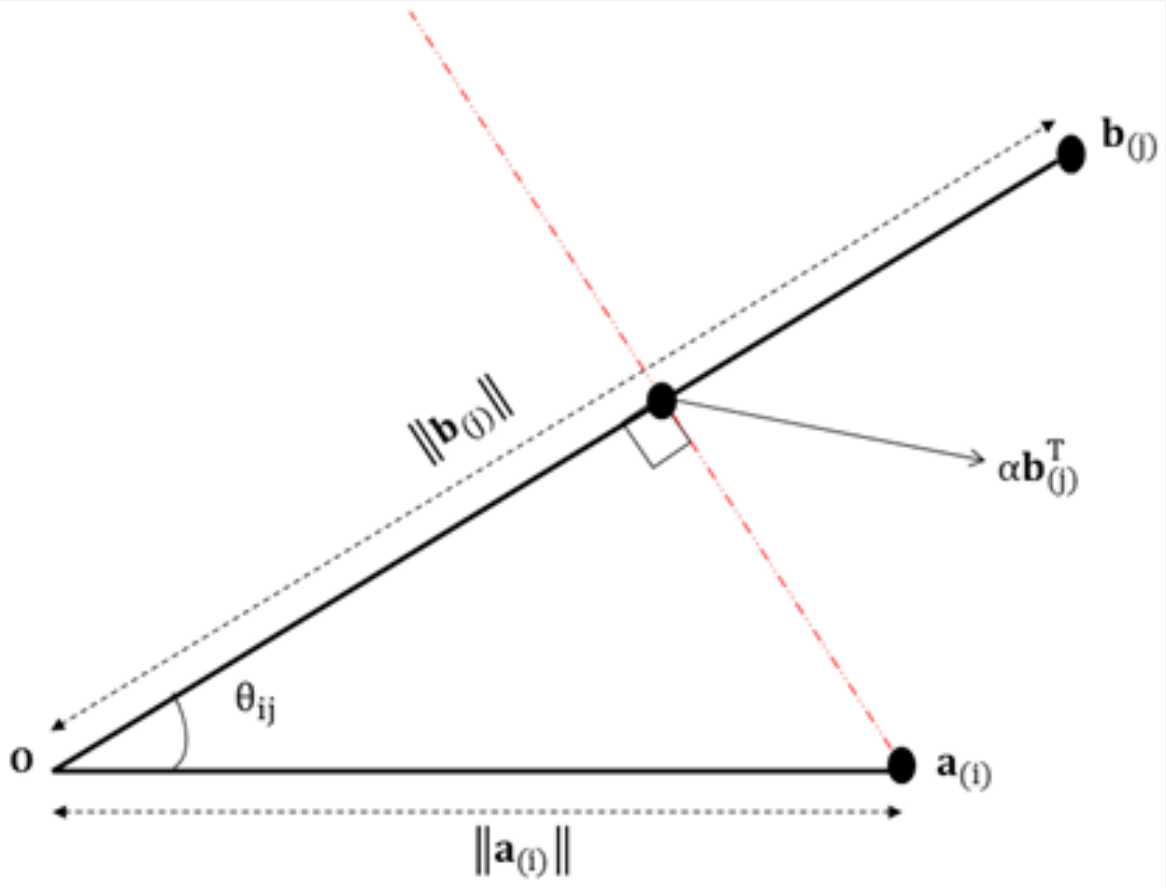

Figure 1: A schematic of the projection of $\mathbf{a}_{(i)}$ on $\mathbf{b}_{(j)}$.

point $\alpha\mathbf{b}_{(j)}^T$ is the projection of $\mathbf{a}_{(i)}$ on $\mathbf{b}_{(j)}$ with a calibration factor α.

The inner product $\mathbf{a}_{(i)}^T\mathbf{b}_{(j)} = ||\mathbf{a}_{(i)}|| \times ||\mathbf{b}_{(j)}|| \times cos(\theta_{ij}) = ||\mathbf{b}_{(j)}|| \times ||\mathbf{a}_{(i)}|| \times cos(\theta_{ij})$ can be written as the product of $||\mathbf{b}_{(j)}||$ and the length of the projection of $\mathbf{a}_{(i)}$ on $\mathbf{b}_{(j)}$ $\Big(||\mathbf{a}_{(i)}|| \times cos(\theta_{ij})\Big)$. All vectors $\mathbf{a}_{(k)}$ with end points on the red dotted line, in Figure 1, through $\mathbf{a}_{(i)}$ and $\alpha\mathbf{b}_{(j)}^T$ will have the same projection and therefore the same length of projection $||\mathbf{a}_{(k)}|| \times cos(\theta_{kj})$. Thus, $\mathbf{a}_{(i)}^T\mathbf{b}_{(j)}$ has a constant value (say, μ^*) for all vectors $\mathbf{a}_{(k)}$ with end points on the red dotted line through $\mathbf{a}_{(i)}$ and $\alpha\mathbf{b}_{(j)}^T$. That is,

$$\mathbf{a}_{(i)}^T\mathbf{b}_{(j)} = \mu^* = \mathbf{a}_{(k)}^T\mathbf{b}_{(j)} \tag{2}$$

for all $\mathbf{a}_{(k)}$ on the red dotted line. Since $\alpha\mathbf{b}_{(j)}^T$ is a point on the red dotted line, $\alpha\mathbf{b}_{(j)}^T\mathbf{b}_{(j)} = \mu^*$. Solving for α yields

$$\alpha = \frac{\mu^*}{\mathbf{b}_{(j)}^T\mathbf{b}_{(j)}}. \tag{3}$$

Equation (3) can be termed the *calibration factor*. Replacing α in $\alpha\mathbf{b}_{(j)}^T$ by eqn.(3) gives the coordinates of the point on the $\mathbf{b}_{(j)}$ axis that is calibrated with a value μ^* as

$$\frac{\mu^*}{\mathbf{b}_{(j)}^T\mathbf{b}_{(j)}}\mathbf{b}_{(j)}^T.$$

An illustration of how to calibrate an axis in the biplot display will be discussed in the next section.

3 Example

The following example is an illustration of a biplot, using the olive oil data from Mevik & Wehrens (2007). This data shows the sensory and chemical quality evaluations of sixteen olive oil samples. There were five chemical quality measurements (Acidity, Peroxide, K232, K270 and DK) taken, and six sensory panel characteristics (Yellow, Green, Brown, Glossy, Transparent and Syrup) were used in this evaluation. The sixteen olive oils are assigned as samples, while the chemical quality measurements and sensory panel characteristics are the variables. As a result, the olive oil data can be viewed as a (16×11) data matrix. This data can be obtained from the **pls** package in R, downloaded freely from CRAN, `http://cran.r-project.org/`. To graphically view this data, we will need an 11-dimensional plot. However, no such plot currently exists. As a result, we can use the biplot.

The row markers $\mathbf{A}$ and the column markers $\mathbf{B}$ are shown in Table 4. To illustrate the calibration of the biplot axes (see Section 2.2), consider the Yellow variable. The column marker vector for this variable, $\mathbf{b}_{(j=6)}$, is given by the sixth row in $\mathbf{B}$. By the definition of a biplot, $\mathbf{a}_{(i)}^T\mathbf{b}_{(6)} = \hat{d}_{i6}$, for $i = 1, 2, \cdots, 16$ and $\mathbf{b}_{(6)}^T = (0.624 \quad -0.016)$. This defines the inner product of the samples and the Yellow variable. Substituting $\mu^* = \hat{d}_{i6}$ in equation (3) gives the calibration factor for the yellow axis as $\alpha_Y = \frac{\hat{d}_{i6}}{0.390}$. For values ranging between -75.6 and 58.0, $\alpha_Y\mathbf{b}_{(6)}^T$ gives the set of tick markers for the Yellow axis. More precisely, with the centred values under the Yellow variable given as

$$d_6 = \begin{pmatrix} -29.48, & -27.48, & -18.17, & -20.68, & 0.92, & -10.17, & 2.92, & -24.48 \\ 14.83, & -5.88, & 20.03, & 22.62, & 17.22, & 16.72, & 20.53, & 20.53 \end{pmatrix},$$

the set of tick markers for the Yellow axis is given by

$$\alpha_Y \mathbf{b}_{(6)}^T = \begin{pmatrix} -47.19, & 1.15, & -29.10, & 0.87, & 1.48, & 0.43, & 4.68, & 1.03 \\ 23.74, & 0.25, & 32.06, & -0.95, & 27.58, & -0.70, & 32.86, & -0.86 \end{pmatrix}.$$

These values are not yet corrected for the mean of Yellow. Correction for the mean of Yellow is done by adding the mean of Yellow to $\alpha_Y \mathbf{b}_{(6)}^T$. That is, $\alpha_Y \mathbf{b}_{(6)}^T + \overline{d}_6$, where $\overline{d}_6 = 50.9$ is the mean of Yellow, as shown in Table 3. Thus, corrected for the mean of Yellow, the set of tick markers for the Yellow axis is given as

$$\begin{pmatrix} 3.7, & 52.0, & 21.8, & 51.7, & 52.4, & 51.3, & 55.6, & 51.9 \\ 74.6, & 51.1, & 82.9, & 49.9, & 78.5, & 50.2, & 83.7, & 50.0 \end{pmatrix}.$$

Rather than using these disproportionate values as the scale markers on the Yellow axis, nicer scale markers can be used, such as (0, 10, 20, 30, 40, 50, 60, 70, 80, 90), as seen below in Figure 2.

The uncentred (and original values) of the olive oil data are shown in Table 2. The asymmetric biplot of this data is shown above in Figure 2. In this figure, the samples of the data are represented by the black points, while the variables are represented by the axes. This biplot also shows a representation of the variance of each variable, represented by the thicker arrow (vector) on each axis. From this display, the standard deviation of Acidity is smaller compared to the others, while DK has a large deviation. This is evident from the length of the vector on these axes.

To read of the data values of the olive oil data from the biplot display in Figure 2, each sample point in the biplot is orthogonally projected onto the axes and their respective values are read off. The resulting values obtained from these projections are referred to as the approximated data values. For example, sample point G1 projected onto the Peroxide and Brown axes yields the values 13.5 and 8.5 respectively, as shown in Figure 3. The approximated values of the olive oil data are shown in Table 1.

Furthermore, several relationships can be deduced from the biplot display (Figure 2), such as a relation between Syrup, K232 and Peroxide. Observing their respective correlation values of 0.69, 0.76 and 0.87 from Figure 4, a fairly good relation exists between them. Another relationships deduction is the relation between K270, Transparent (Transp) and Glossy, and between Green, Yellow and DK. These relationship deductions are done based on the angle between axes. For example, the angle between Glossy and Transparent is acute and larger than the angle between Syrup and K232, corresponding to the former having a higher correlation value of 0.97, while the latter has a correlation value of 0.69, as shown in Figure 4.

Table 1: The approximated olive oil values.

	Acidity	Peroxide	K232	K270	DK	Yellow	Green	Brown	Glossy	Transp	Syrup
G1	0.7	13.2	1.8	0.14	0.001	17.0	76.8	8.4	76.0	69.8	49.3
G2	0.4	13.9	1.8	0.13	-0.001	39.9	47.0	12.2	78.5	74.7	48.9
G3	0.4	11.1	1.6	0.11	-0.002	50.9	35.5	8.4	83.2	80.7	46.5
G4	0.5	13.0	1.8	0.13	0.000	28.7	62.1	9.3	77.9	73.0	48.7
G5	0.5	12.1	1.7	0.12	-0.001	39.0	49.7	8.9	80.4	76.5	47.7
I1	0.3	19.3	2.2	0.15	0.000	34.4	49.3	21.2	71.8	67.2	52.8
I2	0.3	14.0	1.8	0.12	-0.002	50.9	32.9	13.6	80.0	77.4	48.5
I3	0.4	16.2	2.0	0.14	0.000	33.4	53.2	15.6	75.1	70.5	50.7
I4	0.3	13.5	1.7	0.12	-0.002	55.6	27.3	13.4	81.2	79.0	48.0
I5	0.1	20.5	2.2	0.14	-0.001	48.7	29.9	24.9	72.6	69.5	53.0
S1	0.2	10.8	1.5	0.10	-0.003	71.5	9.3	10.4	86.4	86.1	45.5
S2	0.2	9.2	1.4	0.09	-0.004	72.1	9.9	7.7	88.2	88.0	44.4
S3	0.2	12.3	1.6	0.11	-0.003	61.0	21.3	11.9	83.3	81.8	46.9
S4	0.2	12.0	1.6	0.10	-0.003	68.1	12.5	12.2	84.6	83.8	46.5
S5	0.2	10.2	1.5	0.09	-0.003	71.9	9.3	9.4	87.1	86.9	45.0
S6	0.2	10.5	1.5	0.10	-0.003	71.0	10.2	9.9	86.6	86.2	45.3

Table 2: The olive oil values.

	Acidity	Peroxide	K232	K270	DK	Yellow	Green	Brown	Glossy	Transp	Syrup
G1	0.7	12.7	1.9	0.14	0.003	21.4	73.4	10.1	79.7	75.2	50.3
G2	0.2	12.3	1.7	0.12	-0.004	23.4	66.3	9.8	77.8	68.7	51.7
G3	0.3	10.3	1.6	0.12	-0.005	32.7	53.5	8.7	82.3	83.2	45.4
G4	0.7	13.7	1.7	0.17	-0.002	30.2	58.3	12.2	81.1	77.1	47.8
G5	0.5	11.2	1.5	0.12	-0.001	51.8	32.5	8.0	72.4	65.3	46.5
I1	0.3	18.7	2.1	0.14	0.001	40.7	42.9	20.1	67.7	63.5	52.2
I2	0.2	15.3	1.9	0.12	0.000	53.8	30.4	11.5	77.8	77.3	45.2
I3	0.3	18.5	1.9	0.13	0.001	26.4	66.5	14.2	78.7	74.6	51.8
I4	0.4	15.6	1.8	0.10	0.000	65.7	12.1	10.3	81.6	79.6	48.3
I5	0.2	19.4	2.2	0.16	-0.003	45.0	31.9	28.4	75.7	72.9	52.8
S1	0.2	10.5	1.5	0.12	-0.004	70.9	12.2	10.8	87.7	88.1	44.5
S2	0.2	8.1	1.5	0.11	-0.002	73.5	9.7	8.3	89.9	89.7	42.3
S3	0.3	12.5	1.6	0.09	-0.002	68.1	12.0	10.8	78.4	75.1	46.4
S4	0.2	11.0	1.6	0.09	-0.003	67.6	13.9	11.9	84.6	83.8	48.5
S5	0.2	10.8	1.3	0.09	-0.003	71.4	10.6	10.8	88.1	88.5	46.7
S6	0.3	11.4	1.4	0.09	-0.004	71.4	10.0	11.4	89.5	88.5	47.2

Table 3: The column means of the olive oil data.

Acidity	Peroxide	K232	K270	DK	Yellow	Green	Brown	Glossy	Transp	Syrup
0.3	13.3	1.7	0.1	0.0	50.9	33.5	12.3	80.8	78.2	48.0

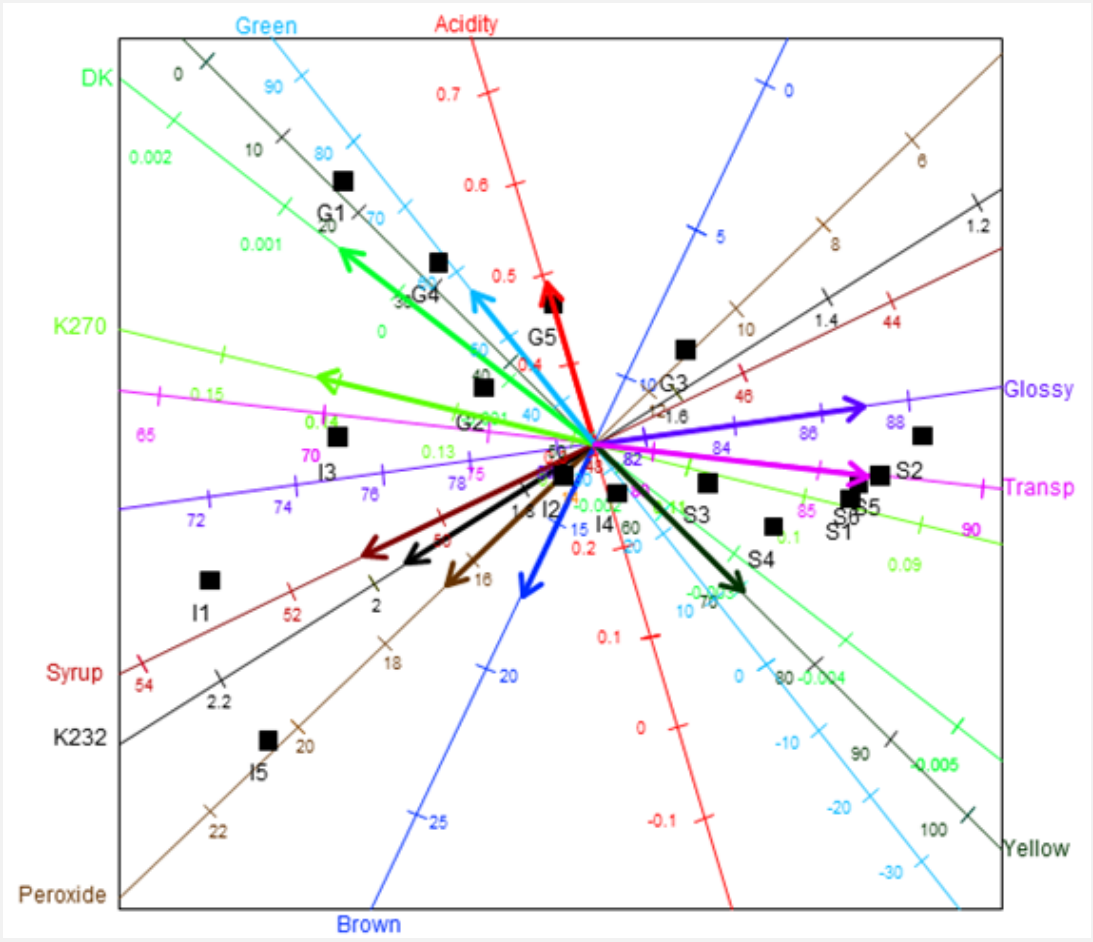

Figure 2: The biplot of the olive oil data.

4 Conclusion

The biplot, a joint graphical display of the rows and of columns of a data matrix, is often referred to as the multivariate version of a scatterplot. This is because it allows for the display of rows (samples) as points and each column (variable) by an axis on the same plot. An advantage of the biplot includes the revelation of the association between samples (rows) and/or variables (columns) of a (large) data set. If the roles of the columns and rows of a data matrix are not interchangeable, the resulting biplot will be an asymmetric biplot.

Also, a unique advantage of the biplot over the scatterplot is that the number of data variables to use in the biplot display is not limited. As a result, all the inter-variable relationships are displayed in the single biplot display.

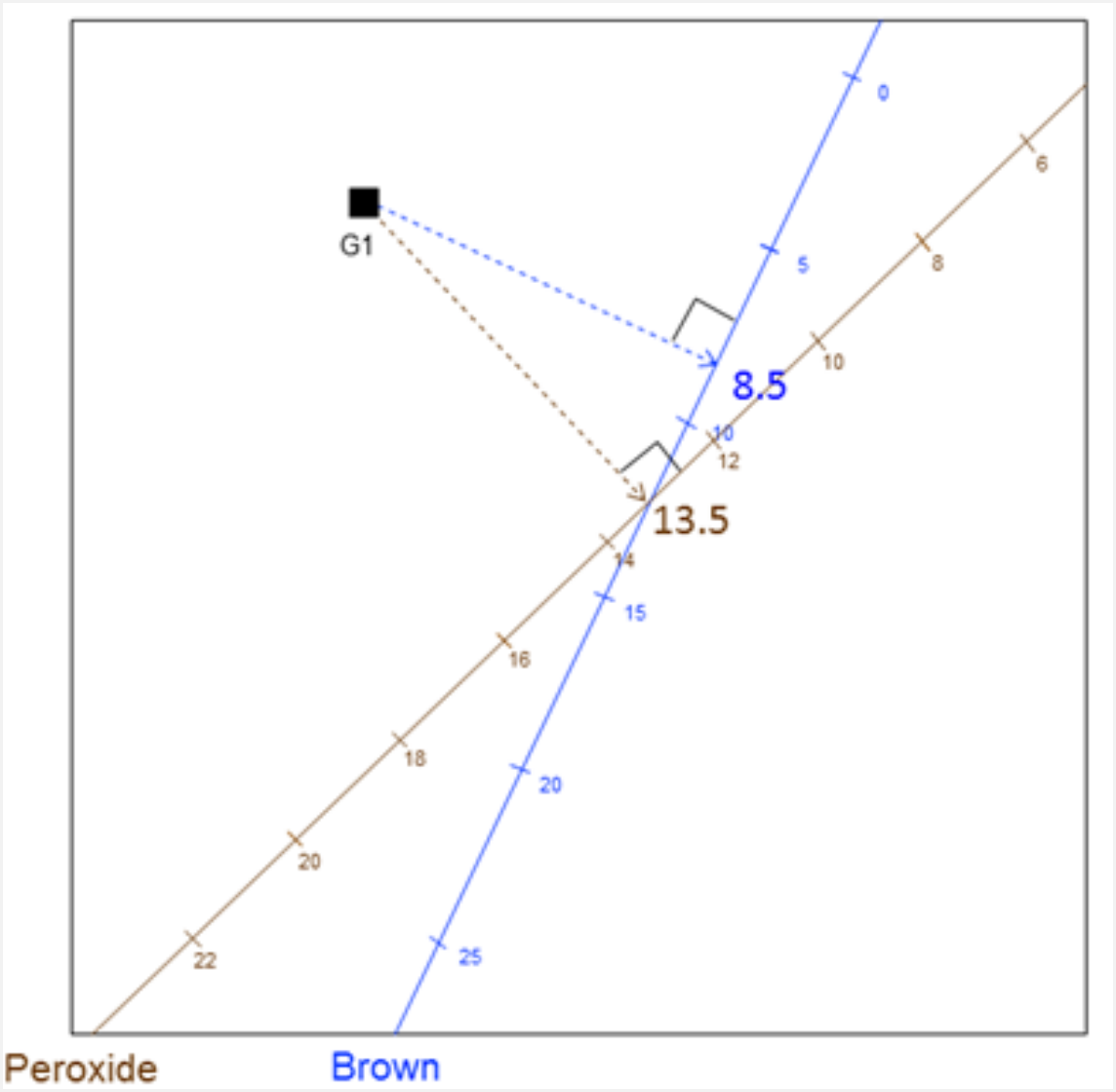

Figure 3: Examples of orthogonal projections in the biplot of the olive oil data.

Software

A collection of functions has been developed in the R language (R Core Team, 2014) to produce the biplot display of the olive oil data in Figure 2. These functions are available in the R package called PLSbiplot1 by Oyedele (2014), and can be found on the Comprehensive R Archive Network (CRAN)'s repository, at `http://cran.r-project.org/`. A detailed documentation for all the routines in this package can be found on the dropbox link, `https:`

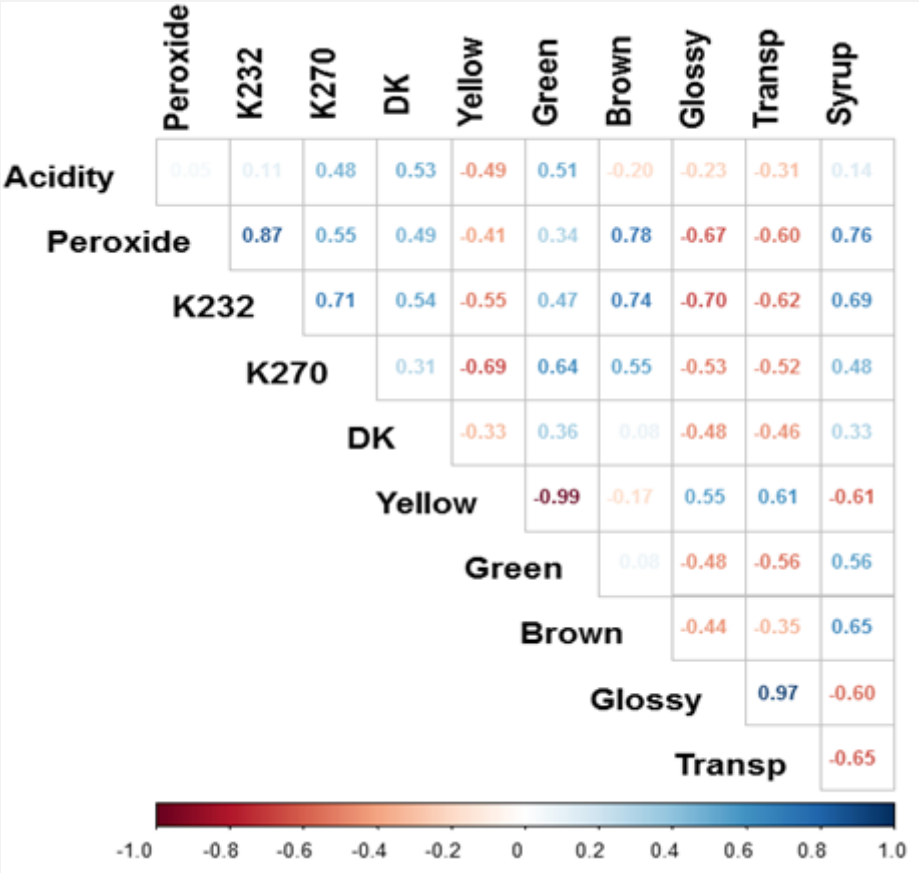

Figure 4: The correlation values of the olive oil data. Nearly empty cells have a value very close to zero.

//www.dropbox.com/sh/wr66u07t1vjm9da/AACg_E4h8MvgOHuCXk69yDIya.

The following R code were used to obtain Figure 2

```
#Install the PLSbiplot1 package
#First download the PLSbiplot1_0.1.tar.gz file from the
#CRAN at http://cran.r-project.org/ and install into R.

#Load the PLSbiplot1 package
require(PLSbiplot1)

#Olive oil data
if(require(pls))
```

```
data(oliveoil, package="pls")
Dmat = as.matrix(oliveoil)
dimnames(Dmat) = list(paste(c("G1","G2","G3","G4","G5","I1","I2",
                        "I3","I4","I5","S1","S2","S3","S4","S5","S6")),
                            paste(c("Acidity","Peroxide","K232","K270","
                         DK","Yellow","Green","Brown","Glossy","
                                          Transp","Syrup")))
#The biplot display
PCA.biplot(D=Dmat, method=mod.PCA, ax.tickvec.D=c(8,5,5,7,6,4,5,5,8,7,7))
#Here, the data was approximated using PCA to obtain a lower rank of 2
#Refer to Section 2.1 above.
```

Table 4: The row and column markers A and B.

	Component 1	Component 2
G1	-49.037	8.502
G2	-43.814	1.303
G3	-24.975	11.854
G4	-31.675	5.998
G5	-1.475	-11.163
I1	-18.004	-18.977
I2	3.774	-2.816
I3	-41.389	2.696
I4	25.581	-4.205
I5	-4.864	-14.392
S1	31.296	6.335
S2	35.605	9.690
S3	26.283	-8.117
S4	26.605	1.147
S5	32.776	5.985
S6	33.311	6.157

	Component 1	Component 2
Acidity	-0.003	0.002
Peroxide	-0.044	-0.239
K232	-0.004	-0.015
K270	-0.001	-0.001
DK	0.000	0.000
Yellow	0.624	-0.016
Green	-0.751	0.253
Brown	-0.024	-0.346
Glossy	0.111	0.540
Transparent	0.168	0.665
Syrup	-0.060	-0.159

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