PRINCIPAL COMPONENT ANALYSIS AND BIPLOTS. A BACK-TO-BASICS COMPARISON OF IMPLEMENTATIONS

A PREPRINT

Ettore Settanni Institute for Manufacturing University of Cambridge Cambridge, UK E.Settanni@eng.cam.ac.uk

April 24, 2024

Abstract

Principal Component Analysis and biplots are so well-established and readily implemented that it is just too tempting to give for granted their internal workings. In this note I get back to basics in comparing how PCA and biplots are implemented in base-R and contributed R packages, leveraging an implementation-agnostic understanding of the computational structure of each technique. I do so with a view to illustrating discrepancies that users might find elusive, as these arise from seemingly innocuous computational choices made under the hood. The proposed evaluation grid elevates aspects that are usually disregarded, including relationships that should hold if the computational rationale underpinning each technique is followed correctly. Strikingly, what is expected from these equivalences rarely follows without caveats from the output of specific implementations alone.

Keywords PCA · biplots · matrix decomposition · R

1 Introduction

A food scientist, a bioinformaticist, and a survey researcher walk into a bar... Jokes aside, what could they possibly have in common? The answer is probably PCA—Principal Component Analysis.

Many will find the concept familiar, perhaps even trite. Overviews of this technique leave little room for doubt about its popularity and relevance across disciplines—see e.g., Knox (2018, Ch. 11); Bro and Smilde (2014); Abdi and Williams (2010). Often, PCA is complemented by a biplot—a closely related, yet distinct technique for jointly visualizing observations and variables that typically make up a data matrix (du Toit, Steyn, and Stumpf 1986 Ch. 6; Gower, Lubbe, and LeRoux 2011).

There is no shortage of options at the analysts' fingertip when performing PCA: Tab.1 provides a nonexhaustive list. Base-R alone provides two built-in functions besides several contributed packages' own implementations. For a hands-on summary of some of these functions see e.g., Mayor (2015, Ch. 6); Kumar and Paul (2016, Ch. 4). Several references on multivariate statistics cover both PCA and biplots in the context of base R (e.g., Venables and Ripley 2002, Ch. 11; Everitt and Hothorn 2011, Ch. 3) or dedicated R packages (e.g., Gower, Lubbe, and LeRoux 2011, Ch. 3; Pagès 2014, Ch. 1).

With PCA and biplots being so readily implemented it is tempting to give for granted their internal workings and go about it mechanically through a canned routine of choice. The exception that proves the rule is the package *LearnPCA* (Hanson and Harvey 2022). Its rich set of vignettes is unique in its intent to address the self-directed learner with a view to unpicking methodological aspects of PCA (but not biplots) that R users rarely engage with, and whose importance may be underplayed. It also provides comparative insights into alternative ways of implementing PCA in base R.

	Functions included	
	PCA	Biplots
base-R	<pre>prcomp(), princomp()</pre>	<pre>biplot()</pre>
ade4	dudi.pca()	<pre>scatter()</pre>
amap	acp()	plot()
FactoMineR	PCA()	plot.PCA()
pcaMethods	pca()	<pre>slplot()</pre>
PCAmixdata	PCAmix()	<pre>plot.PCAmix()</pre>
PCAtools	pca()	<pre>biplot()</pre>
psych	principal()	<pre>biplot.psych()</pre>
factoextra		<pre>fviz_pca_biplot()</pre>
ggbiplot		ggbiplot()

Table 1: Selected implementations of PCA and biplots

Against this backdrop, what seems to be missing is—to the best of my knowledge—a comparison of how PCA and biplots are implemented in base R and contributed R packages, and how that compares with an implementation-agnostic understanding of the computational structure of each technique. In this note I attempt such comparison with a view to illustrating discrepancies that users might find elusive, as these arise from seemingly innocuous computational choices made under the hood. By getting back to basics in PCA and biplots I elevate aspects that are usually disregarded.

The remainder is structured as follows. The next section outlines an implementation-agnostic understanding of the computational building blocks in PCA and biplots with the aid of an illustrative example. Using these insights as an evaluation grid, selected implementations are then compared, pinpointing possible points of departure from what is reasonably expected. A closing section summarises key practical implications of these findings.

2 Implementation-agnostic building blocks

The seasoned practitioner might scoff at the idea of yet another overview on PCA and swiftly move past. At the risk of disappointing advanced readers, this section makes a point of reviewing the computational building blocks of PCA and biplots—especially how they come about—as an agnostic stance for comparing the output of specific implementations.

A useful place to start is the visual intuition behind how PCA works—i.e., that a set of data-points can be represented in a lower-dimensional space while preserving relevant information about them. The analogy with image compression often comes to mind (Poole 2014, 607; Peng 2020, Ch. 3). In the simplest case, the data-points are 2-dimensional and the task at hand is to determine their orthogonal projections onto an appropriately defined line, thus obtaining a 1-dimensional representation of those points. While simplistic, the pedagogic merits of a 2-dimensional visual example are emphasised by the popularity of on-line resources such as Starmer (2018) and amoeba (2015). This is the case I will consider throughout this section, by means of an illustrative numerical example. Similar examples can be found elsewhere e.g., Hanson and Harvey (2022); Abdi and Williams (2010). The example is restricted to numerical features, or variables, as PCA does not immediately apply to categorical or binary features—see Kassambara and Mundt (2020)'s taxonomy in the context of package *factoextra*.

2.1 A motivating example

Consider the example in Tab.2, and Fig.1. The first two columns of Tab.2 represent the raw data, which are arranged in a so-called data matrix $\mathbf{X} = [x_{ij}]_{n \times m}$ consisting of i = 1, ..., n observations and j = 1, ..., m features, or variables. In the example n = 6 and m = 2. For each feature j the last two rows of Tab.2 give its mean $\bar{x}_j = \frac{1}{n} \sum_i x_{ij}$, and sample variance $s_{x_j}^2 = \frac{1}{n-1} \sum_i (x_{ij} - \bar{x}_j)^2$. In R this is just: apply(X, 2, mean) and apply(X, 2, var), respectively.

The columns of Tab.2 denoted as **Y** correspond to the centred data matrix, which is also of size $n \times m$, with generic element $y_{ij} = x_{ij} - \bar{x}_j$. The operation of centring **X** is often expressed in matrix notation as $\mathbf{Y} = \mathbf{X} - \frac{1}{n} \mathbf{1} \mathbf{1}^T \mathbf{X}$, where **1** is a unit vector of appropriate dimension (Venables and Ripley 2002, 302; Gower, Lubbe, and LeRoux 2011). In **R** this is accomplished with: $\mathbf{Y} \leq \operatorname{apply}(\mathbf{X}, \mathbf{2}, \operatorname{function}(\mathbf{x}) \ (\mathbf{x} - \operatorname{mean}(\mathbf{x})))$.

		Feat	ures			Optimal	projections, P	C1	Optimal projections, PC2				
	$Raw [\mathbf{X}] \qquad Centred [\mathbf{Y}]$		Proj. coord		Dist of proj. from		Proj. coord		Dist of proj. from				
	feat1	feat2	feat1	feat2	feat1	feat2	origin $[\mathbf{z}_{\bullet 1}]$	observ.	feat1	feat2	origin $[\mathbf{z}_{\bullet 2}]$	observ.	
А	10.00	6.00	4.17	2.37	4.44	1.59	-4.72	0.83	-0.28	0.78	-0.83	4.72	
В	11.00	4.00	5.17	0.37	4.70	1.68	-4.99	1.39	0.47	-1.31	1.39	4.99	
С	8.00	5.00	2.17	1.37	2.35	0.84	-2.50	0.56	-0.19	0.53	-0.56	2.50	
D	3.00	3.00	-2.83	-0.63	-2.71	-0.97	2.88	0.36	-0.12	0.34	-0.36	2.88	
E	2.00	2.80	-3.83	-0.83	-3.66	-1.31	3.89	0.50	-0.17	0.48	-0.50	3.89	
F	1.00	1.00	-4.83	-2.63	-5.12	-1.83	5.44	0.85	0.29	-0.80	0.85	5.44	
mean	5.83	3.63	0.00	0.00	0.00	0.00	0.00	0.75	0.00	0.00	0.00	4.07	
sample var.	18.97	3.13	18.97	3.13	18.88	2.41	21.28	0.14	0.09	0.72	0.81	1.41	

Table 2: An illustrative example with m = 2 features and a n = 6 observations





Figure 1: Visualisation of selected information from Tab.2. Left: scatterplot of centred data-points corresponding to \mathbf{Y} with orthogonal projections on two principal components represented by score vectors $\mathbf{z}_{\bullet 1}$ (red) and $\mathbf{z}_{\bullet 2}$ (blue); purple arrows represent distances between points and porjection. Right: plot of observations using principal component scores as transformed coordinates.

The mean and sample variance for the centred data are also shown in the last two rows of Tab.2. For each feature j the mean is characteristically zero: $\bar{y}_j = \frac{1}{n} \sum_i y_{ij} = \frac{1}{n} \sum_i x_{ij} - \bar{x}_j = 0$. Yet the sample variance is the same as the raw data's: $s_{y_j}^2 = \frac{1}{n-1} \sum_i (y_{ij} - \bar{y}_j)^2 = \frac{1}{n-1} \sum_i (x_{ij} - \bar{x}_j - 0)^2 = s_{x_j}$.

Contrary to what many think, so long as the quantities represented in \mathbf{X} are expressed in the same units, or if they scale well e.g., through a logarithmic transformation, it is not compulsory to manipulate the data further (see e.g., Venables and Ripley 2002).

Having centred the data, each row of **Y** can be interpreted as the coordinates of a point in the Cartesian plane corresponding to an observation (row header). The n = 6 observations can then be plotted as shown in Fig.1, left-hand side. The same figure also shows two lines passing through the origin—what is commonly referred to as *principal components*—and the orthogonal projections of the centred data-points' onto each. For a given point, its projection is found from intersecting a component, say the red line, and its perpendicular passing through that point (see e.g., Marecek 2017, Ch. 3). The position of an orthogonal projection onto a principal component, being 1-dimensional, is just its distance from the origin—or PCA *score*. The sign of a score, however, depends on which quadrant in which the projection falls with respect to the origin. For the two principal components in our example, the respective *scores* are denoted in Tab.2 by vectors $\mathbf{z}_{\bullet 1}$ (red line) and $\mathbf{z}_{\bullet 2}$ (blue line).

What we see at work in Fig.1 is a key tenet of PCA, albeit streamlined: a set of 2-dimensional data-points is transformed into a set of 1-dimensional points, which are appropriately arranged along a line, or principal component. In the context of PCA a set of data-points is "appropriately" represented in a lower-dimensional space when most information about its variance is retained. In our example, the more dispersed the projected data-points along a 1-dimensional line, the better.

But how are the lines and projections in Fig.1 arrived at, so that one can claim they are optimal? This aspect will be discussed next, and will inform an implementation-agnostic evaluation grid.

2.2 Computational aspects of PCA

To understand how the data-points' projections are positioned along a 1-dimensional *principal component*, one can imagine rotating the lines shown in Fig.1 (left) until the variance of the projections' distances from the origin—i.e., the variance of the *scores* in $\mathbf{z}_{\bullet 1}$ and $\mathbf{z}_{\bullet 1}$ —is maximal. For the first principal component in our example, or PC1 (blue line), the last row in Tab.2 shows that such variance is 21.3. This equals the sum of the variances along the projections' coordinates, see columns 5 and 6 of Tab.2. Typically, the variance of a principal component's scores is expressed as a fraction of the total variance along the the columns of \mathbf{Y} . For PC1 in our example, the maximal projections' variance achieved accounts for about 96% of the projected points'.

A well-established approach to obtain the optimal *scores* is to seek appropriate *linear combinations* of the original data-points' coordinates (e.g., Jolliffe 2004, Ch. 1 & 3; du Toit, Steyn, and Stumpf 1986, Ch. 9). In our example, the coordinates are represented by the columns of the centred data matrix \mathbf{Y} , and a linear combination of interest is the matrix-vector product:

$$\mathbf{z} = \mathbf{Y}\mathbf{a} = \begin{bmatrix} a_1 y_{11} + a_2 y_{12} = z_1 \\ \vdots \\ a_1 y_{i1} + a_2 y_{i2} = z_i \\ \vdots \\ a_1 y_{n1} + a_2 y_{n2} = z_n \end{bmatrix}$$
(1)

where $\mathbf{a} = [a_1, a_2]^T$ is the vector of unknown linear combination weights, commonly referred to as *loadings*; and \mathbf{z} is a vector of unknown principal component *scores* that position the projections of the data-points in \mathbf{Y} along an optimally defined 1-dimensional line or *principal component*, as discussed.

The process of finding \mathbf{z} revolves around the sample variance of its elements. The data being centred, \mathbf{z} has mean $\bar{z} = \frac{1}{n} \sum_{i} z_{i} = 0$, from which it follows that:

$$\operatorname{Var} \left(\mathbf{z} \right) = \frac{1}{n-1} \sum_{i} \left(z_{i} - \bar{z} \right)^{2}$$
$$= \frac{1}{n-1} \left(\mathbf{Y} \mathbf{a} - \bar{z} \right)^{T} \cdot \left(\mathbf{Y} \mathbf{a} - \bar{z} \right)$$
$$= \frac{1}{n-1} \mathbf{a}^{T} \mathbf{Y}^{T} \mathbf{Y} \mathbf{a}$$
$$= \mathbf{a}^{T} \mathbf{S} \mathbf{a}$$
(2)

where $\mathbf{S} = \frac{1}{n-1} \mathbf{Y}^T \mathbf{Y}$ is the sample covariance matrix of \mathbf{Y} . In R this is simply: $\mathbf{S} \leftarrow \text{cov}(\mathbf{Y})$.

Based on the above, one must choose **a** to maximize $Var(\mathbf{z})$ while respecting orthogonality constraints (Jolliffe 2004, 4; Venables and Ripley 2002, 303; Everitt and Hothorn 2011, Ch. 3). Since. from Equation 2, $Var(\mathbf{z}) = \mathbf{a}^T \mathbf{S} \mathbf{a}$, this is typically framed as a mathematical program:

$$\begin{array}{l} \max_{\mathbf{a}} \quad \mathbf{a}^T \mathbf{S} \mathbf{a} \\ \text{s.t.} \quad \mathbf{a}^T \mathbf{a} = 1 \end{array}$$
(3)

As it turns out, solving the program in Equation 3 for \mathbf{a} is equivalent to finding the principal eigenvector of \mathbf{S} . To see how that is so, I examine the first-order conditions for a constrained maximum using Lagrange multipliers (Jolliffe 2004, 4):

$$\frac{d\mathbf{a}^{T}\mathbf{S}\mathbf{a}}{d\mathbf{a}} - \frac{d}{d\mathbf{a}}\lambda\left(\mathbf{a}^{T}\mathbf{a} - 1\right) = 0$$

$$2\mathbf{a}^{T}\mathbf{S} - 2\lambda\mathbf{a}^{T} = 0$$

$$(\mathbf{S} - \lambda\mathbf{I})\mathbf{a} = 0$$
(4)

where the vector derivative $\frac{d\mathbf{a}^T \mathbf{S} \mathbf{a}}{d\mathbf{a}} = 2\mathbf{a}^T \mathbf{S}$ is a special result of the general rule $\frac{d\mathbf{a}^T \mathbf{S} \mathbf{a}}{d\mathbf{a}} = \mathbf{a}^T (\mathbf{S}^T + \mathbf{S})$ when **S** is symmetric (Binmore and Davies 2001, 162), which is the case for covariance matrices. The form of Equation 4 is typical of an eigenvalue problem in linear algebra (e.g. Poole 2014, Ch. 4), and promptly solved in **R** using the function **eigen(S)**, which in our example yields the eigenvalues of **S**

eigen(S)\$values

[1] 21.28 0.81

denoted as the vector $\boldsymbol{\lambda} = \begin{bmatrix} \lambda_1 & \lambda_2 \end{bmatrix}^T$; and the corresponding eigenvectors, juxtaposed

eigen(S)\$vectors

[,1] [,2]
[1,] -0.94 0.34
[2,] -0.34 -0.94

denoted by the matrix $\mathbf{V} = [\mathbf{a}_{\bullet 1} \quad \mathbf{a}_{\bullet 2}]$. The above suggests there are two linear combinations—i.e., as many as there are features—that could satisfy Equation 1. Jolliffe (2004, 5) demonstrates that the same reasoning leading to Equation 4 applies recursively beyond the first *principal component*.

If one considers only the linear combination associated with the largest eigenvalue $\lambda = \lambda_1 = 21.28$ and the corresponding eigenvector $\mathbf{a} = \mathbf{a}_{\bullet 1} = [-0.94, -0.34]^T$ of **S**, Equation 1 yields the *scores* vector $\mathbf{z} = \mathbf{z}_{\bullet 1}$ shown in Tab. 2. Choosing $\mathbf{a} = \mathbf{a}_{\bullet 2} = [0.34, -0.94]^T$ yields $\mathbf{z} = \mathbf{z}_{\bullet 2}$, instead.

These vectors may be juxtaposed to form a *scores* matrix $\mathbf{Z} = [\mathbf{z}_{\bullet,1} \quad \mathbf{z}_{\bullet,2}] = \mathbf{YV}$. Each column of the *scores* matrix \mathbf{Z} is a lower-dimensional representation from which one can reconstruct the 2-dimensional data-points in \mathbf{Y} (Gower, Lubbe, and LeRoux 2011). For example, columns 5 and 6 in Tab.2 are reconstructed as $\mathbf{Y}_{PC1} = \mathbf{z}_{\bullet 1} \mathbf{a}_{\bullet 1}^T$. In R this is: outer(Z[,1], eigen(S)\$vectors[,1]).

Combining Equations 4 and 2 brings about an often overlooked equivalence between the variance along a given *scores* vector \mathbf{z} and the corresponding eigenvalue λ of \mathbf{S} :

V

$$\begin{aligned} \operatorname{Tar}\left[\mathbf{z}\right] &= \mathbf{a}^T \mathbf{S} \mathbf{a} \\ &= \mathbf{a}^T \lambda \mathbf{a} \\ &= \lambda \end{aligned} \tag{5}$$

For example, assuming $\mathbf{z} = \mathbf{z}_{\bullet 1}$ one verifies in R that:

```
Z <- Y %*% eigen(S)$vectors
all.equal(apply(Z,2,var)[1], eigen(S)$values[1])</pre>
```

[1] TRUE

Although it is simplistic to assume two features, the first two principal components have well-established uses for visualising the outputs of PCA, even when there are more than two features. Traditionally, a 2-dimensional visualisation of PCA is attained by combining the first two principal components in a plot as shown in Fig.1 (right), where the vectors $\mathbf{z}_{\bullet,1}$ and $\mathbf{z}_{\bullet,2}$ provide the "transformed" system of coordinates and the original n = 6 observations are plotted accordingly. In the presence of more than two features one would typically retain the first two components with the caveat that the quality of such an approximation is given by the relative weight of the two largest eigenvalues of the covariance matrix \mathbf{S} . From Equation 5, this is equivalent to the proportion of variance associated with the first two principal components relative to the variance of the projected data-points.

$\mathbf{2.3}$ Alternative approaches: Singular Value Decomposition

The computational building blocks described so far emphasise the logical path from seeking a variancemaximising linear combination in Equation 1 to solving the eigenvalue problem in Equation 4. In practice, the preferred way to obtain *loadings* and *scores* is by doing a Singular Value Decomposition (SVD) of the rectangular matrix Y (e.g., Jolliffe 2004, Ch. 3; Hanson and Harvey 2022):

$$\mathbf{Y} = \mathbf{U}\mathbf{D}\mathbf{V}^T \tag{6}$$

which is equivalent to the command svd(Y) in R. With reference to our simple example, Equation 6 generates the following standard outputs (Poole 2014, Ch. 7):

• A matrix $\mathbf{U} = \begin{bmatrix} \mathbf{u}_{\bullet,1} & \mathbf{u}_{\bullet,3} \end{bmatrix}$ formed with the "left" eigenvectors of \mathbf{Y} :

svd(Y)\$u

##		[,1]	[,2]
##	[1,]	-0.46	0.41
##	[2,]	-0.48	-0.69
##	[3,]	-0.24	0.28
##	[4,]	0.28	0.18
##	[5,]	0.38	0.25
##	[6,]	0.53	-0.42

• A matrix $\mathbf{V} = \begin{bmatrix} \mathbf{v}_{\bullet 1} & \mathbf{v}_{\bullet 2} \end{bmatrix}$ formed with the "right" eigenvectors of \mathbf{Y}

svd(Y)\$v

[,1] [,2]
[1,] -0.94 -0.34
[2,] -0.34 0.94

which is analogous to the juxtaposed *loadings* vectors. Yet using V to indicate both $[\mathbf{a}_{\bullet 1} \quad \mathbf{a}_{\bullet 2}]$ from Equation 4 and $\begin{bmatrix} \mathbf{v}_{\bullet 1} & \mathbf{v}_{\bullet 2} \end{bmatrix}$ is an abuse of notation, since the elements' signs may differ.

- A vector $\boldsymbol{\ell} = \begin{bmatrix} l_1 & l_2 \end{bmatrix}^T$ of "singular values" of \mathbf{Y} , which is typically diagonalised to form the matrix $\mathbf{D} = \begin{bmatrix} l_1 & 0\\ 0 & l_2 \end{bmatrix}$ in Equation 6:

svd(Y)\$d

[1] 10.32 2.01

It is worth emphasising that the singular values in ℓ are distinct from, but related to the eigenvalues in λ (e.g., Hanson and Harvey 2022; Jolliffe 2004, 38). In our example, such relationship is:

$$\ell = (n-1)^{1/2} \begin{bmatrix} \lambda_1^{1/2} & \lambda_2^{1/2} \end{bmatrix}$$

= $(n-1)^{1/2} \begin{bmatrix} \sqrt{\operatorname{Var}[\mathbf{z}_{\bullet,1}]} & \sqrt{\operatorname{Var}[\mathbf{z}_{\bullet,1}]} \end{bmatrix}$
= $(n-1)^{1/2} \begin{bmatrix} \sigma_1 & \sigma_2 \end{bmatrix}$ (7)

where $\sigma_j = \text{s.d.}[\mathbf{z}_{\bullet j}]$; and $\lambda_j = \text{Var}[\mathbf{z}_{\bullet j}]$, based on Equation 5. One can verify in **R** that:

all.equal(sqrt((nrow(Y)-1)*eigen(S)\$values), sqrt(nrow(Y)-1)*apply(Z,2,sd))

[1] TRUE

To obtain the *scores* matrix \mathbf{Z} from an SVD, one right-multiplies both sides of Equation 6 by \mathbf{V} :

$$\begin{aligned} \mathbf{Y}\mathbf{V} &= \mathbf{U}\mathbf{D}\mathbf{V}^T\mathbf{V} \\ &= \mathbf{U}\mathbf{D} \\ &= \mathbf{Z}_{SVD} \end{aligned} \tag{8}$$

In practice, \mathbf{Z}_{SVD} and $\mathbf{Z} = \begin{bmatrix} \mathbf{z}_{\bullet,1} & \mathbf{z}_{\bullet,2} \end{bmatrix}$, which is shown in Tab.2, are often used interchangeably. Yet they are only equivalent in absolute values. In our example, one can verify that:

all.equal(abs(unname(U %*% D)), abs(unname(Y %*% eigen(S)\$vector)))

[1] TRUE

2.4 Principal components biplots

The typical PCA plot in Fig.1 (right) may be enriched to become a *biplot*. The difference between these concepts might seem cosmetic: both rely on a "transformed" system of coordinates based on PCA *scores*, but differ in scope as to what they seek to visualise. The former only visualises observations i.e., the rows of the data-matrix; whereas the latter aims to jointly represent observations and features i.e., both the rows and the columns of the data-matrix (Jolliffe 2004, Ch. 5).

On a deeper level, the task of attaining an overlaid representation of a plot of features and a plot of observations in a *biplot* is underpinned by a distinct computational strategy. Whilst it was straightforward to derive the plot in Fig.1 from previous computations, a *biplot* is inherently associated with an SVD of the centred data-matrix (Gower, Lubbe, and LeRoux 2011; Venables and Ripley 2002, Ch. 11; du Toit, Steyn, and Stumpf 1986, Ch. 6; Vu and Friendly 2024).

In the context of principal component biplots, the SVD in Equation 6 serves as the starting point, but is modified so that the diagonal matrix of singular values is "split" based on a parameter $0 \le \alpha \le 1$. Such modification is illustrated below in the context of our simplified example, with just two features:

$$\begin{aligned} \mathbf{Y} &= \mathbf{U}\mathbf{D}\mathbf{V}^{T} \\ &= \mathbf{U}\mathbf{L}^{\alpha}\mathbf{L}^{1-\alpha}\mathbf{V}^{T} \\ &= \begin{bmatrix} \mathbf{u}_{\bullet,1} & \mathbf{u}_{\bullet,2} \end{bmatrix} \begin{bmatrix} l_{1} & 0 \\ 0 & l_{2} \end{bmatrix}^{\alpha} \begin{bmatrix} l_{1} & 0 \\ 0 & l_{2} \end{bmatrix}^{1-\alpha} \begin{bmatrix} \mathbf{v}_{\bullet,1} \\ \mathbf{v}_{\bullet,2} \end{bmatrix}^{\alpha} \\ &= \begin{bmatrix} u_{11}l_{1}^{\alpha} & u_{12}l_{2}^{\alpha} \\ u_{21}l_{1}^{\alpha} & u_{22}l_{2}^{\alpha} \\ \vdots & \vdots \\ u_{n1}l_{1}^{\alpha} & u_{n2}l_{2}^{\alpha} \end{bmatrix} \begin{bmatrix} v_{11}l_{1}^{(1-\alpha)} & v_{21}l_{1}^{(1-\alpha)} \\ v_{12}l_{2}^{(1-\alpha)} & v_{22}l_{2}^{(1-\alpha)} \end{bmatrix} \\ &= \mathbf{A}\mathbf{B}^{T} \end{aligned}$$
(9)

In the presence of more than two features, the right-hand side of Equation 9 yields a rank-2 approximation of the centred data-matrix i.e.,

$$\mathbf{Y} \approx \mathbf{Y}_{(2)} = \mathbf{A}\mathbf{B}^T \tag{10}$$

When $\alpha = 0$ Equation 9 is referred to as a *principal component biplot*, which is of interest here. In our example with just two features, the matrices **A** and **B** take on the following meaning:

• The coordinates of the observations along the principal components are given by $\mathbf{A} = \mathbf{U}$. Based on Equation 8, and using interchangeably \mathbf{Z} and \mathbf{Z}_{SVD} for simplicity, it can be shown that this is equivalent to scaling the PCA plot coordinates given by the *scores* matrix:

$$\mathbf{A} = \mathbf{U}$$

= $\mathbf{Z}\mathbf{D}^{-1}$
= $\begin{bmatrix} \mathbf{z}_{\bullet,1}l_1^{-1} & \mathbf{z}_{\bullet,2}l_2^{-1} \end{bmatrix}$ (11)

• Simultaneously, the coordinates of the features are given by the matrix product $\mathbf{B}^T = \mathbf{D}\mathbf{V}^T$ between the right eigenvectors and the singular values of an SVD. Yet this result can be re-expressed in terms of the *loadings* and *scores*'s St.Dev. Based on Equation 7:

$$\mathbf{B}^{T} = \mathbf{D}\mathbf{V}^{T}$$

$$= \begin{bmatrix} \mathbf{v}_{\bullet,1}l_{1} \\ \mathbf{v}_{\bullet,2}l_{2} \end{bmatrix}$$

$$= (n-1)^{1/2} \begin{bmatrix} \mathbf{v}_{\bullet,1}\sigma_{1} \\ \mathbf{v}_{\bullet,2}\sigma_{2} \end{bmatrix}$$
(12)

In our simple example the matrix \mathbf{A} of observations coordinates is equivalent to the matrix \mathbf{U} of left eigenvectors previously obtained from Equation 6, as expected:

all.equal(Z_svd %*% diag(1/svd(Y)\$d), svd(Y)\$u)

[1] TRUE

whereas the coordinates for the features given by matrix \mathbf{B}^T are:

D %*% t(V)

[,1] [,2]
[1,] -9.71 -3.47
[2,] -0.68 1.89

For our example, a joint representation of observations and features based on **A** and **B**, which are characteristic of a principal components biplot, is shown in Fig.2.

What is clear from Equations 11 and 12 is that there is more to Fig.2 than just overlaying a crude plot of *loadings* over a plot of PCA *scores*—which happens frequently in practice. If the observations' and features' coordinates are jointly computed as shown, one can verify certain identities between the columns of matrix **B** and the standard deviation of the corresponding features, or their correlation. Such properties are often overlooked, but useful for comparative purposes and will be illustrated next.

2.5 Biplot properties linked to features

The literature often states that, for a given feature j the length of the vector formed by its coordinates on a biplot should be equivalent to the feature's standard deviation (St.Dev.) σ_j (e.g., Venables and Ripley 2002, 312; du Toit, Steyn, and Stumpf 1986, 108). This statement is hardly self-evident and might generate some confusion. To demonstrate it, I follow Jolliffe (2004, 77) and left-multiply both sides of Equation 9 by \mathbf{Y}^T :

$$\mathbf{Y}^{T}\mathbf{Y} = \mathbf{Y}^{T}\mathbf{A}\mathbf{B}^{T}$$

$$= \mathbf{B} \left(\mathbf{U}\mathbf{L}^{0}\right)^{T} \left(\mathbf{U}\mathbf{L}^{0}\right) \mathbf{B}^{T}$$

$$= \mathbf{B}\mathbf{U}^{T}\mathbf{U}\mathbf{B}^{T}$$

$$(n-1)\mathbf{S} = \mathbf{B}\mathbf{B}^{T}$$
(13)



Figure 2: Biplot of observations and features for an illustrative example based on SVD. The superposed dual axes (coloured grey) reflect the different scale of the features' coordinates.

where $\mathbf{A} = \mathbf{U}\mathbf{L}^{\alpha}$ from Equation 9, and $\alpha = 0$ is characteristic of a principal components biplot. Also, the columns of \mathbf{U} are orthonormal hence $\mathbf{U}^T\mathbf{U} = \mathbf{I}$. As before, \mathbf{S} is the covariance matrix of \mathbf{Y} .

Next I focus on a generic diagonal element s_{jj} of the covariance matrix **S** on the left-hand side of Equation 13 to show how the St.Dev. σ_j^{feat} of the *j*-th feature relates to the length of vector $\mathbf{b}_{j\bullet}$, which corresponds to the *j*-th column of matrix \mathbf{B}^T in Equation 12:

$$(n-1)s_{jj} = \mathbf{b}_{j\bullet}^{T}\mathbf{b}_{j\bullet}$$

$$\sigma_{j}^{\text{feat}} = (n-1)^{-\frac{1}{2}} \|\mathbf{b}_{j\bullet}\|_{2}$$

$$= \sqrt{\frac{1}{n-1}\sum_{k} (v_{jk}l_{k})^{2}}$$

$$= \sqrt{\sum_{k} \left(v_{jk}\sqrt{\lambda_{k}}\right)^{2}}$$
(14)

where $l_j = (n-1)^{1/2} \sqrt{\lambda_j}$ based on Equation 7. For our example, one can verify in R that: all.equal(sqrt(diag(S)), apply(t(B),2,function(x){norm(x,"2")})/sqrt(nrow(Y)-1))

[1] TRUE

Confusions may arise due to the form of the right-hand side in Equation 14. For instance, it would be imprecise to conclude—as the phrasing in some references might suggest—that the vector whose length equals the St.Dev. of a given feature j is the corresponding column of the matrix \mathbf{B}^T in Equation 12. Also, it would be misleading to expect that Equation 14 holds for a rank-2 approximation when there are more than two features, see Equation 10.

A second property associated with principal components biplots is that the cosine similarity between a pair of vectors of features coordinates is equivalent to the correlation coefficient between these features, assuming these have been centred (Jolliffe 2004, 77; du Toit, Steyn, and Stumpf 1986, 108). In our example, the presence of two features simplifies the task of illustrating this point.

The two features vectors shown in Fig.2 (purple-coloured) correspond to the columns of **B** in Equation 12. I denote these as $\mathbf{b}_{\bullet 1}$ and $\mathbf{b}_{\bullet 2}$. Squaring the 2-norm of their difference $\|\mathbf{b}_{\bullet 1} - \mathbf{b}_{\bullet 2}\|_2^2$ leads to the following "textbook" equivalence—for details see Binmore and Davies (2001, 18):

$$\cos\theta = \frac{\langle \mathbf{b}_{\bullet 1}, \mathbf{b}_{\bullet 2} \rangle}{\|\mathbf{b}_{\bullet 1}\|_2 \cdot \|\mathbf{b}_{\bullet 2}\|_2}$$
(15)

which is the definition of cosine similarity. In Equation 15 the angle in radians between two features vectors is θ ; and $\langle \cdot, \cdot \rangle$ denotes the inner product between them. What is rarely shown is that Equation 15 is equivalent to the *correlation* between the two features in our simple example. This equivalence can be proved starting from the correlation coefficient between two columns of matrix **Y**:

$$\operatorname{corr}_{\mathbf{y}_{\bullet 1}, \mathbf{y}_{\bullet 2}} = \frac{\langle \mathbf{y}_{\bullet 1}, \mathbf{y}_{\bullet 2} \rangle}{\|\mathbf{y}_{\bullet 1}\|_{2} \cdot \|\mathbf{y}_{\bullet 2}\|_{2}}$$
(16)

Recalling Equations 11 and 12, I denote the *i*-th row of matrix A as $\mathbf{u}_{i\bullet}$ and rephrase the inner product in Equation 16 as:

$$\langle \mathbf{y}_{\bullet 1}, \mathbf{y}_{\bullet 2} \rangle = \langle [\mathbf{u}_{1\bullet} \cdot \mathbf{b}_{\bullet 1} \dots \mathbf{u}_{i\bullet} \cdot \mathbf{b}_{\bullet 1} \dots \mathbf{a}_{n\bullet} \cdot \mathbf{b}_{\bullet 1}], [\mathbf{u}_{1\bullet} \cdot \mathbf{b}_{\bullet 2} \dots \mathbf{u}_{i\bullet} \cdot \mathbf{b}_{\bullet 2} \dots \mathbf{u}_{n\bullet} \cdot \mathbf{b}_{\bullet 2}] \rangle$$
$$= (\mathbf{U}\mathbf{b}_{\bullet 1})^T \mathbf{U}\mathbf{b}_{\bullet 2}$$
(17)

The equivalence in Equation 17 also applies to the denominator of Equation 16 since, for a given feature j, $\|\mathbf{y}_{\bullet j}\|_2 = \sqrt{\langle \mathbf{y}_{\bullet j}, \mathbf{y}_{\bullet j} \rangle}$. Hence, substituting Equation 17 in Equation 16 yields:

$$\frac{\langle \mathbf{y}_{\bullet 1}, \mathbf{y}_{\bullet 2} \rangle}{\|\mathbf{y}_{\bullet 1}\|_{2} \cdot \|\mathbf{y}_{\bullet 2}\|_{2}} = \frac{\mathbf{b}_{\bullet 1}^{T} \mathbf{U}^{T} \mathbf{U} \mathbf{b}_{\bullet 2}}{\sqrt{\mathbf{b}_{\bullet 1}^{T} \mathbf{U}^{T} \mathbf{U} \mathbf{b}_{\bullet 1}} \sqrt{\mathbf{b}_{\bullet 2}^{T} \mathbf{U}^{T} \mathbf{U} \mathbf{b}_{\bullet 2}}}$$
$$= \frac{\mathbf{b}_{\bullet 1}^{T} \mathbf{b}_{\bullet 2}}{\sqrt{\mathbf{b}_{\bullet 1}^{T} \mathbf{b}_{\bullet 1}} \sqrt{\mathbf{b}_{\bullet 2}^{T} \mathbf{b}_{\bullet 2}}}$$
$$= \frac{\langle \mathbf{b}_{\bullet 1}, \mathbf{b}_{\bullet 2} \rangle}{\|\mathbf{b}_{\bullet 1}\|_{2} \cdot \|\mathbf{b}_{\bullet 2}\|_{2}}$$
$$\operatorname{corr}_{\mathbf{y}_{\bullet 1}, \mathbf{y}_{\bullet 2}} = \cos \theta \tag{18}$$

where $\mathbf{U}^T \mathbf{U} = \mathbf{I}$ is a property of the "left" eigenvectors matrix from Equation 9. In our example, one can verify that the cosine similarity between $\mathbf{b}_{\bullet 1}$ and $\mathbf{b}_{\bullet 2}$ is $\cos \theta = 0.84$, which indeed equivalent to the correlation coefficient between $\mathbf{y}_{\bullet 1}$ and $\mathbf{y}_{\bullet 2}$:

```
cos_theta_ab <- (B[1,] %*% B[2,]) / (norm(B[1,], "2")*norm(B[2,], "2"))
all.equal(as.numeric(cos_theta_ab), as.numeric(cor(Y[,1], Y[,2])))</pre>
```

[1] TRUE

3 Discussion of comparative insights

This section develops the computational building blocks summarised earlier, into an implementation-agnostic evaluation grid, and discusses how specific implementations compare within such grid. The implementations examined here are those listed in Tab.1, with key comparative insights summarised upfront in Tab.3 and Tab.4 below. Within these tables, the proposed evaluating grid informs the chosen column headers. The following subsections detail how these insights came about.

			Loadings (eige	envectors)	Eigen/singul	ar values	PCA scores		
			Cov. mat.	SVD right.	Cov. mat.	SVD	Cov. mat.	SVD, left	Variance
	Function	$M.D.^1$	$\mathbf{V} = \left[\mathbf{a}_{j} ight]_{n imes m}$	$ \mathbf{v}_j = \mathbf{a}_j $	$\boldsymbol{\lambda} = \left[\lambda_j\right]_{n \times 1}$	$\frac{\ell_j}{\sqrt{n-1}} = \sqrt{\lambda_j}$	$\mathbf{z}_j = \mathbf{Y} \mathbf{a}_j$	$\mathbf{z}_j = \mathbf{u}_j \ell_j$	$\operatorname{Var}\left[\mathbf{z}_{j}\right] = \lambda_{j}$
SVD-based									
base-R	prcomp()	a		rotation		$ t s extsf{dev} = \sqrt{\lambda_j}$		x	•
pcaMethods	pca()	a		loadings		$ t s extsf{Dev} eq \sqrt{\lambda_j}$		scores	•
PCAtools	pca()	a		loadings		$ ext{sdev} eq \sqrt{\lambda_j}$		rotated	•
ggbiplot	getsvd()								
Eigenproblme	e								
base-R	<pre>princomp()</pre>	b	loadings			$ t s extsf{dev} = \sqrt{\lambda_j}$	scores		
ade4	dudi.pca()	b	c1			$\texttt{eig} = \sqrt{\lambda_j}$	li		
amap	acp()	с	loadings			$\texttt{eig} = \sqrt{\lambda_j}$	scores		
psych	<pre>principal()</pre>	d	$loadings^2$		values		\mathtt{scores}^2		
Gen. SVD-ba	sed								
FactoMineR	PCA()	a		svd\$V		$rac{\ell_j}{\sqrt{n}} = \texttt{svd}\\texttt{vs}		ind\$coord	0
PCAmixdata	PCAmix()	a		svd\$V		$\frac{\ell_j}{\sqrt{n}} = \text{svd}$ \$vs		ind\$coord	0
factoextra	getpca()					v			

Table 3: Selected implementations, PCA focus

Note: The evaluation grid appears in the column headings. \circ indicates an equivalence that holds with caveats. ¹ Matrix being decomposed: (a) **Y**; (b) n^{-1} **Y**^T**Y**; (c) **Y**^T**Y**; (d) **S** ² These outputs correspond to, respectively: $\mathbf{a}_j \sqrt{\lambda_j}$ and $\mathbf{z}_j \sqrt{\lambda_j}$

		Observ. coord.		Feat. coord.		Feat. coord. properties	
	Function	$\begin{array}{l} \text{Scaled} \\ \mathbf{A} = \mathbf{U} \end{array}$	As is ¹ $\mathbf{A} = \mathbf{Z}$	Scaled $\mathbf{B}^T = \mathbf{D}\mathbf{V}^T$	As is ¹ $\mathbf{B} = \mathbf{V}$	St. Dev. (single feat.) $\ \mathbf{b}_j\ (n-1)^{1/2} = \sigma_j$	Corr. coeff. (feat. pair) $\operatorname{corr}_{\mathbf{y}_i,\mathbf{y}_j} = \cos\theta_{ij}$
SVD-based							
base-R	<pre>biplot()</pre>	0		0		0	0
pcaMethods	slplot()		•		•		
PCAtools	<pre>biplot()</pre>		•		•		
ggbiplot	ggbiplot()		0	0		0	0
Eigenproblem	L						
base-R	<pre>biplot()</pre>	0		0		0	0
ade4	<pre>scatter()</pre>		•		•		
amap	plot()		•		•		
psych	<pre>biplot.psych()</pre>		٠		•		
Gen. SVD-ba	sed						
FactoMineR	plot.PCA()		•	•			
PCAmixdata	<pre>plot.PCAmix()</pre>			•			
factoextra	<pre>fviz_pca_biplot()</pre>		•	•			

Table 4: Selected implementations, principal component biplots ($\alpha = 0$)

Note: The evaluation grid appears in the column headings. \circ indicates an equivalence that holds with caveats. ¹ Equivalent to the PCA scores matrix; ² Equivalent to the loadings matrix.

	Raw d	ata \mathbf{X}			PCA scores $\mathbf{Z}_{SVD} = \mathbf{U}\mathbf{D}$			PCA scores \mathbf{Z}				Biplot ${\bf U}$		
	feat1	feat2	feat3	feat4	PC1	PC2	PC3	PC4	PC1	PC2	PC3	PC4	PC1	PC2
А	10.00	6.00	12.00	5.00	-7.44	1.16	-0.89	-0.04	7.44	-1.16	-0.89	-0.04	-0.51	0.27
В	11.00	4.00	9.00	7.00	-5.70	-1.51	1.92	-0.03	5.70	1.51	1.92	-0.03	-0.39	-0.35
С	8.00	5.00	10.00	6.00	-4.58	-0.18	-1.08	0.13	4.58	0.18	-1.08	0.13	-0.31	-0.04
D	3.00	3.00	2.50	2.00	4.94	2.63	0.51	-0.38	-4.94	-2.63	0.51	-0.38	0.34	0.61
E	2.00	2.80	1.30	4.00	6.26	0.67	0.32	0.55	-6.26	-0.67	0.32	0.55	0.43	0.16
F	1.00	1.00	2.00	7.00	6.51	-2.77	-0.79	-0.23	-6.51	2.77	-0.79	-0.23	0.44	-0.64
mean	5.83	3.63	6.13	5.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
sample var.	18.97	3.13	22.25	3.77	42.95	3.73	1.32	0.10	42.95	3.73	1.32	0.10	0.20	0.20

Table 5: PCA scores for an illustrative example with m = 4 features and n = 6 observations. Matrix **Z** obtained by eigendecomposition of the covariance matrix **S**; matrix **Z**_{SVD} obtained by SVD of matrix **Y**; Last two columns: observations' coordinates on the biplot also from SVD

To provide a benchmark, Tab.5 extends the illustrative example to include more than two features. Fig.3 shows the corresponding biplot for a rank-2 approximation assuming that the first two components are retained. The tables show that specific functions may share the same algebraic rationale, yet differ in how the relevant computations are carried out for each building block.

The grid includes verification equivalences corresponding to Equations 5, 14, and 18 i.e., relationships that should hold if the computational rationale underpinning each technique—illustrated in previous sections—is followed correctly. Strikingly, these equivalences rarely follow without caveats from the output of specific implementations alone.

3.1 Group 1: SVD

The first group of **R** implementations considered here has a common trait: the function svd() is at work under the hood, providing what is needed to obtain a *scores matrix*, as per Equation 8, as well as the coordinates for both observations and features in a principal component biplot, as per Equation 9. This is specifically the case for Base-R, functions like prcomp() and biplot(), although some caveats apply in the latter case.

For example, the command $test_pcal < -prcomp(X, scale = FALSE)$ applies svd() under the hood to the centred data matrix Y. The returned output x corresponds to the PCA *scores* in columns 7-8 in Tab.5, whereas rotation, returns the matrix of right eigenvectors or *loadings*.

One aspect that stands out from Tab.3 is that, unlike other implementations in this group, prcomp() satisfies Equation 7, which verifies the relationship between the eigenvalues of the covariance matrix **S**, the St.Dev. of the scores, and the singular values from an SVD:

```
all.equal(test_pca1$sdev*sqrt(nrow(Y)-1), svd(Y)$d)
```

[1] TRUE

As a corollary, the function also satisfies Equation 5:

all.equal(as.numeric(test_pca1\$sdev^2), as.numeric(apply(test_pca1\$x,2,var)))

[1] TRUE

The script stats:::prcomp.default reveals how this is achieved: the output sdev returns the singular values from the SVD divided by $\sqrt{n-1}$, consistently with Equation 7:

all.equal(svd(Y)\$d/sqrt(nrow(Y)-1), test_pca1\$sdev)

[1] TRUE

In base-R, a principal component biplot can be obtained from prcomp() via the biplot() function. Although users are presented with a graphical output, biplot() does not return the jointly computed coordinates



Figure 3: Biplot of observations and features (shown as numbers) for an extended example based on SVD. The superposed dual axes outside the plot reflect the different scale of the features' coordinates.

for features and observations. The function's script stats:::biplot.prcomp reveals good alignment with Equations 11 and 12, except for an imprecision in how the singular values are arrived at—which explains the caveats for this function in Tab.3.

Specifically, biplot.prcomp computes the singular values from the output sdev of a prcomp object. How it does so depends on the argument pc.biplot: the default setting is FALSE, with TRUE denoting that a principal component biplot is desired. Contrary to what one may expect, when pc.biplot=TRUE the function sets the singular values equal to sdev, disagreeing with Equation 7, which in turn affects Equations 11, 12 and 14. Surprisingly, when pc.biplot=FALSE the singular values are computed in a fashion similar to Equation 7, although it is erroneously assumed that sdev returns the singular values divided by \sqrt{n} instead of $\sqrt{n-1}$, the latter being the case for prcomp().

Due to these assumptions, when the argument pc.biplot is (contestably) FALSE the singular values returned by biplot.prcomp are close to, but different from ℓ from Equation 7:

```
lam <- test_pca1$sdev*sqrt(nrow(test_pca1$x))
all.equal(lam, svd(Y)$d)</pre>
```

[1] "Mean relative difference: 0.08712907"

With the singular values thus obtained, biplot.prcomp computes the matrix of observations coordinates A from the scores matrix consistently with Equation 11. Yet the result differs from what Equation 11 suggests, and hence from what is shown in Tab.5and Fig.3:

all.equal(unname(sweep(test_pca1\$x,2,lam,"/")), svd(Y)\$u)

[1] "Mean relative difference: 0.09544512"

The caveat in Tab.4 acknowledges that the equivalence $\mathbf{A} = \mathbf{U}$ could be attained with minor changes in how singular values are computed by **biplot.prcomp**, namely:

```
sv <- test_pca1$sdev*sqrt(nrow(Y)-1)
all.equal(unname(sweep(test_pca1$x,2,sv,"/")), unname(svd(Y)$u))</pre>
```

[1] TRUE

Similar caveats apply to the features' coordinates. In principle, the underlying computations in biplot.prcomp are consistent with Equation 12, which yields matrix **B**, except that these results are also affected by how singular values are computed. In our example, the features' coordinates produced by biplot() are different from matrix **B** in Equation 12—which is displayed in Fig.3:

```
B <- t(D %*% t(V))
all.equal(unname(sweep(test_pca1$rotation,2,lam,"*")), B)</pre>
```

[1] "Mean relative difference: 0.08712907"

Just like the base-R functions examined so far, several curated packages rely on conventional SVD, too. In particular, *PcaMethods* (Stacklies et al. 2007) and *PCAtools* (Blighe and Lun 2023) extend traditional PCA methods to handle computational challenges that are specific to bioinformatics data. While both packages offer a homonym function pca(), they differ in the extent to which they rely on base-R function. For the implementation pcaMethods::svdPca, reliance on prcomp() is explicit upon examination of the function's script, and promptly ascertained. For example:

```
test_pca2 <- pcaMethods::pca(Y, method = "svd")
all.equal(test pca2@scores, test pca1$x[,1:2])</pre>
```

[1] TRUE

So long as the selected method in pcaMethods::svdPca is svd the equivalence with prcomp() can be verified in a similar fashion for loadings and sDev.

With regards to PCAtools::pca, the analogy with prcomp() is less straightforward to identify as it relies on another package, *BiocSingular*, to carry out an SVD. Yet the results associated with a so-called "exact" SVD are, once again, equivalent to prcomp(). For example:

```
test_pca3 <- PCAtools::pca(X, transposed = T)
all.equal(as.matrix(test_pca3$rotated), test_pca1$x)</pre>
```

[1] TRUE

The equivalence with prcomp() can be verified in a similar fashion for loadings and sdev.

Unlike their base-R counterpart, the biplot functions in packages *pcaMethods* and *PCAtools* do not strictly speaking generate a principal components biplot as per Equation 9. The function pcaMethods::slplot displays two separate plots of *scores* and *loadings* whose coordinates are derived, respectively, from he the outputs x and rotation of the function prcomp() without further processing. Despite its name, the function PCAtools::biplot(), too, overlays a scores and a loadings plot.

The packages ggbiplot (Vu and Friendly 2024) is dedicated to biplots. Like biplot() in base-R, also ggbiplot() assumes that an SVD-based PCA be carried out separately e.g., by prcomp(). The documentation acknowledges that PCA implementations may differ in how they go about an SVD, and that get_SVD() seeks to provide a unifying interface. Yet get_SVD() suffers from some imprecisions already encountered for biplot.prcomp e.g., it assumes that the output sdev of a prcomp() object is equivalent to the singular values divided by \sqrt{n} instead of $\sqrt{n-1}$. For the singular values thus defined, both get_SVD() and biplot.prcomp return the same observations' coordinates:

```
test_pca4 <- ggbiplot::get_SVD(test_pca1)
all.equal(test_pca4$U[,1:2], sweep(test_pca1$x,2,lam,"/")[,1:2])</pre>
```

[1] TRUE

If Equation 9 was followed, instead, the output U from ggbiplot::get_SVD() would represent the biplot coordinates for the observations, as well as the matrix of left eigenvalues from an SVD. Instead, such output is further processed by the function ggbiplot() as follows: if the desired output is a principal component biplot i.e., if the argument pc.biplot is true, ggbiplot() multiplies U by sdev and, continuing with assumption the input is a prcomp() object, by $\sqrt{n-1}$ as well. Ultimately, this process reverts back to the PCA scores, multiplied by the ratio $\sqrt{n-1}/\sqrt{n}$, hence the caveat in Tab.4:

```
df.u <- as.data.frame(sweep(test_pca4$U[, 1:2], 2, test_pca4$D[1:2], FUN = "*"))
df.u <- df.u * sqrt(nrow(test_pca1$x) - 1)
all.equal(test_pca1$x[,1:2] * sqrt(nrow(Y)-1) / sqrt(nrow(Y)), as.matrix(df.u))</pre>
```

Moving on to the features' coordinates, ggbiplot() operates similarly to Equation 12, except that the scores' St.Dev. sdev from prcomp() are used instead of the singular values **D**. Hence the results not only disagree with Equation 12, but also with biplot.prcomp:

```
df.v <- as.data.frame(sweep(test_pca1$rotation[, 1:2], 2, test_pca4$D[1:2], FUN = "*"))
all.equal(sweep(test_pca1$rotation[,1:2],2,lam[1:2],"*"), as.matrix(df.v))</pre>
```

[1] "Mean relative difference: 0.5917517"

3.2 Group 2: eigenvalue problem

The second group of implementations considered here follows more closely the variance optimisation rationale underlying PCA, and the eigendecomposition problem in Equation 4 concerning the covariance matrix \mathbf{S} . Whilst less prevalent than SVD, R implementations adopting this approach are commonly adopted in the literature—e.g., Mayor (2015); Hanson and Harvey (2022). Yet there may be discrepancies between our agnostic evaluation grid for both base-R and curated packages.

A natural starting point is the function princomp() in base-R. Nearly a homonym of prcomp(), this implementation relies upon the eigenvalues and eigenvectors of the covariance matrix S, rather than the outputs of a data-matrix SVD. Yet princomp() disagrees with Equation 2 in that it uses the number of observations n, not n - 1, as the divisor for the covariance matrix. What is more, the signs of the scores returned by princomp() differ from those computed directly using eig() due to further processing within the function:

```
test_pca5 <- princomp(X, fix_sign = F)
test_pca5_eig <- eigen(1/nrow(Y)*t(Y) %*% Y, symmetric = TRUE)$vectors
all.equal(abs(unname(Y %*% test_pca5_eig)), abs(unname(test_pca5$scores)))</pre>
```

[1] TRUE

Hence, the scores returned by princomp() differ in sign from Z shown in Tab.5 despite both being obtained from eig().

When PCA is implemented using princomp() instead of prcomp(), the eigenvalues do not equal the variance of the scores as in Equation 5:

all.equal(as.numeric(test_pca5\$sdev^2), as.numeric(apply(test_pca5\$scores,2,var)))

[1] "Mean relative difference: 0.2"

An object form princomp() can serve as an input to the functions biplot() and ggbiplot::ggbiplot() examined earlier. Hence, the same caveats discussed before apply, with the difference that now both functions are correct in assuming that the the singular values from an SVD are equivalent to multiplying the output sdev of princomp() times \sqrt{n} :

all.equal(as.numeric(svd(Y)\$d), as.numeric(test_pca5\$sdev*sqrt(nrow(Y))))

[1] TRUE

An option which is very close to princomp() in base-R is the function dudi.pca() from the package *ade4*(Thioulouse et al. 2018). Both functions define the covariance matrix of the centred data-points in similar terms, thus generating comparable outputs for PCA scores

```
test_pca6 <- ade4::dudi.pca(X, center = TRUE, scale = FALSE, scannf = FALSE, nf = ncol(Y))
all.equal(unname(as.matrix(test_pca6$li)), unname(as.matrix(test_pca5$scores)))</pre>
```

Similar equivalences hold for the eigenvectors (loadings) and eigenvalues of covariance matrix. The implementation in dudi.pca(), too, disagrees with Equation 5:

all.equal(as.numeric(test_pca6\$eig), as.numeric(apply(test_pca6\$li,2,var)))

[1] "Mean relative difference: 0.2"

Package *amap* (Lucas 2022) provides a different take on the covariance matrix with its function $\mathtt{amap:::acp()}$, which computes the eigenvalues and eigenvectors of $\mathbf{Y}^T \mathbf{Y}$, unlike the previous options:

```
test_pca7 <- amap:::acp(X, reduce = FALSE)
test_pca7_eig <- eigen(t(Y) %*% Y, symmetric = FALSE)
all.equal(unname(test_pca7_eig$vectors), unname(test_pca7$loadings))</pre>
```

[1] TRUE

Confusingly, the function's output **eig** returns the square roots of the eigenvalues:

all.equal(sqrt(test_pca7_eig\$values), test_pca7\$eig)

[1] TRUE

In absolute values, the scores and loadings generated by acp() are comparable to those obtained in the previous cases, as well as with those in Tab.5. Oddly, the output sdev of the function acp() is computed directly as the St.Dev. of such scores:

all.equal(test_pca7\$sdev, apply(test_pca7\$scores, 2, sd))

[1] TRUE

Yet the equivalence in Equation 5 is not satisfied:

```
all.equal(unname(test_pca7_eig$values), apply(unname(test_pca7$scores), 2, var))
```

[1] "Mean relative difference: 0.8"

Unlike the implementations described so far, the function principal() from the package *psych* (Revelle, W. 2024) runs an eigendecomposition of the covariance matrix **S**, consistently with our evaluation grid. Except that the meaning of "loadings" is peculiarly defined as the eigenvectors rescaled by the square root of the eigenvalues. This is reminiscent of—but not identical to—the feature's coordinate in a biplot obtained in Equation 12.

If principal() is applied to the centred data matrix, and if the implicit scaling just mentioned is corrected, then the scores are equivalent, in absolute values, with those shown in Tab.5:

```
test_pca8 <- psych::principal(Y, nfactors = 0, cor="cov", rotate = "none")
test_pca8_adjscor <- sweep(unname(test_pca8$scores), 2, sqrt(test_pca8$values), "*")
all.equal(abs(test_pca8_adjscor), abs(unname(Z)))</pre>
```

[1] TRUE

Similar considerations apply to the outputs loadings and values. The latter returns the covariance matrix's eigenvalues, and satisfies the equivalence in Equation 5 provided that the scores are once again corrected from their implicit scaling:

```
all.equal(unname(test_pca8$values), apply(test_pca8_adjscor, 2, var))
```

All three packages considered in this section offer visualisation facilities for generating a combined plot of the PCA *scores* and *loadings*. Examples include scatter() for dudi.pca() objects; plot(), for acp() objects; and biplot() for principal() objects. Yet none of these functions seems to jointly compute the features' and observations' coordinates according to Equation 9, hence one could question whether their visual output is a principal component biplot.

What is more, objects generated by dudi.pca() can also be an input to the function ggbiplot() discussed in the previous section. A word of caution, however, is necessary as this biplot implementation may not agree with Equation 9 due to how get_SVD() chooses the equivalent of the left and right eigenvector matrices needed to generate a biplot—in addition to the caveats already mentioned.

3.3 Group 3: generalised SVD

The final group of implementations shares an intent to move beyond some of the restrictions concerning what type of data can be handled by PCA, allowing for the inclusion, for example, of "mixed" data. Another commonality is that the underlying computational device is the so-called "generalised" SVD (Abdi and Williams 2010, Appendix B). None of these characteristics seem to have equivalent implementations in base-R.

The most prominent package in this group is probably FactoMineR (Lê, Josse, and Husson 2008), whose functions PCA() is of particular interest here (e.g., Pagès 2014, Ch. 1). This implementation is underpinned by a generalised SVD function svd.triplet(), which also operates under the hood of packages such as PCAmixdata (Chavent et al. 2022).

As in previous cases, the PCA scores are equivalent, in absolute values, to those in Tab.5. Since the results of the generalised SVD are available as part of the outputs of PCA(), users can directly verify that the PCA scores are obtained consistently with Equation 8:

```
test_pca9 <- FactoMineR::PCA(X, scale.unit = FALSE)</pre>
```

```
D <- diag(test_pca9$svd$vs)
all.equal(test_pca9$ind$coord, test_pca9$svd$U %*% D)</pre>
```

[1] TRUE

The singular values in this generalised SVD are related to the eigenvalues of the covariance matrix whose elements are divided by \sqrt{n} instead of $\sqrt{n-1}$, which we encountered previously:

```
all.equal(test_pca9$eig, test_pca9$svd$vs^2)
```

[1] TRUE

all.equal(test_pca9\$eig, unname(eigen(1/nrow(Y)*t(Y) %*% Y)\$values))

[1] TRUE

However, this implementation too disagrees with the equivalence between the scores' variance and covariance matrix's eigenvalues in Equation 5:

all.equal(apply(test_pca9\$ind\$coord,2,var) , test_pca9\$eig)

[1] "Mean relative difference: 0.16666667"

Moving on to the biplot implementations in this group, it is worth noting that PCA() generates coordinates for both features and observations and it automatically produces a plot for each when called. The observations features are simply the scores, whereas the features' coordinates correspond to matrix **B** in Equation 12:

```
all.equal(test_pca9$var$coord, test_pca9$svd$V %*% D)
```

Based on the above it seems reasonable to conclude that visualisation devices like FactoMineR:: plot.PCA() and PCAmixdata::plot.PCAmix() do not generate, strictly speaking, a principal component biplot. The package *factoextra* (Kassambara and Mundt 2020) provides additional visualisation facilities building on the output generated by PCA(), such as the function fviz_pca_biplot(). Yet I could not ascertain an immediate connection with Equation 9.

It is worth noting that PCA() and fviz_pca_biplot() hint to the relationship between how features correlate and the angles formed by the vectors that represent their coordinates on a biplot (see e.g., Pagès 2014, Ch. 1; Kassambara 2017). Despite the terminology used, these metrics bear little resemblance with the properties concerning the the cosine of the angle between features' vectors on a principal components biplot, or their lengths, from Equations 14 and 18.

4 Concluding remarks

PCA and biplots are well-established techniques, and when it comes to resources illustrating how they are done in practice, **R** users are spoiled for choice. Whilst most resources hint to the underpinning matrix decomposition approaches, it is not customary to dwell on how key computational building blocks come about. Users are often left with a rather procedural understanding of PCA and biplots tied to specific implementations. Also, the overwhelming prevalence of SVD-based approaches can obscure the rationale with which one arrives at such concepts as *scores* and *loadings*.

In a context where implementing PCA and biplots has become somewhat a conditioned reflex, one can hardly resist the temptation to give for granted the internal workings. Yet in this note I have taken a back-to-basics approach to comparing PCA and biplots implementations in base R and a selection of contributed R packages. This approach highlighted useful equivalences that should hold if the computational rationale underpinning each technique is followed correctly.

Findings suggest that discrepancies from an implementation-agnostic understanding of PCA and biplots do arise, in both base R and contributed R packages, from seemingly innocuous computational choices made under the hood. Surprisingly, the identified verification equivalences rarely follow without caveats from the output of specific implementations alone. What is more, biplots are often just a misnomer due to imprecisions in how the underlying computational aspects are dealt with.

Base-R implementations such as prcomp() and biplot() appear to be most convincingly aligned with what one expects from the fundamental algebra of PCA and biplots, although some caveats apply in the case of biplot that might call for minor amendments. Despite being based on an SVD, functions like prcomp() adhere more closely to our evaluation grid than princomp() or psych::principal(). Functions with richer capabilities and better visualisation devices, which are understandably more popular amongst user, are harder to reconcile with an implementation-agnostic understanding of PCA and biplots. This is the case for packages like *FactoMineR* and *ggbiplot*.

This work has no pretence of comprehensiveness, and only some of the scripts could be reviewed in an attempt to pinpoint possible discrepancies from the proposed evaluation grid. Other resources provide more hands-on comparative outlooks that might speak to practitioners better than this note does; yet they rarely include biplots or offer an implementation-agnostic perspective.

Despite its limitations, the hoped for outcome of this note is to raise awareness that getting back-to-basic in PCA and biplot—two techniques practically given for granted—helps to elevate aspects that are usually disregarded for comparative purposes, and to address discrepancies that users continue to find elusive despite the extensive resources available for their implementation.

References

Abdi, H., and L. J. Williams. 2010. "Principal Component Analysis." WIREs Computational Statistics 2 (4): 433-59. https://doi.org/https://doi.org/10.1002/wics.101.

amoeba. 2015. "Answer to: Making Sense of Principal Component Analysis, Eigenvectors and Eigenvalues." Cross Validated. 2015. https://stats.stackexchange.com/q/140579.

Binmore, K., and J. Davies. 2001. Calculus. Cambridge: Cambridge University Press.

- Blighe, K., and A. Lun. 2023. *PCAtools: PCAtools: Everything Principal Components Analysis.* https://doi.org/10.18129/B9.bioc.PCAtools.
- Bro, R., and A. K. Smilde. 2014. "Principal Component Analysis." Anal. Methods 6: 2812-31. https://doi.org/10.1039/C3AY41907J.
- Chavent, M., V. Kuentz-Simonet, A. Labenne, and J. Saracco. 2022. "Multivariate Analysis of Mixed Data: The r Package PCAmixdata." https://arxiv.org/abs/1411.4911.

du Toit, S. H. C., A. G. W. Steyn, and R. H. Stumpf. 1986. *Graphical Exploratory Data Analysis.* Springer. Everitt, B., and T. Hothorn. 2011. An Introduction to Applied Multivariate Analysis with r. Springer.

Gower, J. C., S. Lubbe, and N. LeRoux. 2011. Understanding Biplots. Chichester: Wiley.

- Hanson, Bryan A., and David T. Harvey. 2022. LearnPCA: Functions, Data Sets and Vignettes to Aid in Learning Principal Components Analysis (PCA). https://CRAN.R-project.org/package=LearnPCA.
- Jolliffe, I. T. 2004. Principal Component Analysis. 2nd ed. Springer.
- Kassambara, A. 2017. "PCA Principal Component Analysis Essentials." STHDA. 2017. http: //www.sthda.com/english/articles/31-principal-component-methods-in-r-practical-guide/ 112-pca-principal-component-analysis-essentials/#r-packages.
- Kassambara, A., and F. Mundt. 2020. Factoextra : Extract and Visualize the Results of Multivariate Data Analyses. https://cran.r-project.org/web/packages/factoextra/readme/README.html.
- Knox, S. W. 2018. Machine Learning: Topics and Techniques. 1st ed. Wiley.
- Kumar, A., and A. Paul. 2016. Mastering Text Mining with r. Pakt Publishing.
- Lê, S., J. Josse, and F. Husson. 2008. "FactoMineR: A Package for Multivariate Analysis." Journal of Statistical Software 25 (1): 1–18. https://doi.org/10.18637/jss.v025.i01.
- Lucas, A. 2022. Amap: Another Multidimensional Analysis Package. https://CRAN.R-project.org/package=amap.
- Marecek, L. 2017. Intermediate Algebra. OpenStax. https://openstax.org/books/ intermediate-algebra/pages/preface.
- Mayor, E. 2015. Learning Predictive Analytics with r. Pakt Publishing.
- Pagès, J. 2014. Multiple Factor Analysis by Example Using r. 1st ed. Chapman; Hall/CRC.
- Peng, R. D. 2020. "Exploratory Data Analysis with r SVD and PCA." 2020. https://bookdown.org/ rdpeng/exdata/dimension-reduction.html#svd-and-pca.
- Poole, D. 2014. Linear Algebra : A Modern Introduction. 4th ed. Brooks Cole.
- Revelle, W. 2024. Psych: Procedures for Psychological, Psychometric, and Personality Research. Evanston, Illinois: Northwestern University. https://CRAN.R-project.org/package=psych.
- Stacklies, W., H. Redestig, M. Scholz, D. Walther, and J. Selbig. 2007. "pcaMethods a Bioconductor Package Providing PCA Methods for Incomplete Data." *Bioinformatics* 23: 1164–67. https://doi.org/ 10.1093/bioinformatics/btm069.
- Starmer, J. 2018. "StatQuest: Principal Component Analysis (PCA), Step-by-Step." [media] Youtube. 2018. https://youtu.be/FgakZw6K1QQ?si=R0WqV5NwFNNKCXVv.
- Thioulouse, J., S. Dray, Dufour A.–B, A. Siberchicot, T. Jombart, and S. Pavoine. 2018. *Multivariate Analysis of Ecological Data with ade4*. Springer.
- Venables, W. N., and B. D. Ripley. 2002. Modern Applied Statistics with s. 4th ed. Springer.
- Vu, V. Q., and M. Friendly. 2024. *Ggbiplot: A Grammar of Graphics Implementation of Biplots*. https://CRAN.R-project.org/package=ggbiplot.