Reading

Nature Biotechnology **26**, 303 - 304 (2008)
doi:10.1038/nbt0308-303

What is principal component analysis?

Markus Ringnér[1]

Principal component analysis is often incorporated into genome-wide expression studies, but what is it and how can it be used to explore high-dimensional data?

PCA as a tool to Quantify and Visualise

Multivariate Analysis

Multiple Regression / two way-ANOVA / mixed models / machine learning algorithms

Ordination methods

What is the difference between these two pairwise correlation matrices?

	X_1	X_2	X_3	X_4	X_5
X_1	1.00	0.80	0.90	0.78	0.87
X_2	0.80	1.00	0.76	0.87	0.78
X_3	0.90	0.76	1.00	0.78	0.89
X_4	0.78	0.87	0.78	1.00	0.95
X_5	0.87	0.78	0.89	0.95	1.00

	X_1	X_2	X_3	X_4	X_5
X_1	1.00	0.87	0.96	0.04	0.05
X_2	0.87	1.00	0.95	0.03	0.07
X_3	0.96	0.95	1.00	0.04	0.05
X_4	0.04	0.03	0.04	1.00	0.84
X_5	0.05	0.07	0.05	0.84	1.00

What is the difference between these two pairwise correlation matrices?

	X_1	X_2	X_3	X_4	X_5
X_1	1.00	0.80	0.90	0.78	0.87
X_2	0.80	1.00	0.76	0.87	0.78
X_3	0.90	0.76	1.00	0.78	0.89
X_4	0.78	0.87	0.78	1.00	0.95
X_5	0.87	0.78	0.89	0.95	1.00

One dimension

	X_1	X_2	X_3	X_4	X_5
X_1	1.00	0.87	0.96	0.04	0.05
X_2	0.87	1.00	0.95	0.03	0.07
X_3	0.96	0.95	1.00	0.04	0.05
X_4	0.04	0.03	0.04	1.00	0.84
X_5	0.05	0.07	0.05	0.84	1.00

Two dimensions

Ordination analyses

- Uncover, organize and summarize the main patterns of variation in a set of variables measured over multiple observations.

- Patterns of variation are structured in a reduced space with smaller number number of dimensions.

- Reduction is possible because often variables are associated (e.g., correlated). Dimensions represent combinations (e.g., linear combinations of variables).

Ordination analyses

A procedure for adapting a multidimensional swarm of data points in such a way that when it is projected onto a reduced number of dimensions any intrinsic pattern will become apparent.

Adapted from Connie Clark

Ordination analyses – uncover and organize data; a quick example:

Species

Site	B	I	D	A	H	E	G	C
4	1	0	1	0	0	0	0	1
1	0	0	0	1	0	0	0	0
7	0	0	0	0	1	1	1	0
8	0	1	0	0	1	0	1	0
6	0	0	1	0	0	1	1	0
5	0	0	1	0	0	1	0	1
10	0	1	0	0	0	0	0	0
2	1	0	0	1	0	0	0	0
9	0	1	0	0	1	0	0	0
3	1	0	0	1	0	0	0	1

Ordination analyses – uncover and organize data; a quick example:

Species

Site	B	I	D	A	H	E	G	C
4	1	0	1	0	0	0	0	1
1	0	0	0	1	0	0	0	0
7	0	0	0	0	1	1	1	0
8	0	1	0	0	1	0	1	0
6	0	0	1	0	0	1	1	0
5	0	0	1	0	0	1	0	1
10	0	1	0	0	0	0	0	0
2	1	0	0	1	0	0	0	0
9	0	1	0	0	1	0	0	0
3	1	0	0	1	0	0	0	1

=

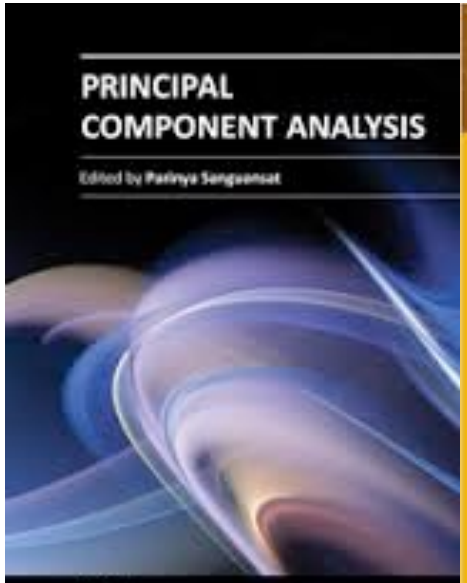
Species

Sites	A	B	C	D	E	G	H	I
1	1	0	0	0	0	0	0	0
2	1	1	0	0	0	0	0	0
3	1	1	1	0	0	0	0	0
4	0	1	1	1	0	0	0	0
5	0	0	1	1	1	0	0	0
6	0	0	0	1	1	1	0	0
7	0	0	0	0	1	1	1	0
8	0	0	0	0	0	1	1	1
9	0	0	0	0	0	0	1	1
10	0	0	0	0	0	0	0	1

Ordination methods

- **Principal Component Analysis (PCA)**
- Correspondence Analysis (CA)
- Principal Coordinate Analysis (PCoA)
- Discriminant Function Analysis (DFA)
- Principal Curve Analysis
- Etc, etc, etc…

Principal components analysis (PCA) is perhaps the most common technique used to summarize patterns among variables in multivariate datasets.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Edited by Parinya Sanguansat
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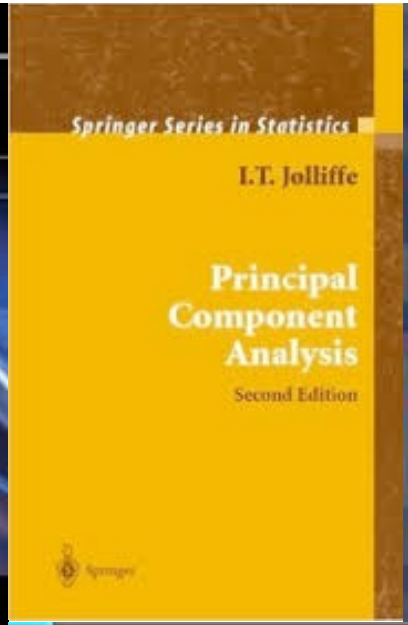
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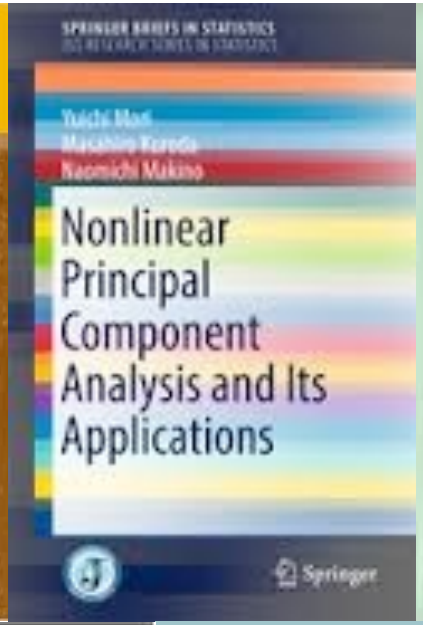
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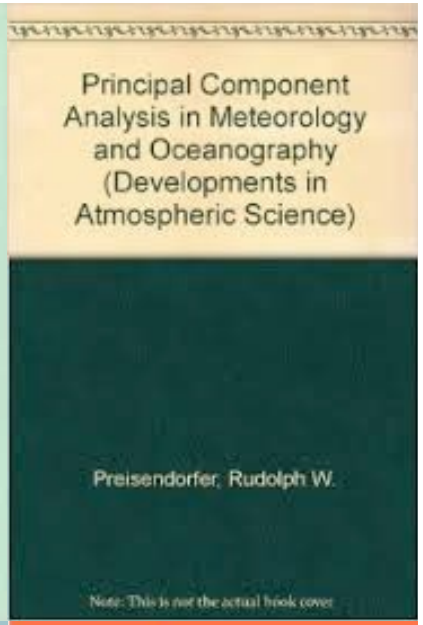
Principal Component
Analysis in Meteorology
and Oceanography
(Developments in
Atmospheric Science)
Preisendorfer, Rudolph W.
Note: This is not the actual book cover


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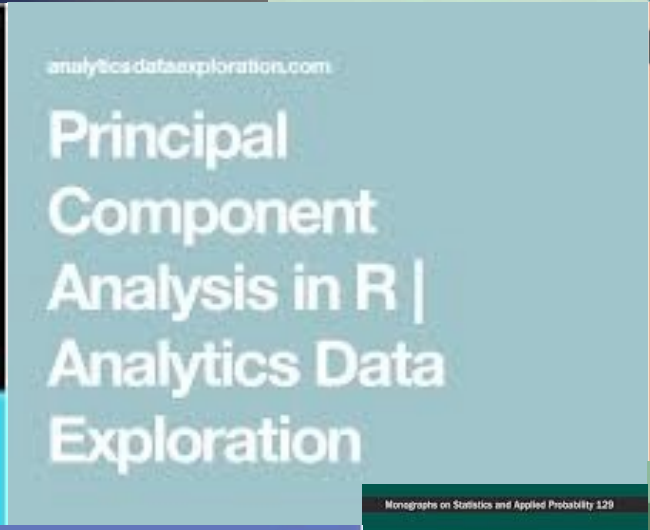
MULTIDISCIPLINARY APPLICATIONS
Edited by Parinya Sanguansat


Principal
Component Analysis
Contributors: Maria Manfreda et al.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Analysis in R |
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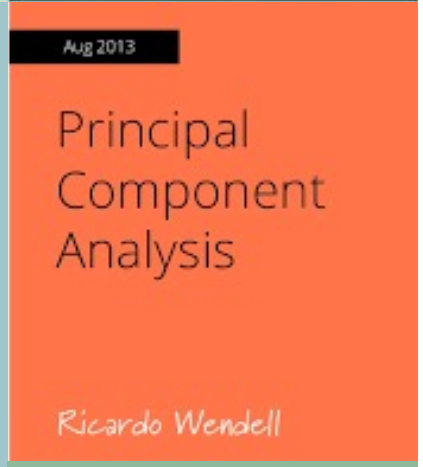
Aug 2013
Principal
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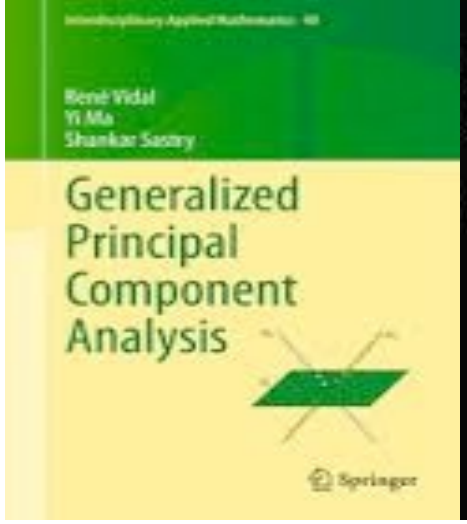
Analysis
Ricardo Wendell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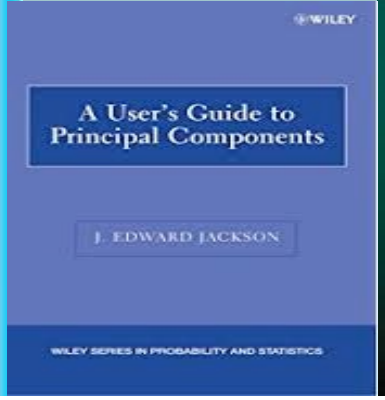
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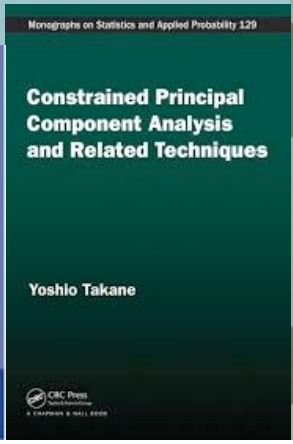
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Yoshio Takane
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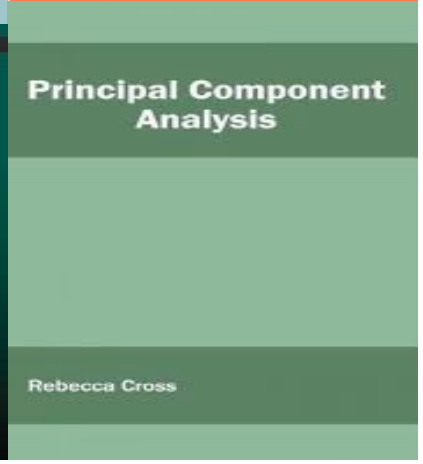
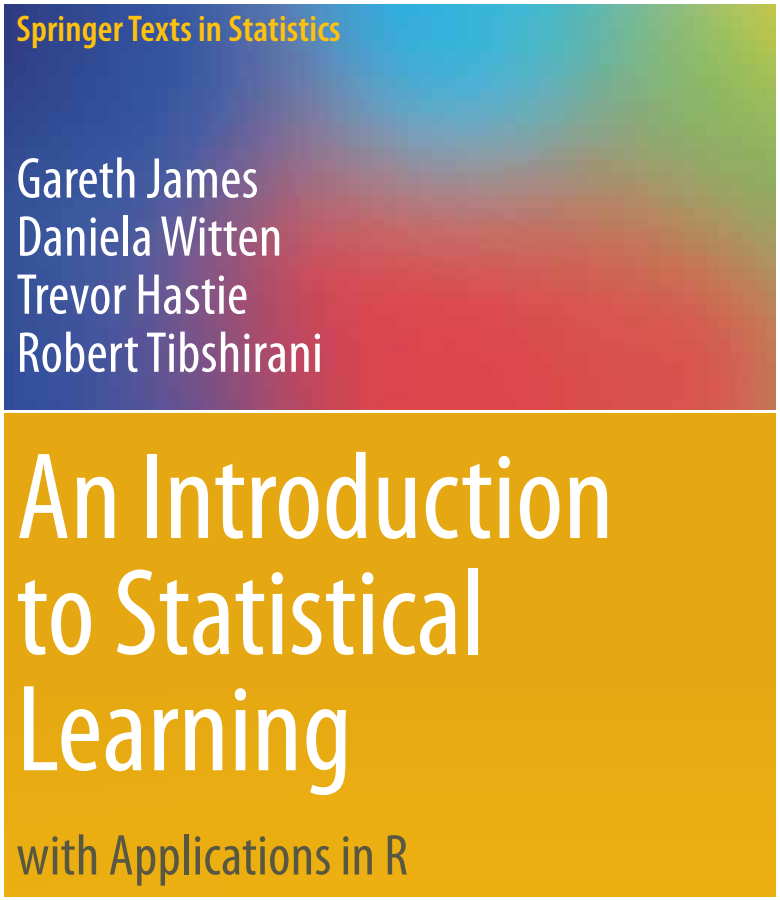

Principal Component
Analysis
Rebecca Cross

Some treat Principal Component Analysis (PCA) as an unsupervised learning method (an exploratory technique such as k-means)



Supervised *versus* unsupervised learning techniques

- Techniques for unsupervised learning are fast growing in a number of fields, particularly biology.

- A cancer researcher might assay gene expression levels in 100 patients with breast cancer. They might then look for subgroups among the breast cancer samples, or among the genes, in order to obtain a better understanding of the disease.

- A search engine might choose what search results to display to a particular individual based on the click histories of other individuals with similar search patterns. These statistical learning tasks, and many more, can be performed via unsupervised learning techniques.

Adapted from James et al. 2013

Supervised *versus* unsupervised learning techniques

In contrast, unsupervised learning is often much more challenging. The exercise tends to be more subjective, and there is no simple goal for the analysis, such as prediction of a response.

Unsupervised learning is often performed as part of an exploratory data analysis.

Hard to assess the results obtained given that there is no universally accepted mechanism for performing cross-validation or validating results on an independent data set; there is no way to check how the models does because we don't know the true answer—the problem is unsupervised.

Adapted from James et al. 2013

Examples of Principal Component Analysis

Principal components analysis (PCA) - example 1

A subtype of childhood acute lymphoblastic leukaemia with poor treatment outcome: a genome-wide classification study

Monique L Den Boer, Marjon van Slegtenhorst*, Renée X De Menezes, Meyling H Cheok, Jessica G C A M Buijs-Gladdines, Susan T C J M Peters, Laura J C M Van Zutven, H Berna Beverloo, Peter J Van der Spek, Gaby Escherich†, Martin A Horstmann†, Gritta E Janka-Schaub†, Willem A Kamps‡, William E Evans, Rob Pieters‡*

Summary

Background Genetic subtypes of acute lymphoblastic leukaemia (ALL) are used to determine risk and treatment in children. 25% of precursor B-ALL cases are genetically unclassified and have intermediate prognosis. We aimed to use a genome-wide study to improve prognostic classification of ALL in children.

Lancet Oncol 2009; 10: 125–34

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Quantification and Visualisation

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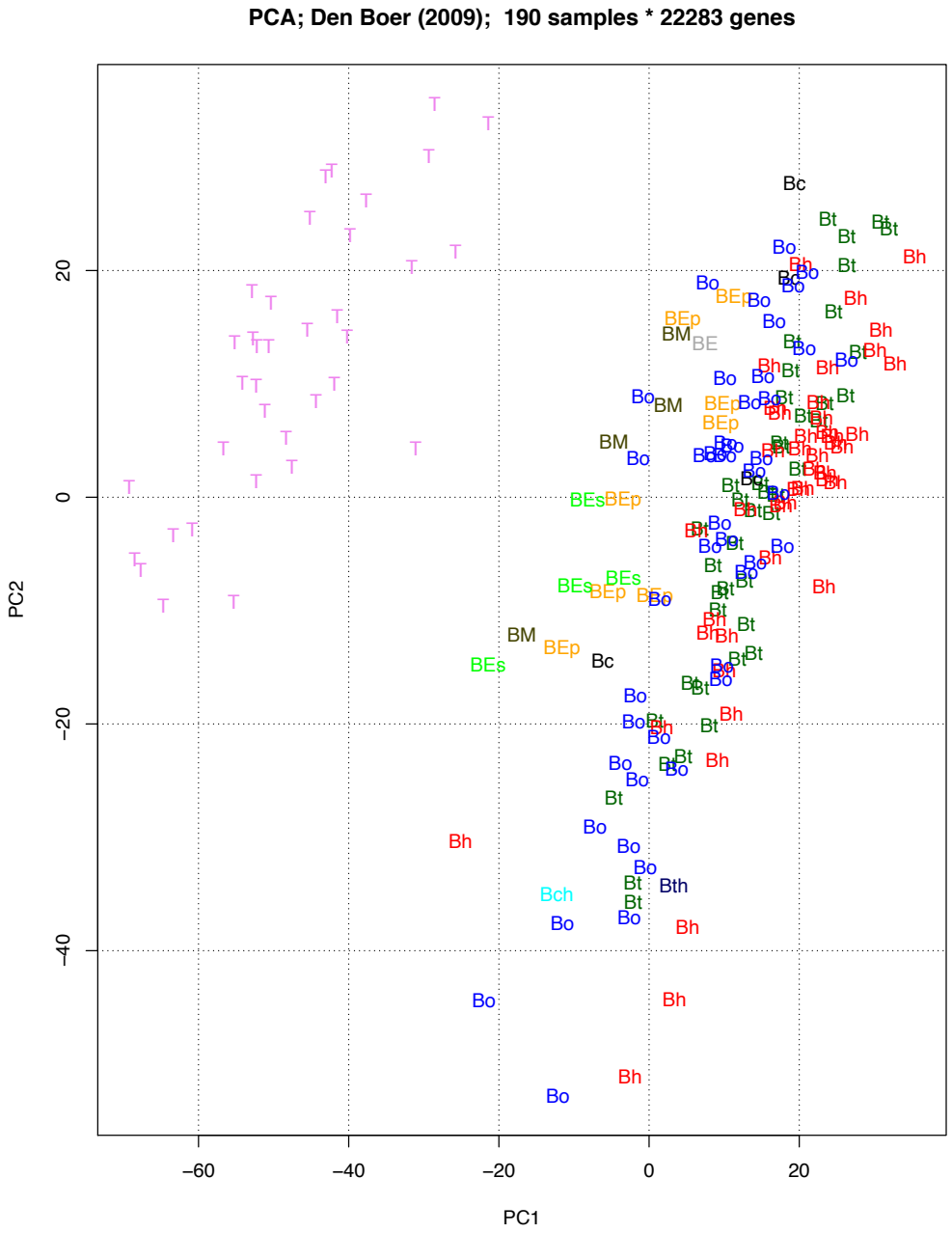
Data matrix: 190 observations by 22283 columns

Gene expression (22283 genes)

Gene expression (190 patients)

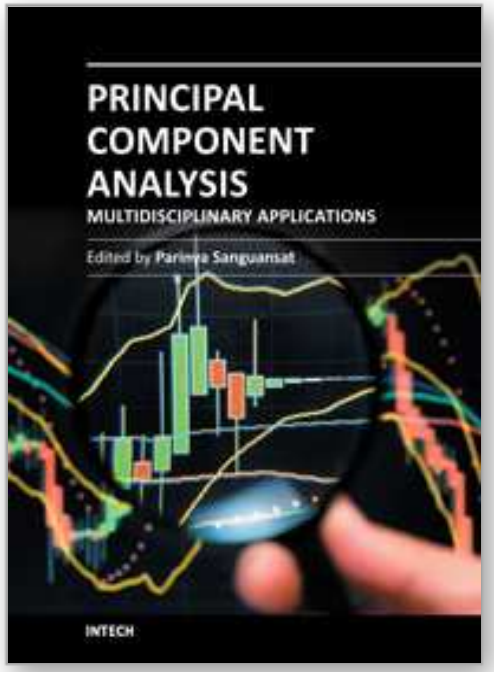
Principal components analysis (PCA) - example 1



Each letter is a patient. Labels stand for different lymphoblastic leukaemia (ALL) types.

Data matrix: 190 observations by **22283** columns.

Principal components analysis (PCA) - example 2



PCA – A Powerful Method for Analyze Ecological Niches

Franc Janžekovič and Tone Novak
University of Maribor, Faculty of Natural Sciences and Mathematics, Department of Biology, Maribor Slovenia

Principal components analysis (PCA) - example 2

2.1 Environmental niche of three hymenopteran and two spider species

Between 1977 and 2004, 63 caves and artificial tunnels were ecologically investigated in Slovenia; the three most abundant Hymenoptera species found in these studies have been ecologically evaluated (details in Novak et al. 2010a). In the caves, many environmental data were collected, as follows. The following abbreviations of the environmental variables are used: Dist-E = distance from entrance; Dist-S = distance from surface; Illum = illumination; PCS = passage cross-section; Tair =air temperature; RH = relative air humidity; Tgr = ground temperature; HY = substrate moisture. The hymenopteran spatial niche breadth was originally represented by nine variables.

Data matrix: 63 observations (caves) by 9 columns

Environmental variables (9)

63 caves

Franc Janžekovič and Tone Novak
University of Maribor, Faculty of Natural Sciences and Mathematics, Department of Biology, Maribor Slovenia

Principal components analysis (PCA) - example 2

(pairwise correlation among environmental variables)

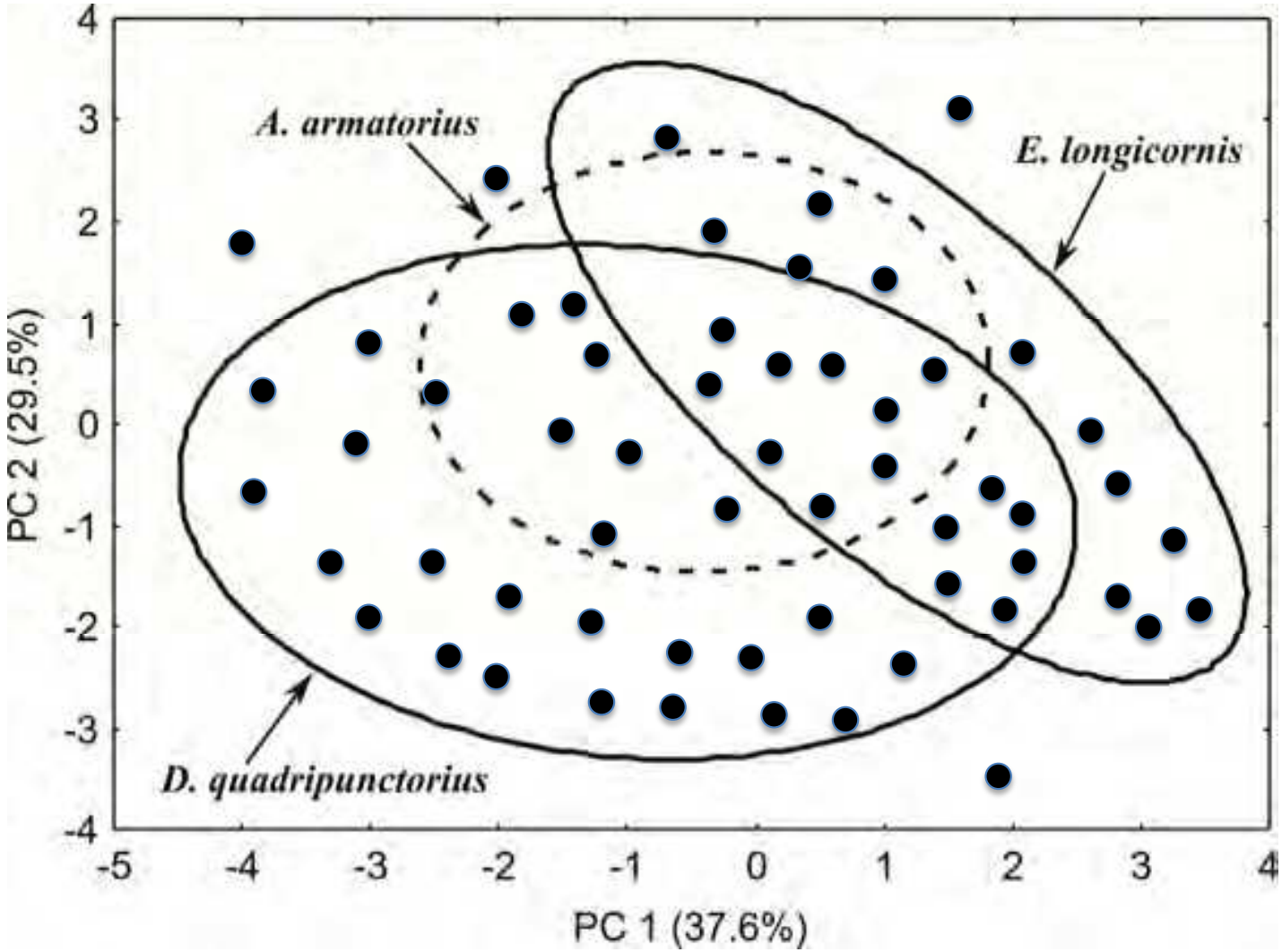
	1	2	3	4	5	6	7	8	9
1 Air temperature	1.00 ---								
2 *arc-sin* relative air humidity	0.15 0.133	1.00 ---							
3 Ground temperature	**0.94** **<0.001**	0.18 0.079	1.00 ---						
4 *arc-sin* substrate moisture	**0.388** **<0.001**	**0.59** **<0.001**	**0.37** **<0.001**	1.00 ---					
5 Airflow	**-0.48** **<0.001**	**-0.36** **<0.001**	**-0.43** **<0.001**	**-0.55** **<0.001**	1.00 ---				
6 Distance from entrance	**-0.34** **<0.001**	0.14 0.153	**-0.41** **<0.001**	0.10 0.312	0.04 0.712	1.00 ---			
7 Distance from surface	-0.02 0.837	**0.24** **0.017**	-0.04 0.683	**0.46** **<0.001**	-0.11 0.275	**0.67** **<0.001**	1.00 ---		
8 Passage cross-section	**0.35** **<0.001**	0.17 0.089	**0.23** **0.025**	**0.39** **<0.001**	**-0.40** **<0.001**	-0.11 0.274	0.05 0.656	1.00 ---	
9 *log* illumination	**0.45** **<0.001**	-0.18 0.077	**0.46** **<0.001**	-0.04 0.690	-0.07 0.494	**-0.821** **<0.001**	**-0.679** **<0.001**	**0.37** **<0.001**	1.00 ---

Table 1. Pearson correlations coefficient among nine environmental variables. Significant correlations in bold. (Upper row r, lower row p).

Franc Janžekovič and Tone Novak
University of Maribor, Faculty of Natural Sciences and Mathematics, Department of Biology, Maribor Slovenia

Principal components analysis (PCA) - example 2

(niche differences – dots represent different caves ellipsoids are confidence intervals for where species is found)



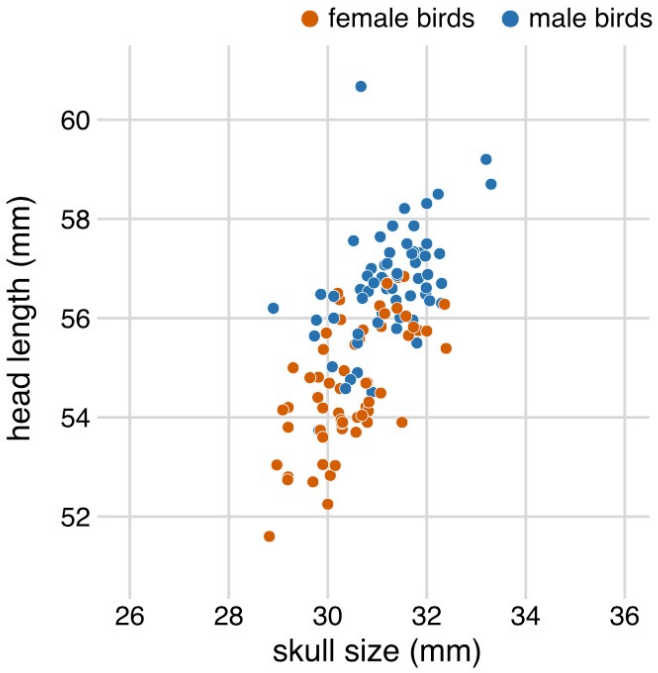
Each dot represents a cave

Fig. 5. Ordination of the nine environmental variables in 1st and 2nd PC axes. Ellipses (95% confidence) represent spatial niches in the three hymenopteran species.

Principal Component Analysis (PCA): A geometric interpretation

PCA finds the coordinate system (called principal components) that best represents the internal variability in the data, essentially re-projecting the data on these coordinate system. As such, PCA represents associations among variables (gene, environmental variables) and data points are re-projected so that the correlations among variables is maximized.

Original data



Source https://wilkelab.org/SDS375/slides/dimension-reduction-1.html#9

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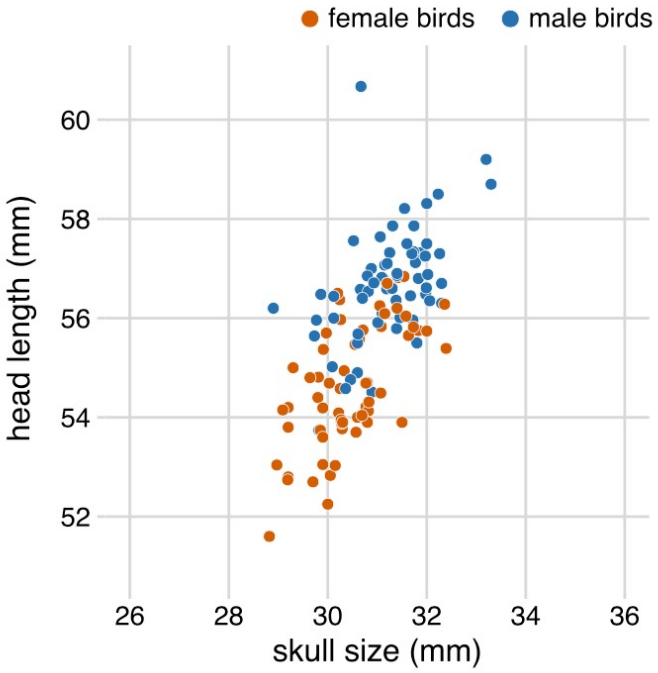
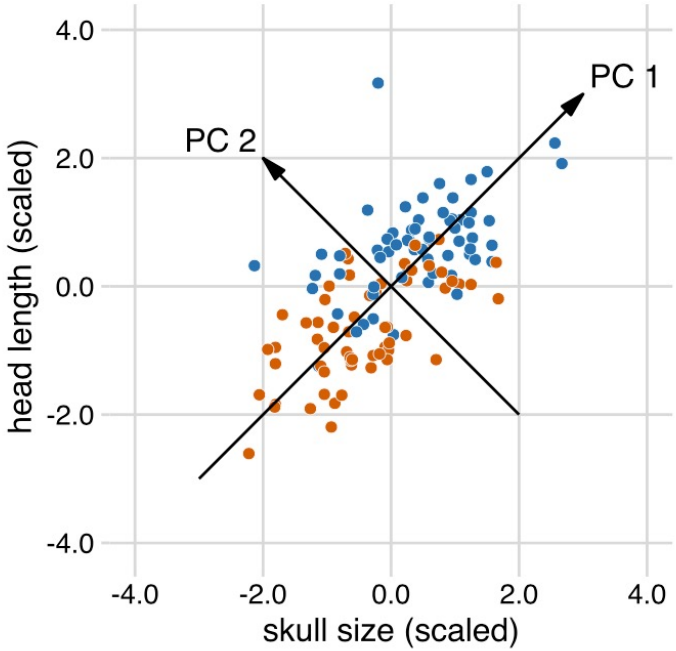


Standardization and PCA fitting



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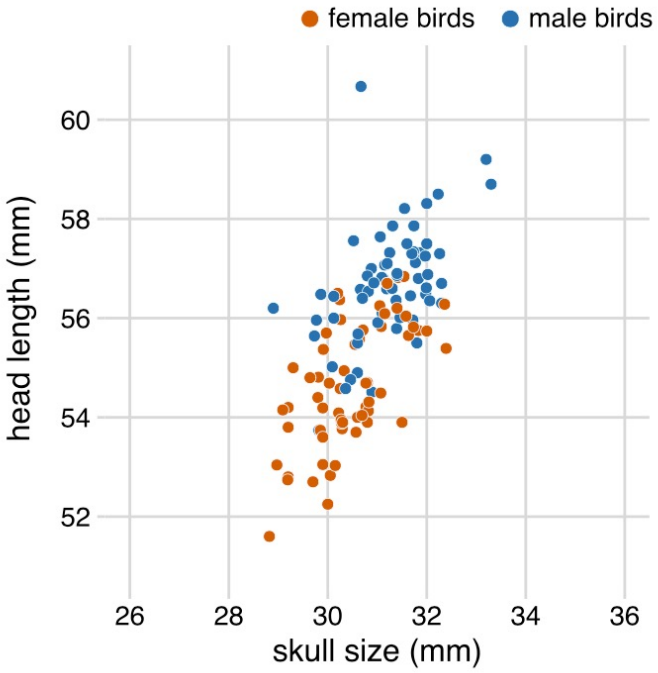

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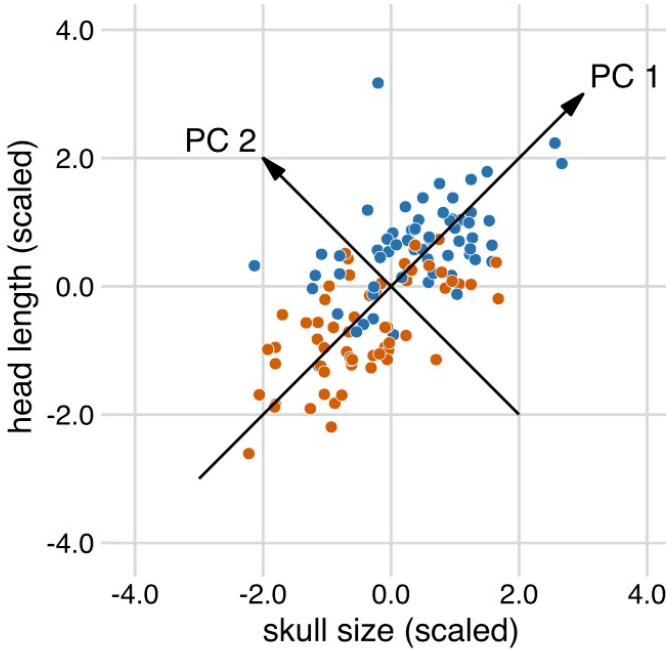
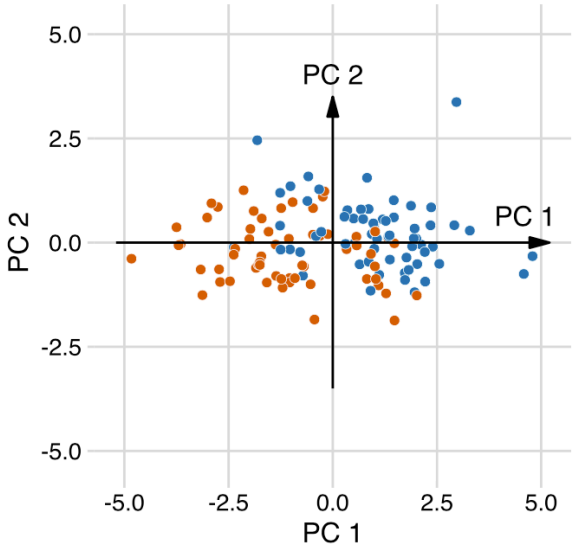


Rotation



PCA aligns their axes with directions of maximum variation in the data

Source https://wilkelab.org/SDS375/slides/dimension-reduction-1.html#9

Principal Component Analysis (PCA): A geometric interpretation

- PCA constructs a new coordinate system (new variables, PCs) which are linear combinations of the original data and which are defined to align the samples along their major axes of variation (assuming linearity).

- Thus, PCA determines the coordinate system that best represents the internal variability in the data, essentially re-projecting the data.

The association among variables need to be measured by either (in most cases):

Correlation Matrix (for variables that have different units or scales, e.g., ph, temperature).

Covariance Matrix (variables have the same units, e.g., body length & body width in cm).

Raw data when variables are in the same units (more difficult to interpret) and calculations differ (very rare to find applications in the literature); rarely used.

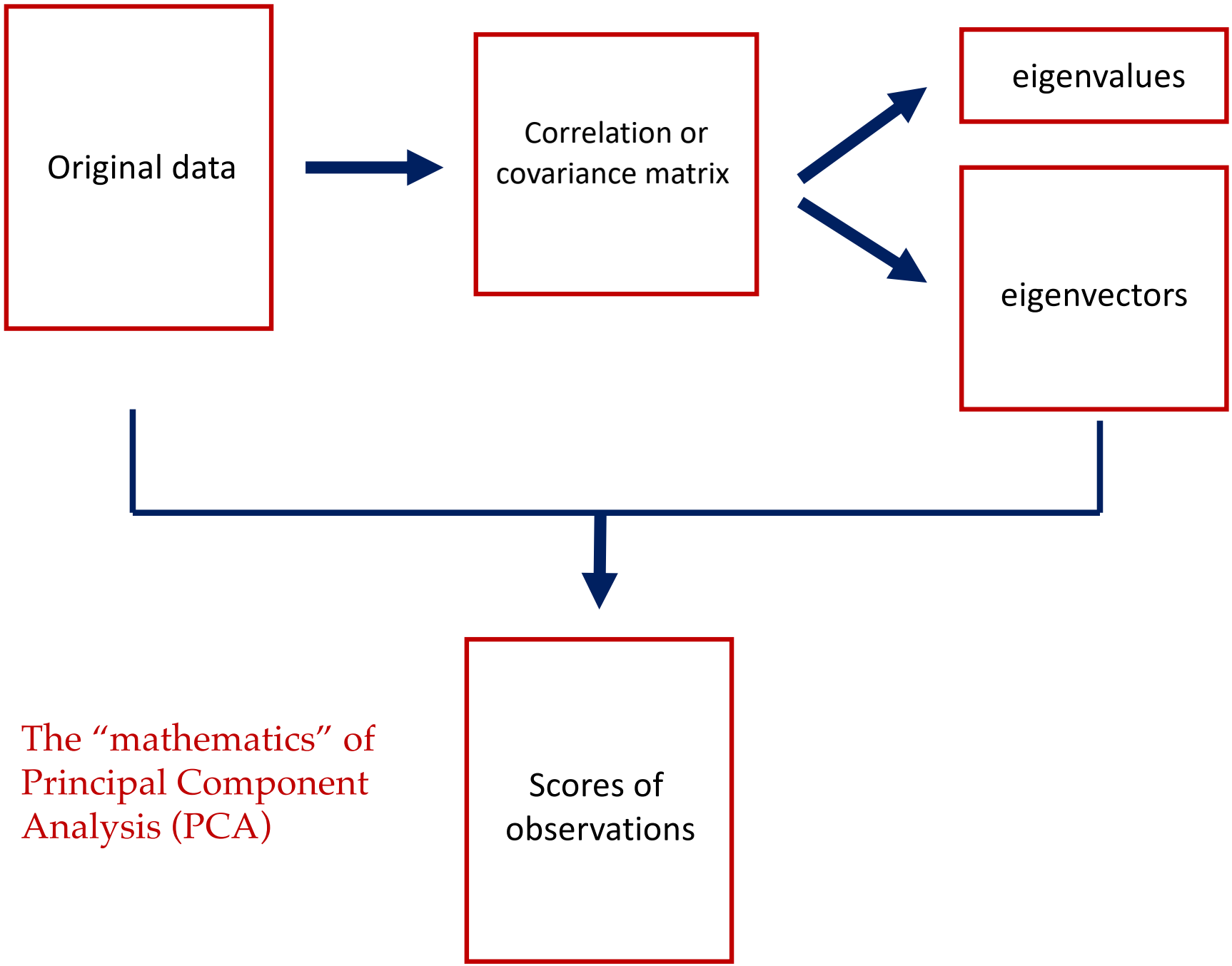
Correlation *versus* covariance

$$COV_{xy} = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{n-1}$$

$$\bar{X} = 0 \;\&\; \bar{Y} = 0 \;\; \therefore s_x = s_x \;\&\; s_y = s_y$$

$$COR_{xy} = \frac{COV_{xy}}{s_x s_y}$$

$$\bar{X} = 0 \;\&\; \bar{Y} = 0 \;\; \therefore s_x = 1 \;\&\; s_y = 1$$



The "mathematics" of Principal Component Analysis (PCA)

The mathematics of Principal Component Analysis (PCA):

Eigen-analysis is a mathematical operation on a *square symmetric* matrix (e.g., pairwise correlation matrix, pairwise covariance matrix).

A *square* matrix has the same number of rows as columns.

A *symmetric* matrix is the same if you switch rows and columns.

square and symmetric matrix

(e.g., pairwise correlation matrix)

	X_1	X_2	X_3	X_4	X_5
X_1	1.00	0.80	0.90	0.78	0.87
X_2	0.80	1.00	0.76	0.87	0.78
X_3	0.90	0.76	1.00	0.78	0.89
X_4	0.78	0.87	0.78	1.00	0.95
X_5	0.87	0.78	0.89	0.95	1.00

The important components of Principal Component Analysis (pun intended)

Principal component analysis presents three important structures:

1 – **Eigenvalues:** represent the amount of variation in the original data summarized by each principal component. The first principal component (PC-1) presents the largest amount, PC-2 presents the second largest amount, and so on.

Eigenvalues

	X_1	X_2	X_3	X_4	X_5
X_1	1.00	0.80	0.90	0.78	0.87
X_2	0.80	1.00	0.76	0.87	0.78
X_3	0.90	0.76	1.00	0.78	0.89
X_4	0.78	0.87	0.78	1.00	0.95
X_5	0.87	0.78	0.89	0.95	1.00

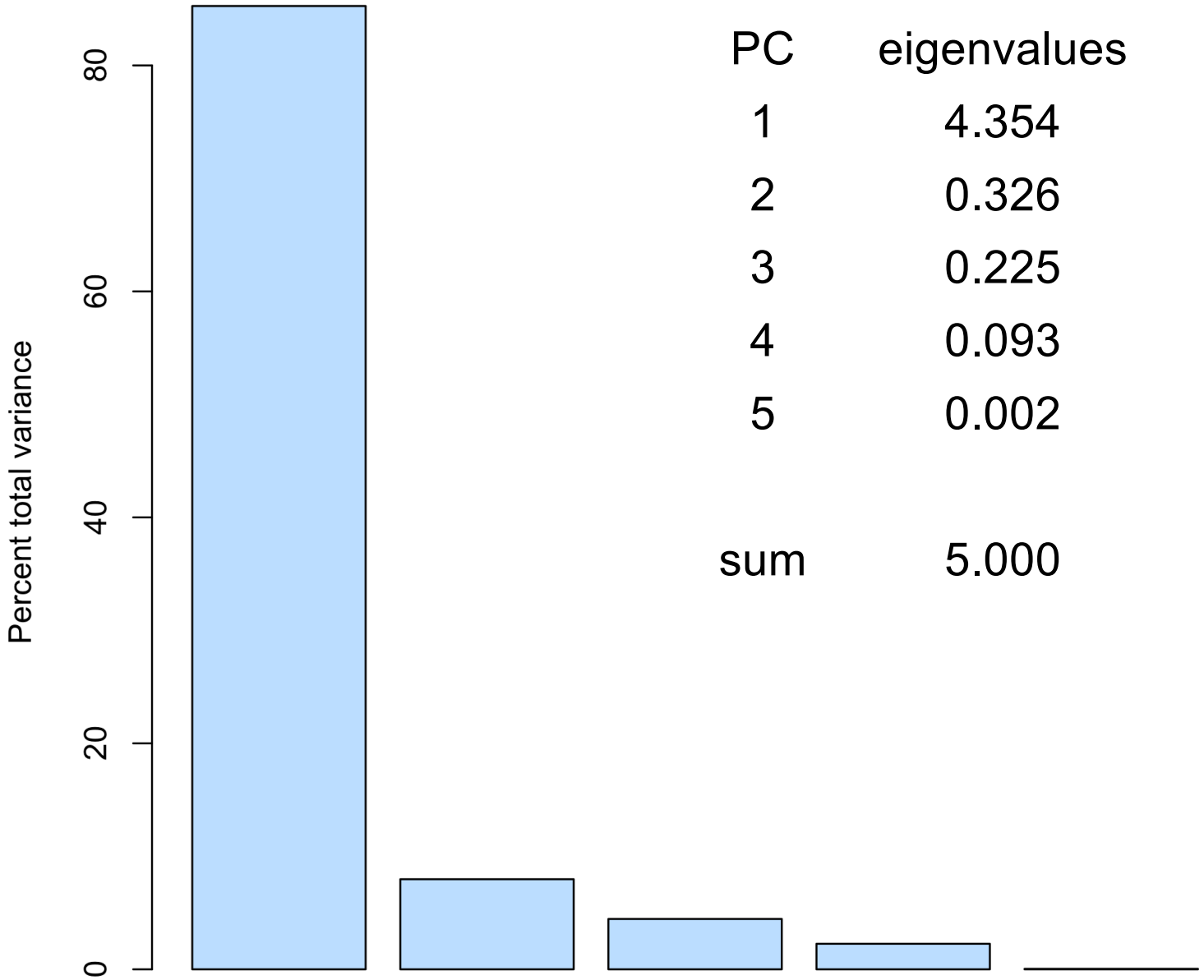
"one dimension"

Eigenvalues:

PC	eigenvalues	%
1	4.354	0.871
2	0.326	0.065
3	0.225	0.045
4	0.093	0.019
5	0.002	0.000
sum	5.000	1.000

"Lower" dimensionality because it kept a large proportion of the variation in the data in the first PC.

Plot of eigenvalue contributions



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2	0.326	0.065
3	0.225	0.045
4	0.093	0.019
5	0.002	0.000
sum	5.000	1.000

Eigenvalues

1.00	0.87	0.96	0.04	0.05
0.87	1.00	0.95	0.03	0.07
0.96	0.95	1.00	0.04	0.05
0.04	0.03	0.04	1.00	0.84
0.05	0.07	0.05	0.84	1.00

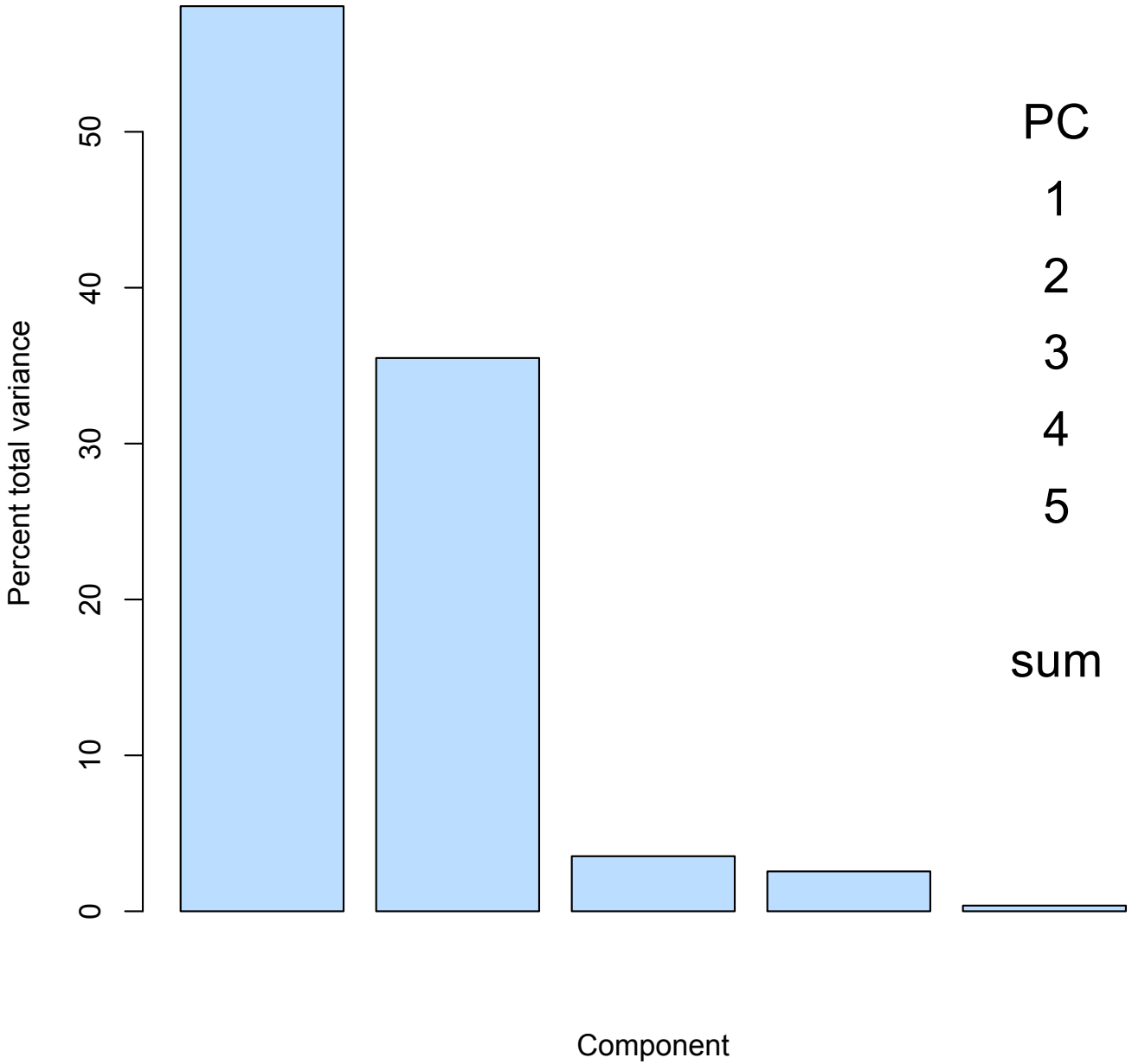
"two dimensions"

Eigenvalues:

PC	eigenvalues	%
1	2.867	0.573
2	1.827	0.365
3	0.167	0.033
4	0.124	0.025
5	0.015	0.003
sum	5.000	1.000

"Higher" dimensionality because two components are needed to summarize variation.

Plot of eigenvalues



PC	eigenvalues	%
1	2.867	0.573
2	1.827	0.365
3	0.167	0.033
4	0.124	0.025
5	0.015	0.003
sum	5.000	1.000

Principal component analysis presents three important structures:

2 - **Eigenvectors:** Each principal component is a linear function with coefficients for each variable.

- Eigenvectors contain these coefficients. High values, positive or negative, represents high association with the component.

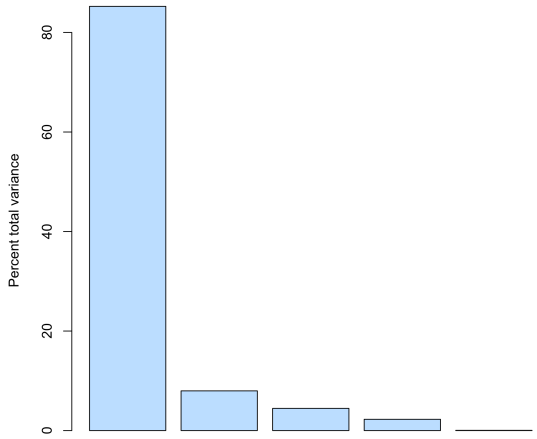
Correlation matrix

	X_1	X_2	X_3	X_4	X_5
X_1	1.00	0.80	0.90	0.78	0.87
X_2	0.80	1.00	0.76	0.87	0.78
X_3	0.90	0.76	1.00	0.78	0.89
X_4	0.78	0.87	0.78	1.00	0.95
X_5	0.87	0.78	0.89	0.95	1.00

"one dimension"

Associated eigenvectors

	PC				
var	1	2	3	4	5
1	0.447	-0.436	0.330	-0.687	0.170
2	0.432	0.533	0.644	0.181	-0.288
3	0.445	-0.534	0.035	0.692	0.192
4	0.450	0.489	-0.413	-0.063	0.619
5	0.462	-0.039	-0.552	-0.109	-0.684



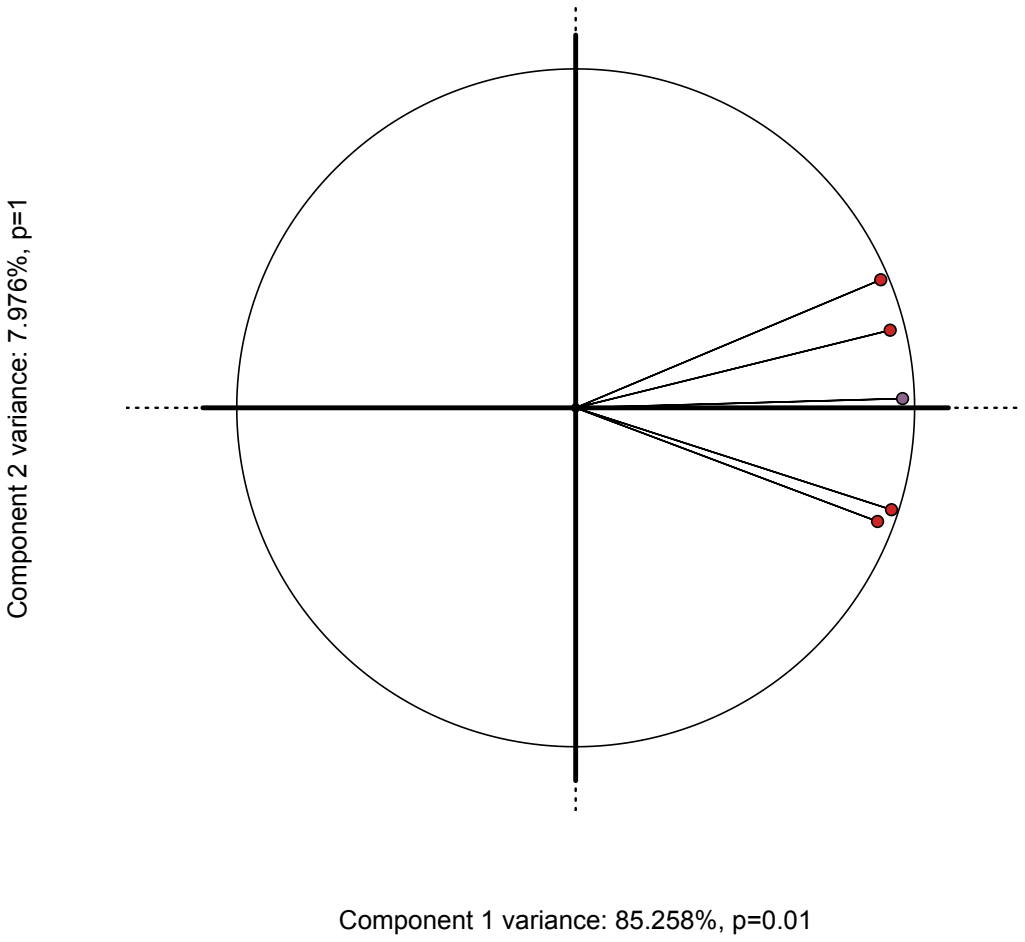
Eigenvectors can be seen as regression coefficients, where the component is the dependent variable. A "one dimension" matrix has only one interpretable principal component.

$$PC\text{-}1=0.447X_1+0.432X_2+0.445X_3+0.450X_4+0.462X_5$$

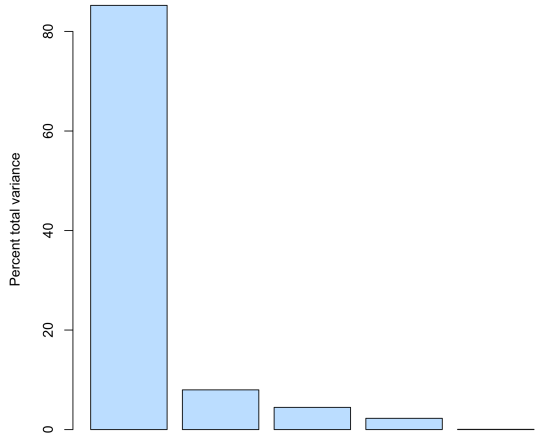
Unlike the numbers after =, this is not a subtraction but a hyphen stating that this is the first and second Principal Components (PC).

	PC				
var	1	2	3	4	5
1	0.447	0.436	0.330	-0.687	0.170
2	0.432	-0.533	0.644	0.181	-0.288
3	0.445	0.534	0.035	0.692	0.192
4	0.450	-0.489	-0.413	-0.063	0.619
5	0.462	0.039	-0.552	-0.109	-0.684

Eigenvectors (simulated data with 1 dimension): only first axis (PC-1) should be interpreted



variable	PC axis 1
1	0.447
2	0.432
3	0.445
4	0.450
5	0.462



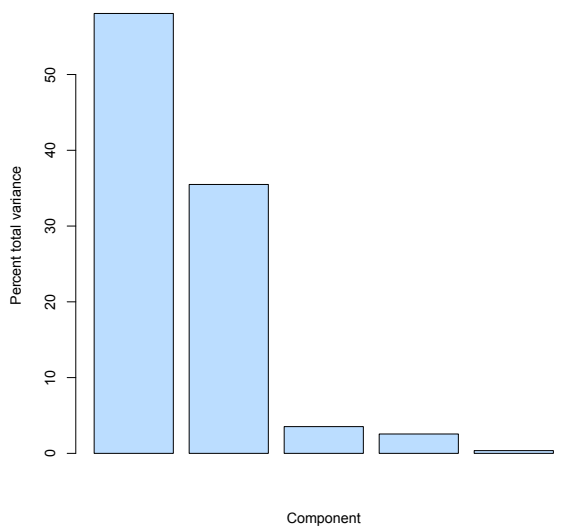
Correlation matrix

	X_1	X_2	X_3	X_4	X_5
X_1	1.00	0.87	0.96	0.04	0.05
X_2	0.87	1.00	0.95	0.03	0.07
X_3	0.96	0.95	1.00	0.04	0.05
X_4	0.04	0.03	0.04	1.00	0.84
X_5	0.05	0.07	0.05	0.84	1.00

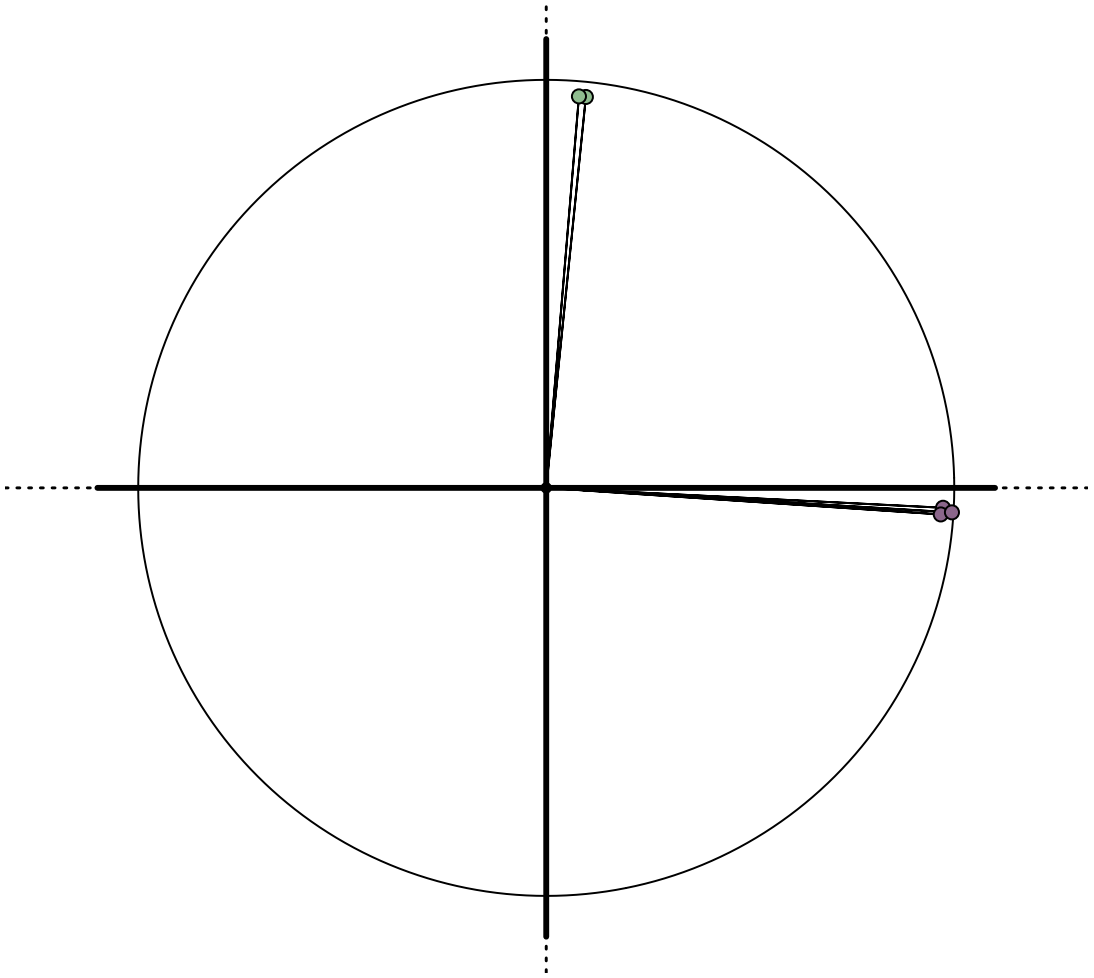
"two dimensions"

Associated eigenvectors (only interpret the first two components (PC)

	PC				
var	1	2	3	4	5
1	0.569	-0.064	0.249	-0.642	0.445
2	0.567	-0.060	-0.298	0.661	0.386
3	0.585	-0.067	0.061	-0.610	-0.806
4	0.072	0.704	0.651	0.273	0.039
5	0.085	0.702	-0.650	-0.277	-0.043

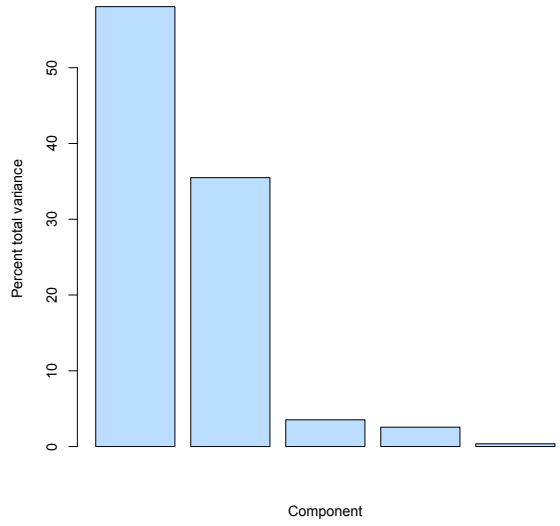


Eigenvectors (simulated data with 2 dimensions): only first two axis (PC-1 & PC-2) should be interpreted



PC axis

var	1	2
1	0.569	-0.064
2	0.567	-0.060
3	0.585	-0.067
4	0.072	0.704
5	0.085	0.702



Principal component analysis presents three important structures:

3 – **Multivariate scores:** Since each component is a linear function of the variables, when multiplying the standardized variables (in the case of correlation matrices) by the eigenvector structure, a matrix containing the position of each observation in each principal component is produced.

The plot of these scores in the first few dimensions, represents the main patterns of variation among the original observations (more in the empirical example).

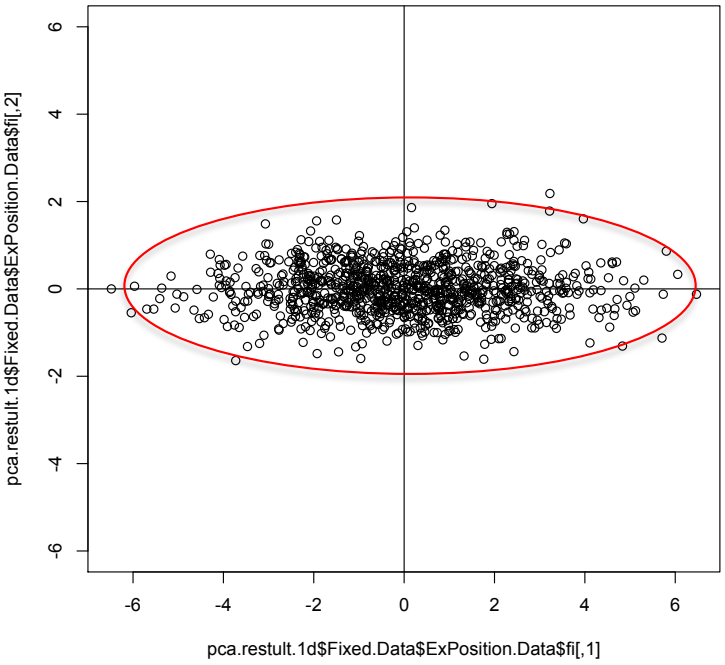
$$PC\text{-}1=0.569X_1+0.567X_2+0.585X_3+0.072X_4+0.085X_5$$

$$PC\text{-}2=-0.064X_1-0.060X_2-0.067X_3+0.704X_4+0.702X_5$$

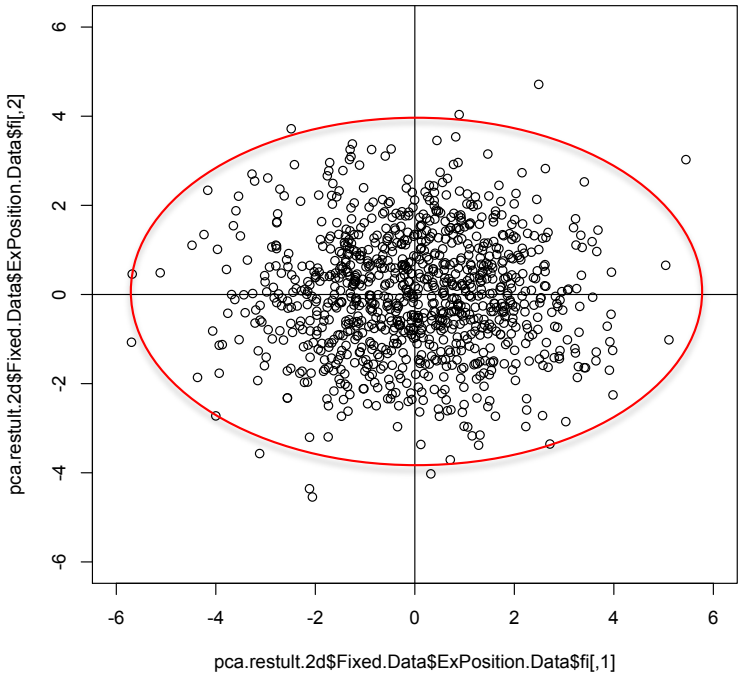
	PC axis	
var	1	2
1	0.569	-0.064
2	0.567	-0.060
3	0.585	-0.067
4	0.072	0.704
5	0.085	0.702

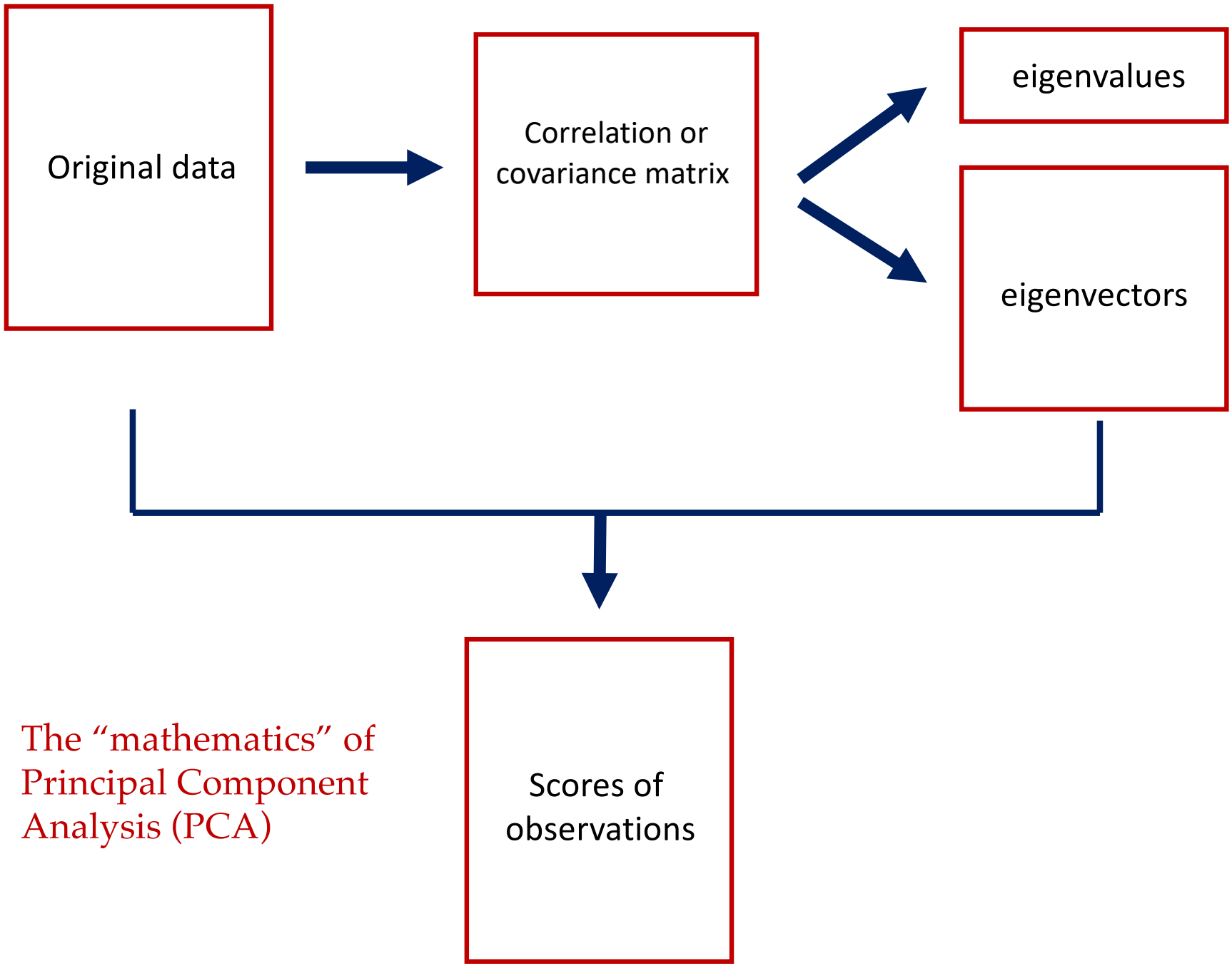
PCA Scores: one versus two dimensions

1D



2D





The "mathematics" of Principal Component Analysis (PCA)

Next lecture: How many PCA dimensions? Inferential frameworks for determining number of axes to interpret and the significance of each variable on each axis (lots of work on this area).

1st) determine how many axes to interpret (i.e., how many PCs capture correlated variation in the data?).

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How many principal components? stopping rules for determining the number of non-trivial axes revisited

Pedro R. Peres-Neto*, Donald A. Jackson, Keith M. Somers

Inferential frameworks for determining number of axes to interpret and the significance of each variable on each axis are usually nor performed.

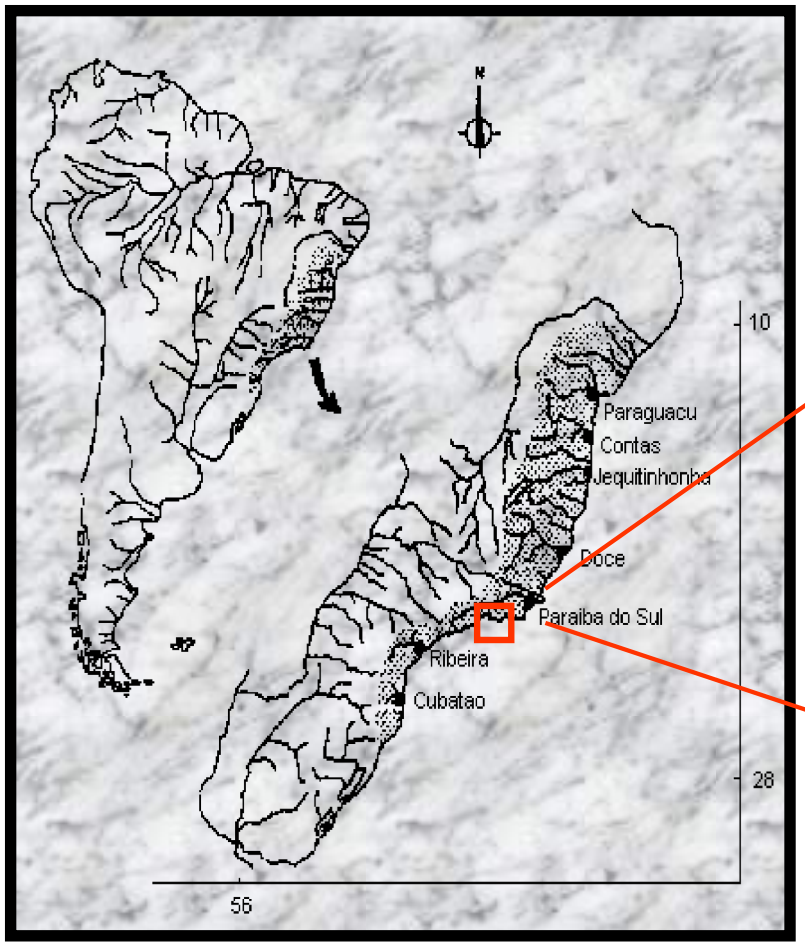
2nd) for each significant axis, determine which variable is significant on each of them.

Ecology, 84(9), 2003, pp. 2347–2363

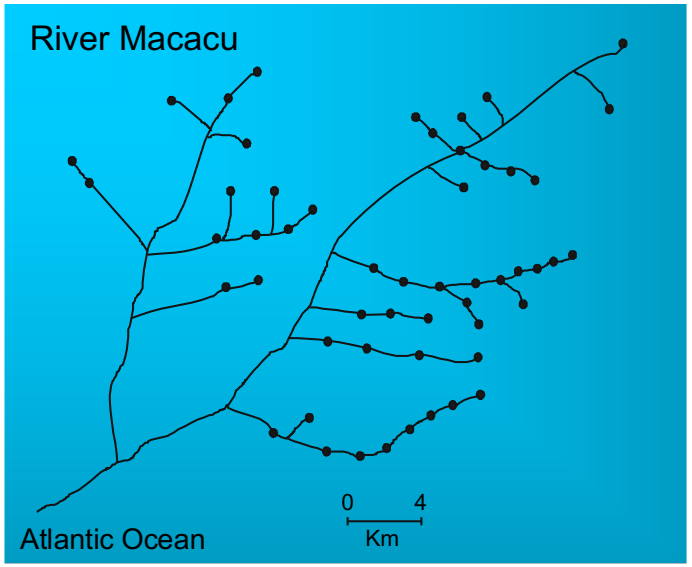
GIVING MEANINGFUL INTERPRETATION TO ORDINATION AXES: ASSESSING LOADING SIGNIFICANCE IN PRINCIPAL COMPONENT ANALYSIS

PEDRO R. PERES-NETO,[1] DONALD A. JACKSON, AND KEITH M. SOMERS

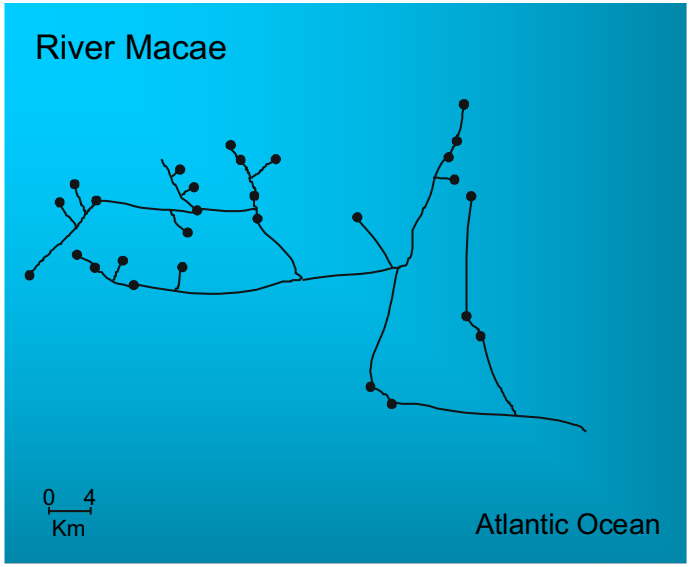
Principal component analysis: a complete example



53 sites



28 sites



What is the correlation structure and differences among streams in terms of their environmental features?

Depth
Depth variation
Current velocity
Current variation
Substrate composition: Boulder, rubble, gravel and sand
Substrate variation (variance in composition)
Stream width variation (irregularity)
Area
Altitude

Oecologia (2004) 140: 352–360
DOI 10.1007/s00442-004-1578-3

COMMUNITY ECOLOGY

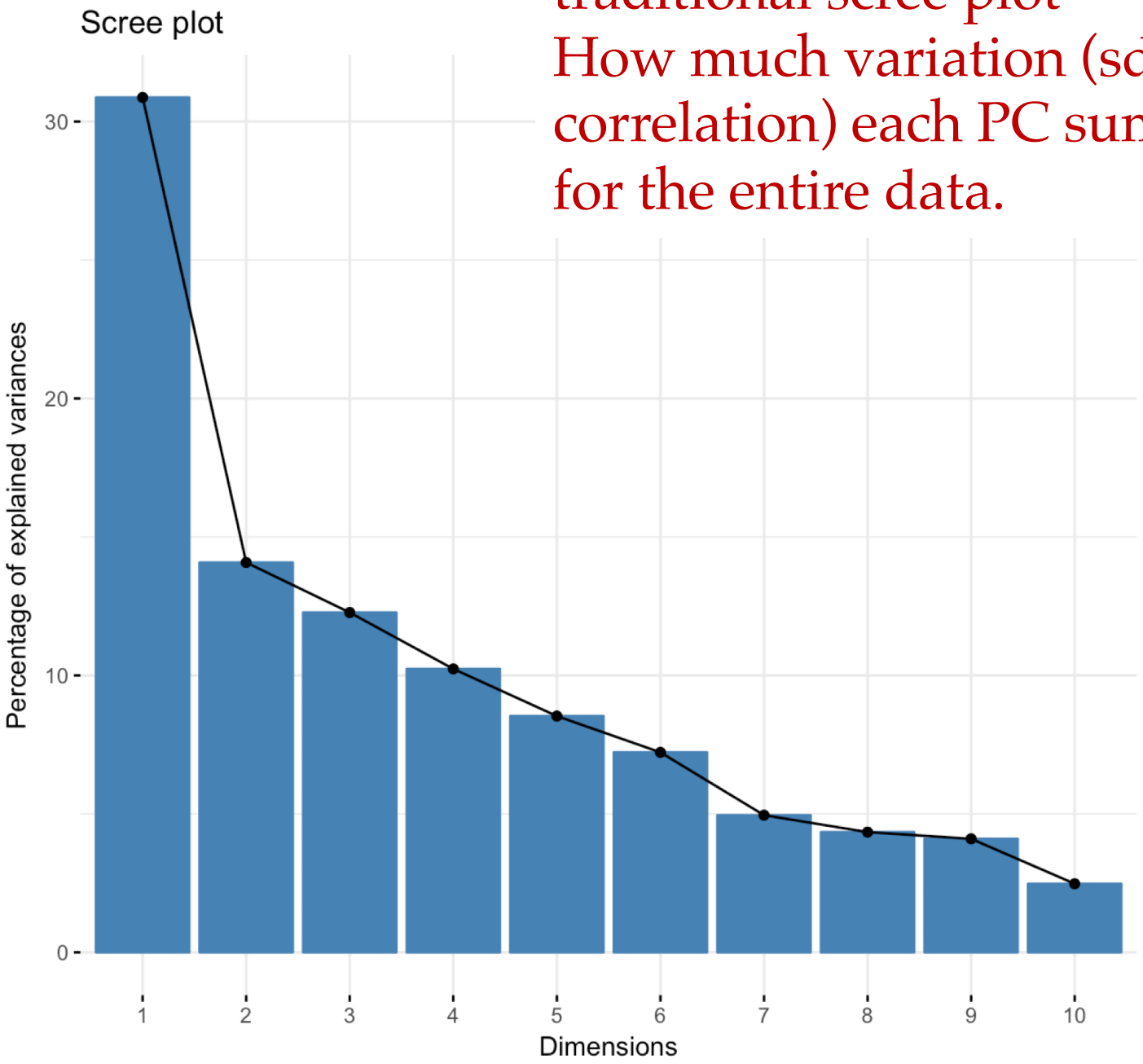
Pedro R. Peres-Neto

Patterns in the co-occurrence of fish species in streams: the role of site suitability, morphology and phylogeny versus species interactions

Correlation matrix

1.00	0.04	0.28	-0.07	0.06	-0.33	-0.02	0.12	-0.02	0.05	0.01	-0.11
0.04	1.00	-0.12	0.85	0.31	0.07	0.07	-0.35	-0.42	0.84	0.86	-0.66
0.28	-0.12	1.00	-0.07	-0.17	-0.08	0.02	0.19	-0.13	-0.13	-0.17	-0.03
-0.07	0.85	-0.07	1.00	0.36	0.17	0.06	-0.44	-0.33	0.71	0.71	-0.57
0.06	0.31	-0.17	0.36	1.00	0.08	-0.33	-0.81	0.33	0.36	0.20	-0.17
-0.33	0.07	-0.08	0.17	0.08	1.00	-0.11	-0.52	0.09	0.00	0.11	0.23
-0.02	0.07	0.02	0.06	-0.33	-0.11	1.00	-0.04	-0.22	0.14	0.05	0.00
0.12	-0.35	0.19	-0.44	-0.81	-0.52	-0.04	1.00	-0.25	-0.39	-0.25	0.04
-0.02	-0.42	-0.13	-0.33	0.33	0.09	-0.22	-0.25	1.00	-0.38	-0.38	0.33
0.05	0.84	-0.13	0.71	0.36	0.00	0.14	-0.39	-0.38	1.00	0.66	-0.58
0.01	0.86	-0.17	0.71	0.20	0.11	0.05	-0.25	-0.38	0.66	1.00	-0.60
-0.11	-0.66	-0.03	-0.57	-0.17	0.23	0.00	0.04	0.33	-0.58	-0.60	1.00

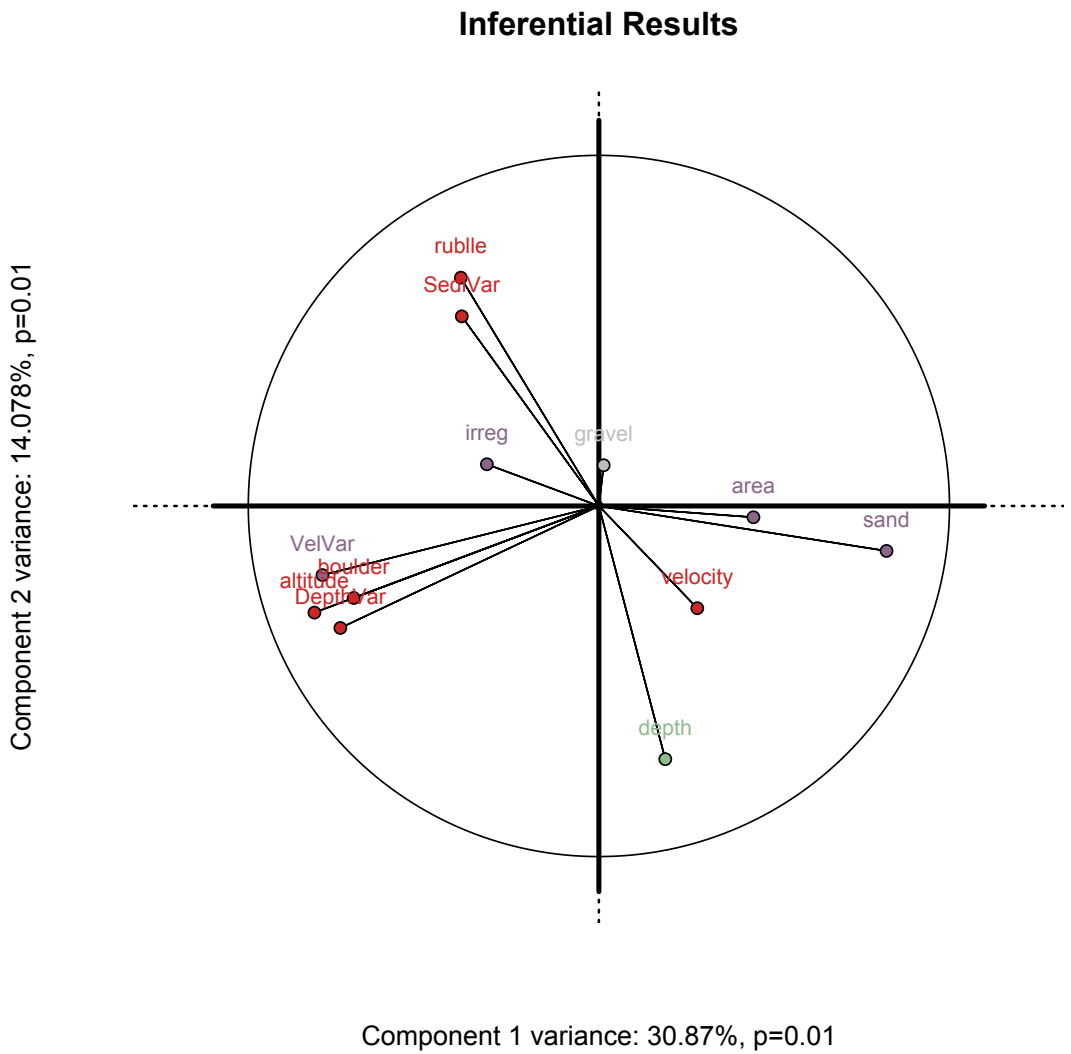
Eigenvalue contribution – the traditional scree plot -
How much variation (sd and correlation) each PC summarizes for the entire data.



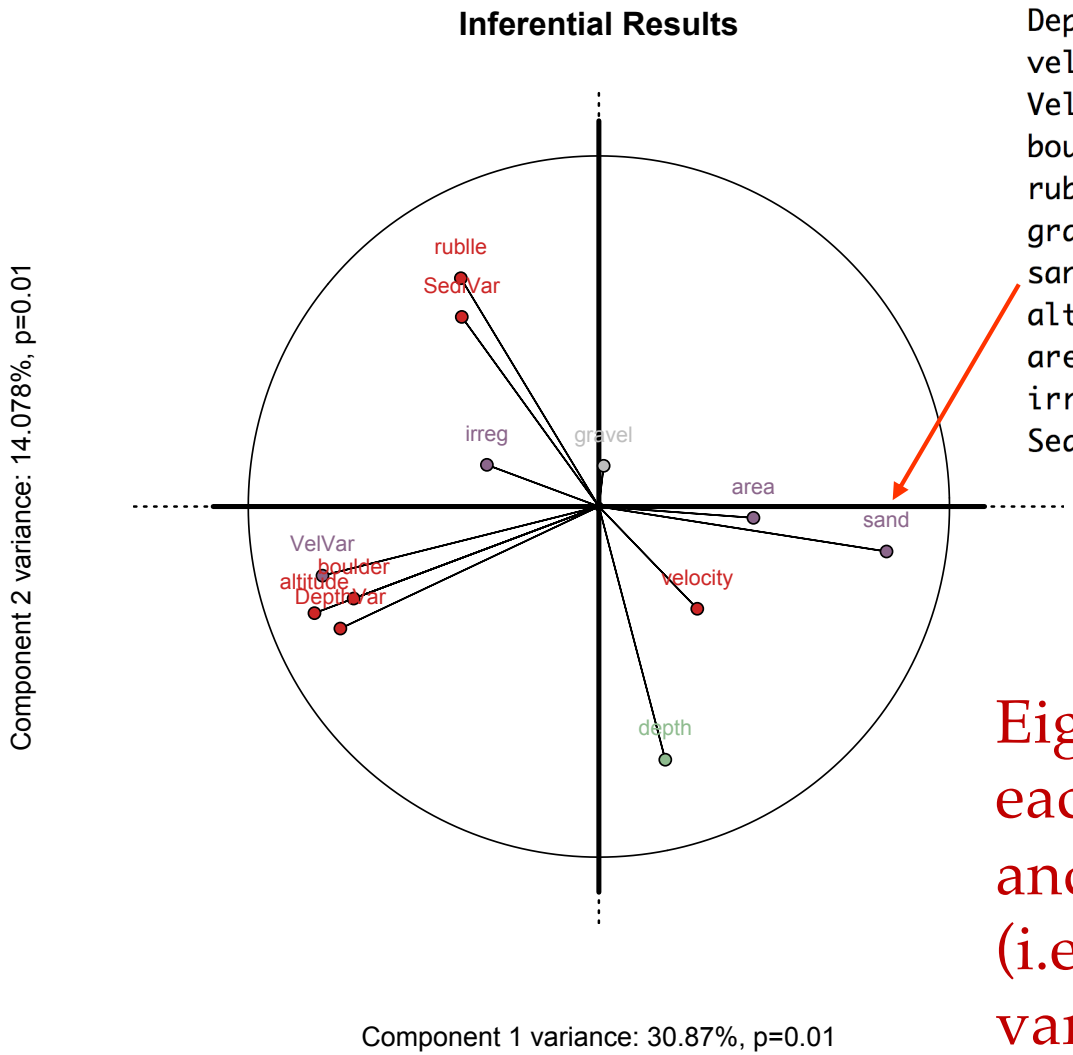
Eigenvector structure (2 first dimensions)

	PC-1	PC-2
depth	0.098416371	-0.55557259
DepthVar	-0.383072589	-0.26772556
velocity	0.145820452	-0.22434910
VelVar	-0.409585483	-0.15169873
boulder	-0.363399847	-0.20189977
rublle	-0.204526467	0.50098773
gravel	0.007091107	0.08935752
sand	0.426264131	-0.09866678
altitude	-0.421467330	-0.23396335
area	0.229031867	-0.02477526
irreg	-0.165951470	0.09149688
SediVar	-0.203159109	0.41607768

Eigenvector plot :



Eigenvector plot :



depth	0.098416371	-0.55557259
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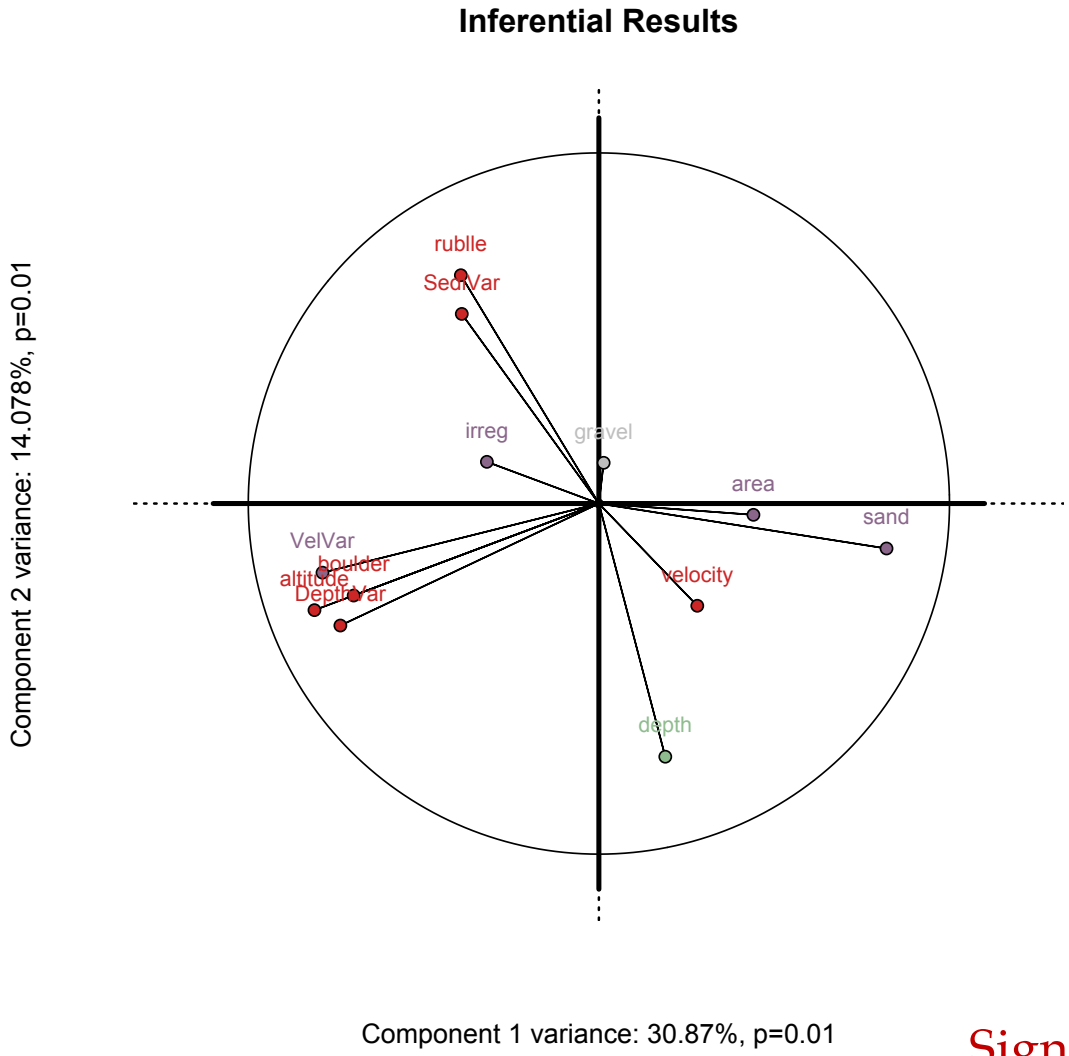
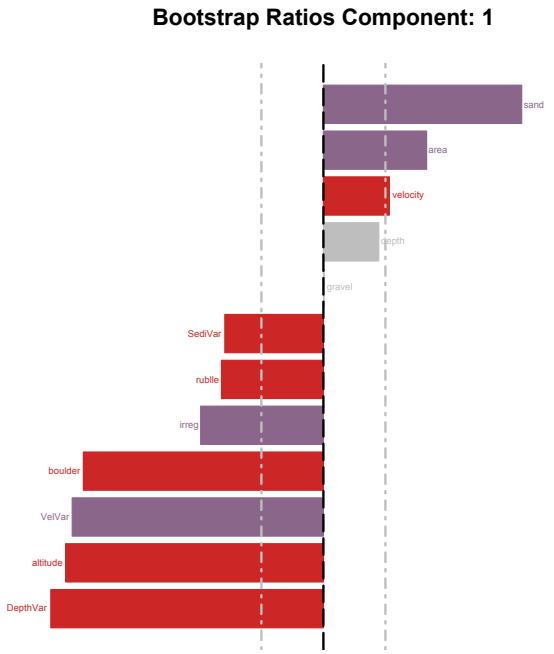
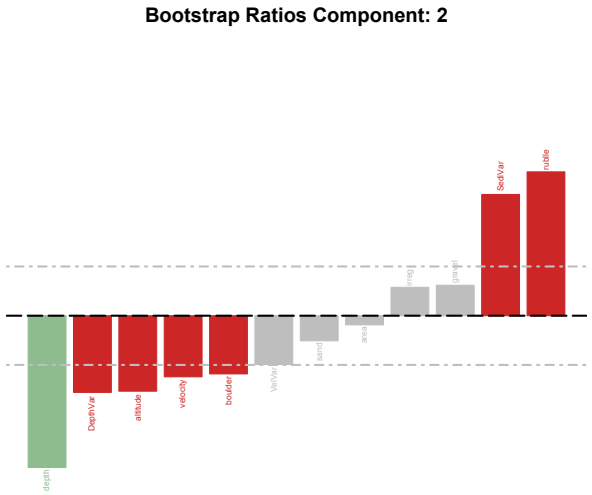
area	0.229031867	-0.02477526
irreg	-0.165951470	0.09149688
SediVar	-0.203159109	0.41607768

Eigenvector coefficients for each variable are plotted and presented as arrows (i.e., correlation of each variable with each principal component).

Eigenvector plot:







Significant variable contributions are determined if the eigenvector coefficient for the variables are beyond the confidence interval.

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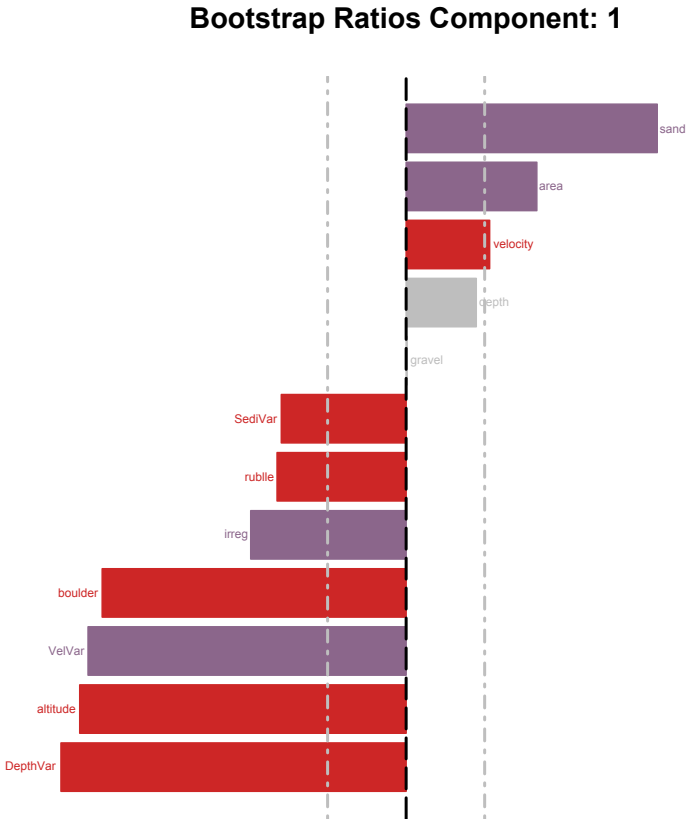
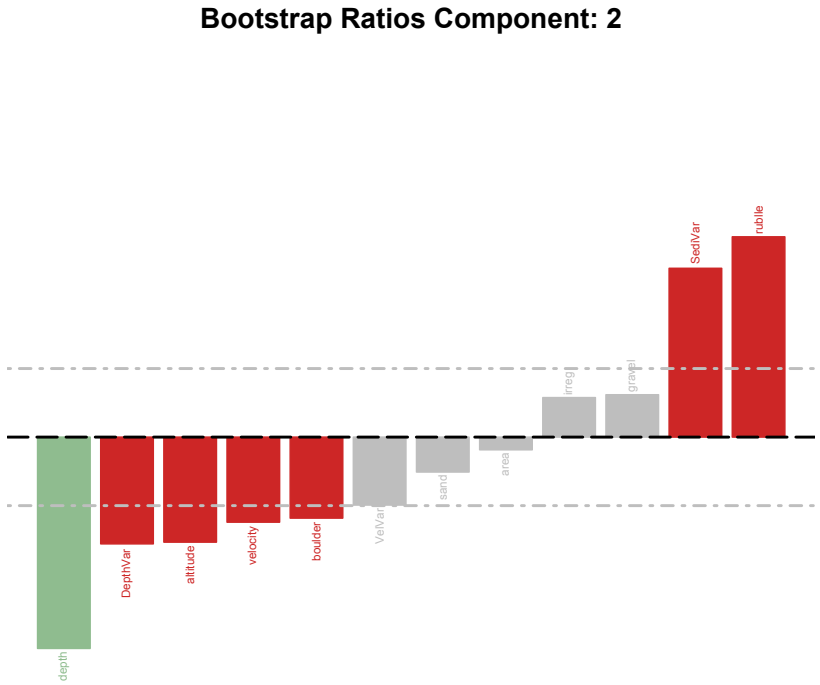
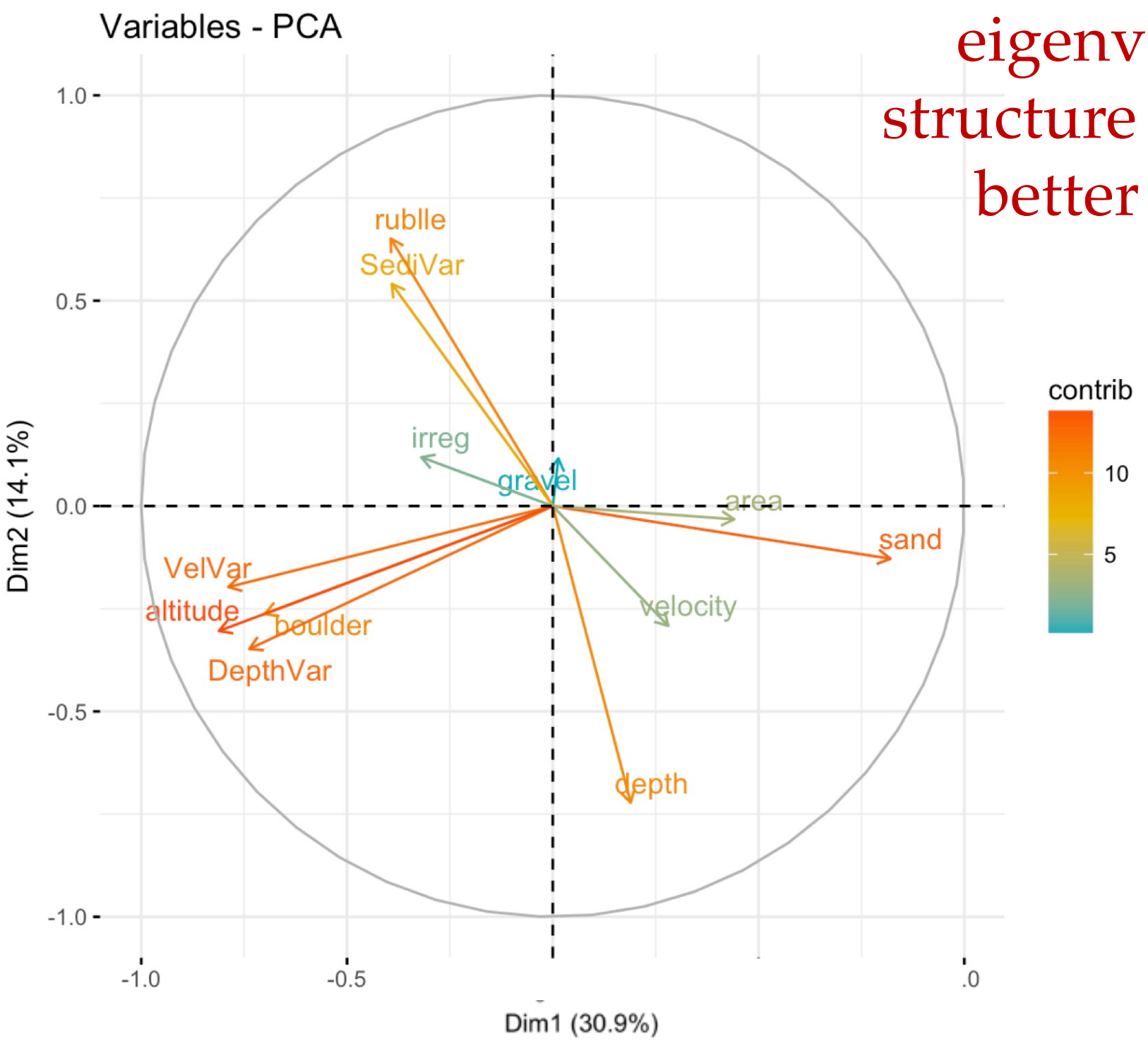
GIVING MEANINGFUL INTERPRETATION TO ORDINATION AXES: ASSESSING LOADING SIGNIFICANCE IN PRINCIPAL COMPONENT ANALYSIS

PEDRO R. PERES-NETO,[1] DONALD A. JACKSON, AND KEITH M. SOMERS



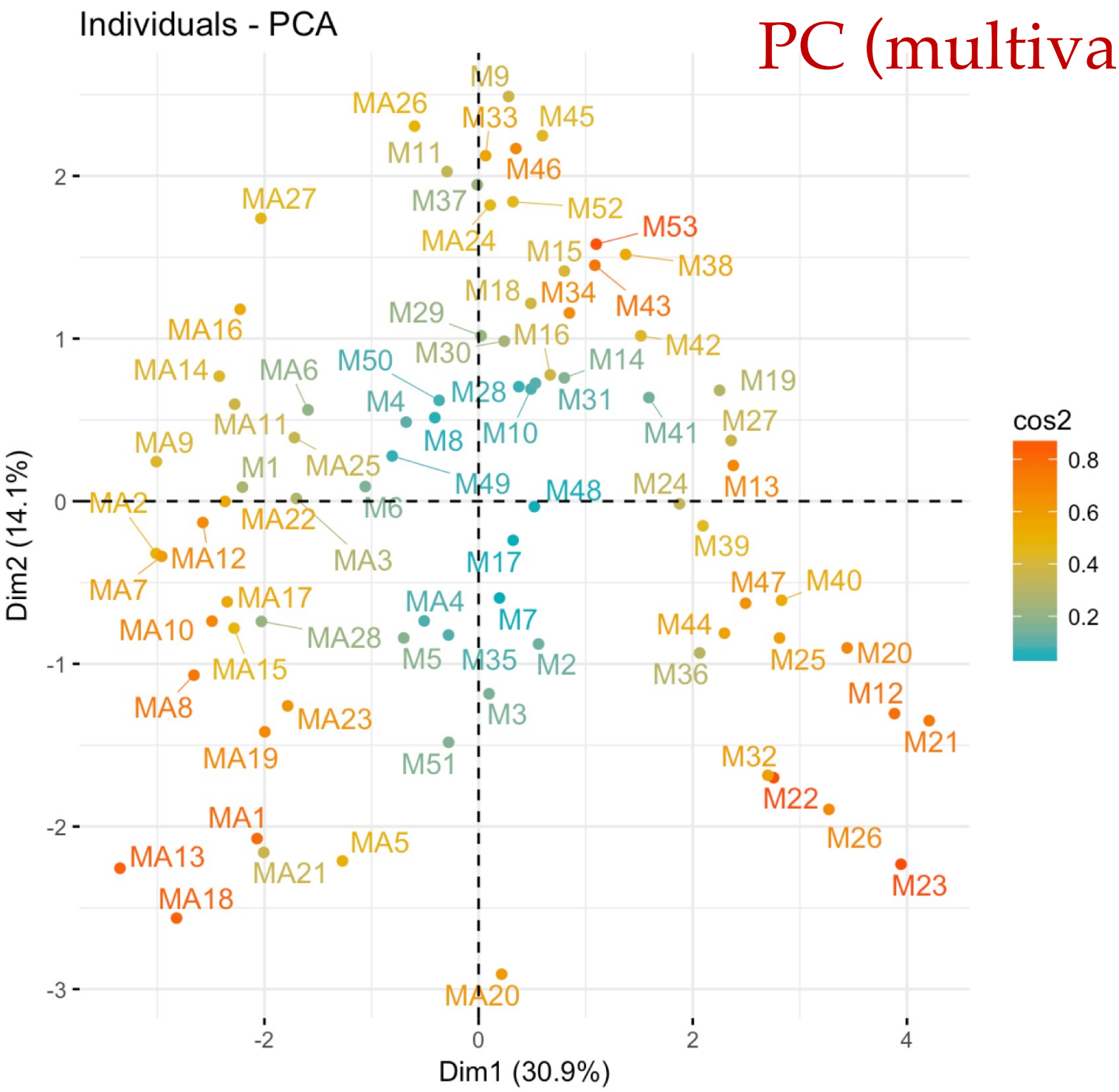


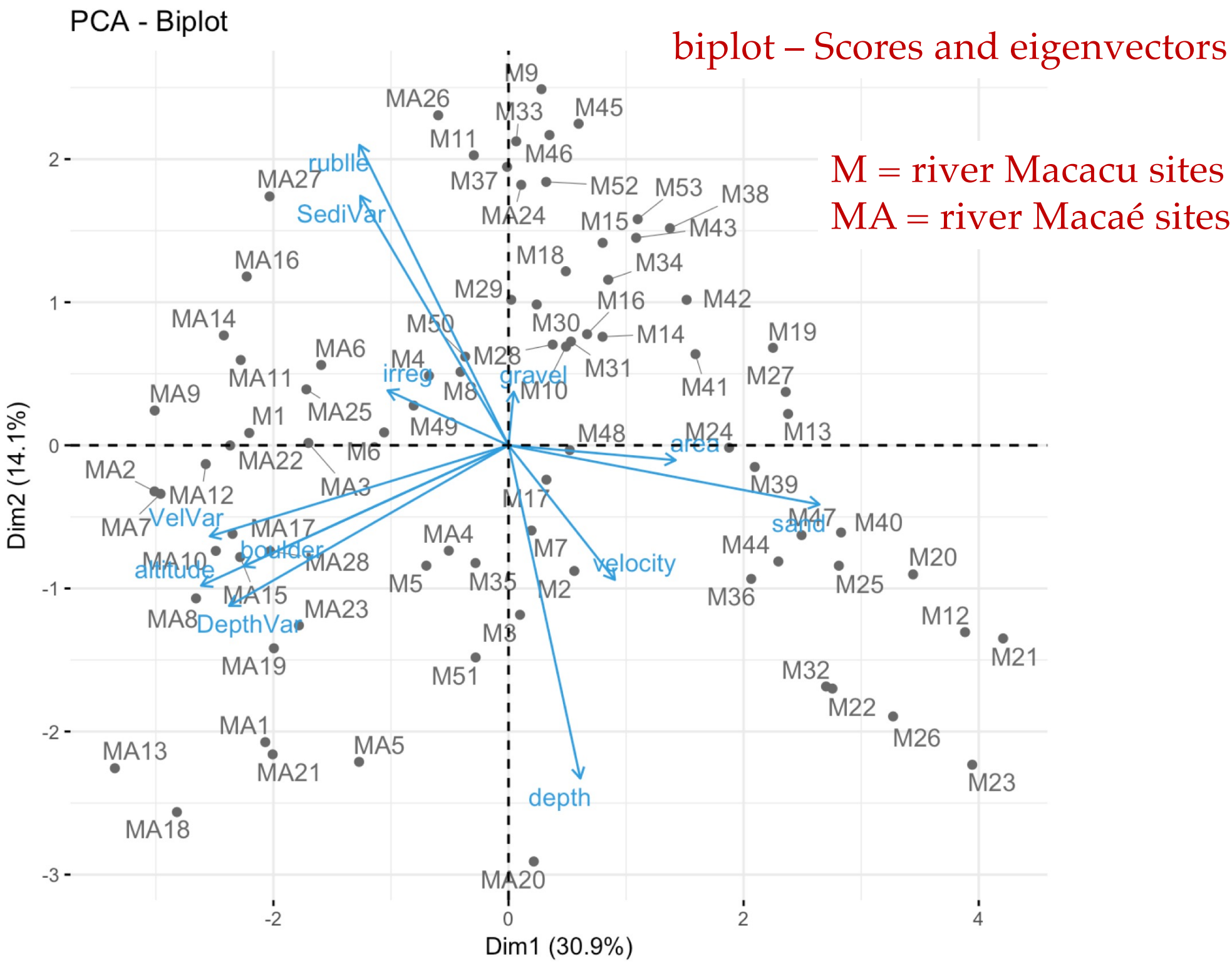
Significant variable contributions are determined if the eigenvector coefficient for the variables are beyond the confidence interval.

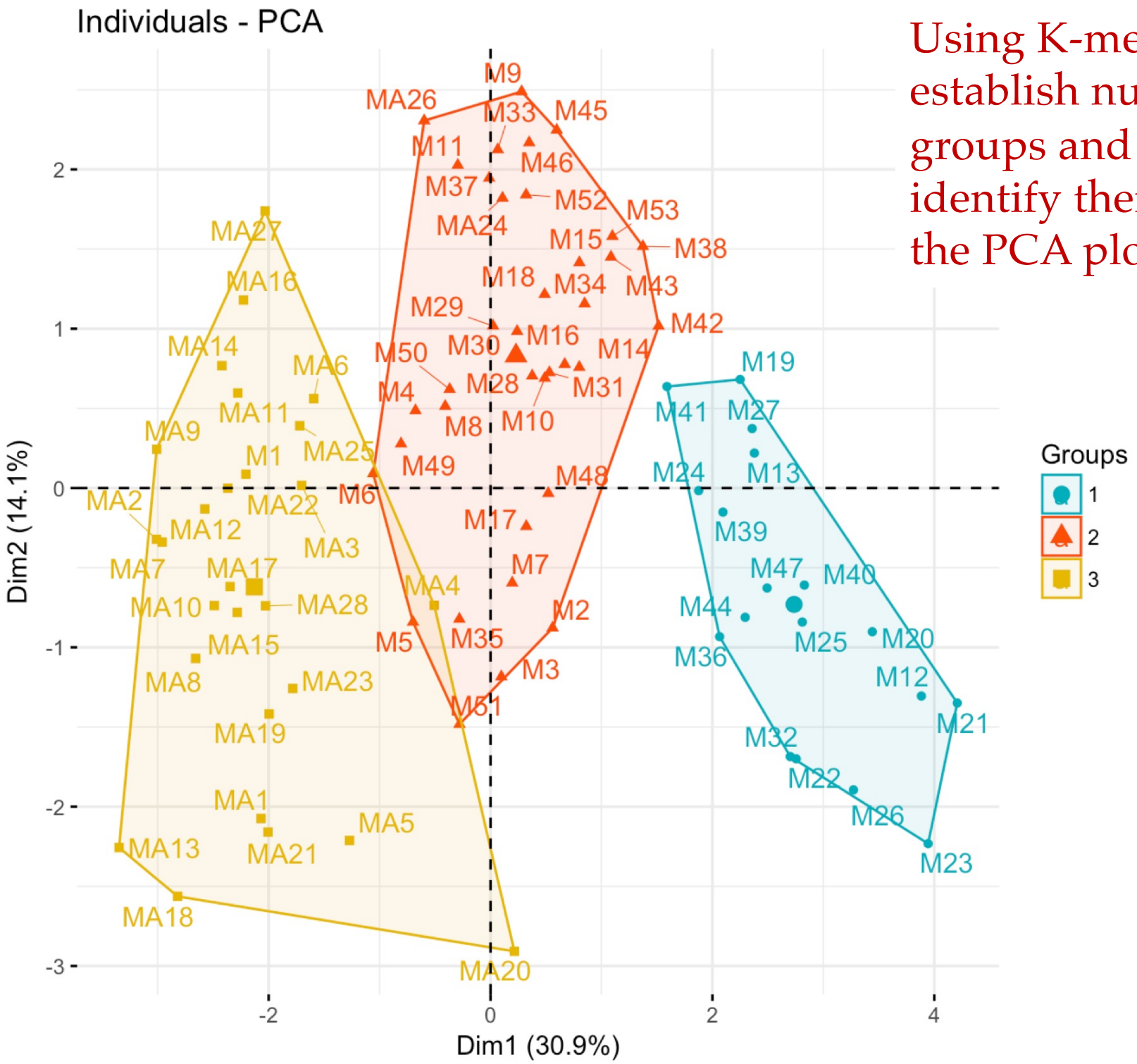


eigenvector structure – much better plot

PC (multivariate) scores




PCA - Biplot
biplot – Scores and eigenvectors
M = river Macacu sites
MA = river Macaé sites
rubble
SediVar
irreg
gravel
area
sand
VelVar
boulder
altitude
DepthVar
velocity
depth
Dim1 (30.9%)
Dim2 (14.1%)



Using K-means to establish number of groups and then identify them the PCA plot

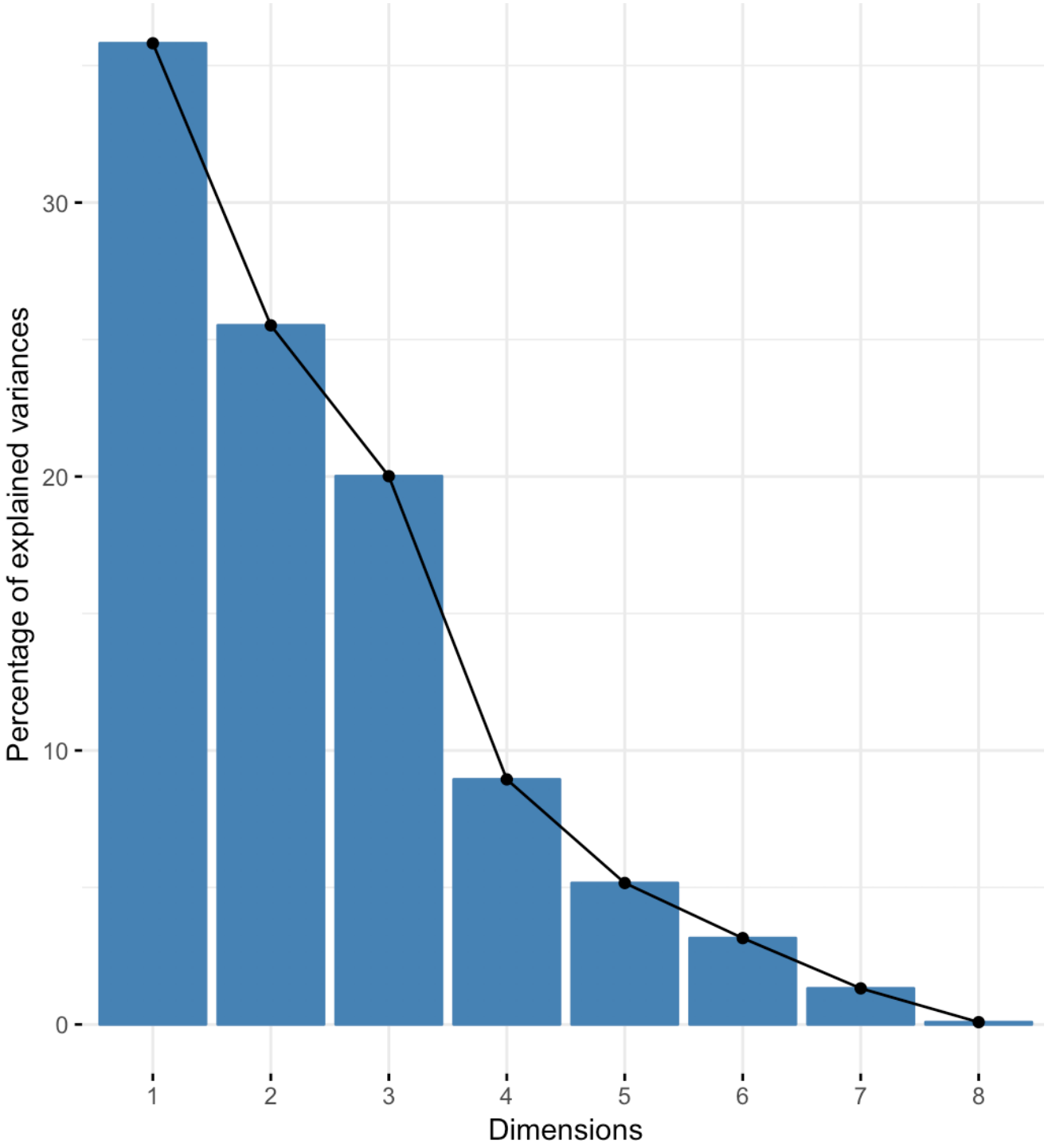
Mapping the environment of our planet – a very “small” example

Long	Lat	avg_prec	avg_ET	avg_VI	avg_Alt	range_Alt	avg_temp	seas_temp	seas_prec
-70.5	-55.344	89.49	222.167	421.958	370.806	2160	38.501	13.97282505	258.8423462
-69.5	-55.344	68.95	241.5	482.354	472.088	2470	32.631	15.6611433	282.420105
-68.5	-55.344	50.23	229	599.458	348.21	1258	38.392	16.68809319	316.756958
-67.5	-55.344	37.9	222.333	623.583	222.572	1047	44.807	22.50125504	323.7763367
-66.5	-55.344	38.94	170.167	498.25	176.965	833	45.774	23.47930336	300.9299011
-70.5	-54.046	47.71	222.167	421.958	174.06	763	54.352	16.45620728	315.1140137
-69.5	-54.046	36.37	241.5	482.354	186.163	786	53.772	17.72191429	331.6278076
-68.5	-54.046	29.06	229	599.458	83.993	342	56.596	20.50442696	354.6487122
-67.5	-54.046	28.69	222.333	623.583	42.762	224	53.089	22.89826965	380.9208679
-73.5	-52.788	149.71	447.167	571.81	287.777	1590	54.122	11.40344238	291.9087524
-72.5	-52.788	54.23	415.333	778.905	267.908	1190	53.38	14.44744396	341.0378723
-71.5	-52.788	26.4	315	867.833	214.992	691	57.626	14.78347588	374.8889771
-70.5	-52.788	18.47	285.167	742.786	148.188	355	61.686	20.54120636	392.6990967
-69.5	-52.788	21.24	158.833	697.405	69.194	263	65.235	23.69093513	386.2383728
-73.5	-51.564	108.16	447.167	562.875	720.814	2785	40.757	11.40344238	291.9087524
-72.5	-51.564	33.43	415.333	761.104	605.359	2000	46.611	14.44744396	341.0378723
-71.5	-51.564	15.04	315	655.229	416.289	861	57.116	14.78347588	374.8889771
-70.5	-51.564	13.15	285.167	622.688	247.667	418	66.142	20.54120636	392.6990967
-69.5	-51.564	15.56	158.833	607.313	161.634	367	69.428	23.69093513	386.2383728
-74.5	-50.373	266.93	512.833	540.292	427.273	2164	60.755	12.20302963	278.6205139
-73.5	-50.373	108.13	353.333	562.875	1127.405	3405	29.841	14.35677052	314.4966431
-72.5	-50.373	31.43	296.333	761.104	568.539	1756	61.505	25.55801201	418.8746643
-71.5	-50.373	13.61	275	655.229	500.653	1080	65.597	26.75129128	476.8866882
-70.5	-50.373	11.79	207.833	622.688	340.328	775	74.516	22.04994202	503.4150391
-69.5	-50.373	13.93	198.167	607.313	171.078	549	83.211	20.19462204	514.8027954
-68.5	-50.373	16.74	134.333	448.188	96.374	463	87.676	22.06239319	502.4994507
-74.5	-49.21	252.75	512.833	547.905	383.44	1567	65.613	8.876086235	275.4307251
-73.5	-49.21	110.05	353.333	497.929	1054.021	3435	36.699	12.14703465	320.0220642
-72.5	-49.21	39.53	296.333	589.905	931.375	1961	48.015	20.98670387	388.9425964
-71.5	-49.21	16.23	275	582.929	768.218	1447	61.56	27.47363091	454.5921631

14909 geographic cells (110Km by 110Km)

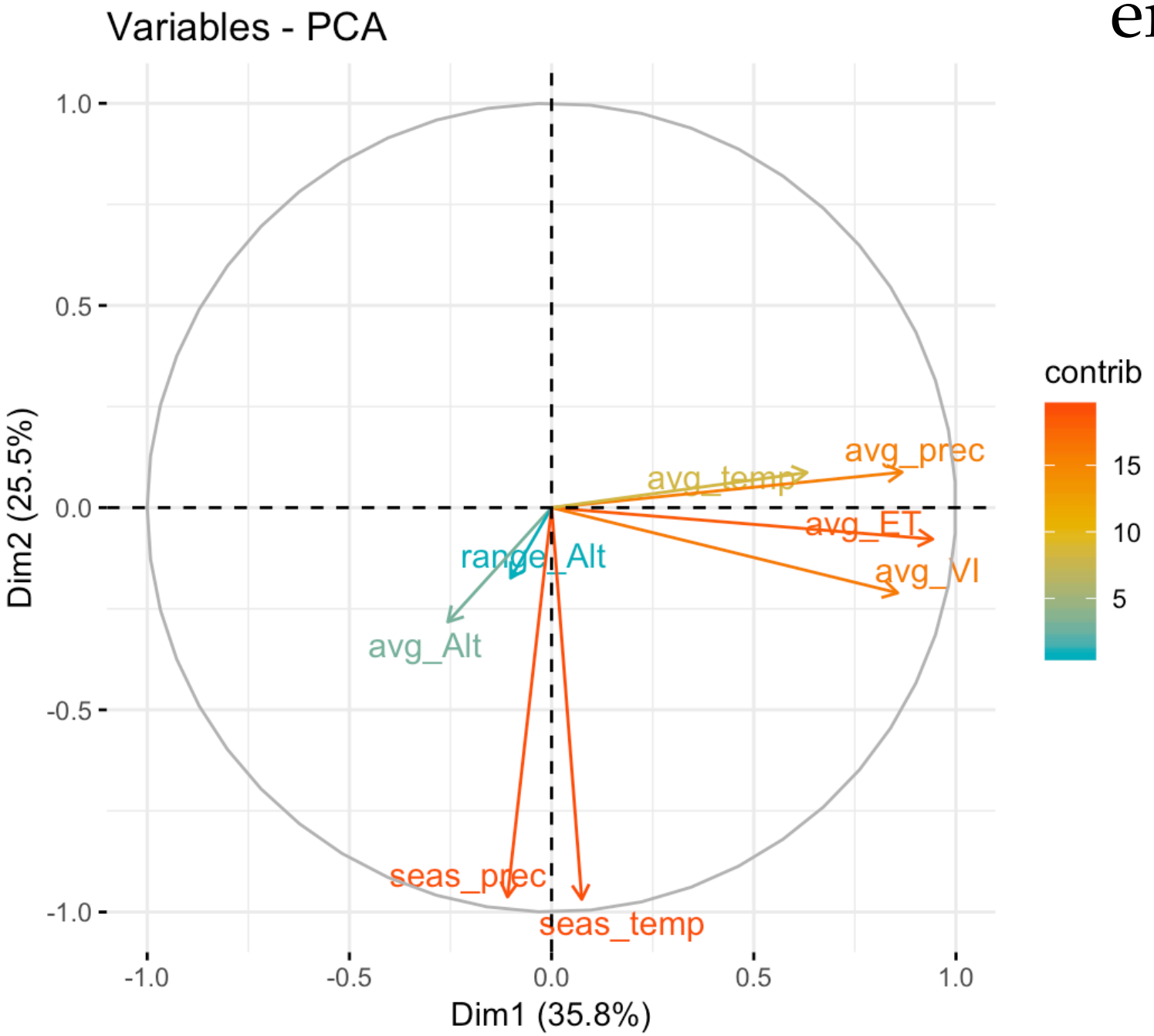
Long	Lat	avg_prec	avg_ET	avg_VI	avg_Alt	range_Alt	avg_temp	seas_temp	seas_prec
-70.5	-55.344	89.49	222.167	421.958	370.806	2160	38.501	13.97282505	258.8423462
-69.5	-55.344	68.95	241.5	482.354	472.088	2470	32.631	15.6611433	282.420105
-68.5	-55.344	50.23	229	599.458	348.21	1258	38.392	16.68809319	316.756958
-67.5	-55.344	37.9	222.333	623.583	222.572	1047	44.807	22.50125504	323.7763367
-66.5	-55.344	38.94	170.167	498.25	176.965	833	45.774	23.47930336	300.9299011
-70.5	-54.046	47.71	222.167	421.958	174.06	763	54.352	16.45620728	315.1140137
-69.5	-54.046	36.37	241.5	482.354	186.163	786	53.772	17.72191429	331.6278076
-68.5	-54.046	29.06	229	599.458	83.993	342	56.596	20.50442696	354.6487122
-67.5	-54.046	28.69	222.333	623.583	42.762	224	53.089	22.89826965	380.9208679
-73.5	-52.788	149.71	447.167	571.81	287.777	1590	54.122	11.40344238	291.9087524
-72.5	-52.788	54.23	415.333	778.905	267.908	1190	53.38	14.44744396	341.0378723
-71.5	-52.788	26.4	315	867.833	214.992	691	57.626	14.78347588	374.8889771
-70.5	-52.788	18.47	285.167	742.786	148.188	355	61.686	20.54120636	392.6990967
-69.5	-52.788	21.24	158.833	697.405	69.194	263	65.235	23.69093513	386.2383728
-73.5	-51.564	108.16	447.167	562.875	720.814	2785	40.757	11.40344238	291.9087524
-72.5	-51.564	33.43	415.333	761.104	605.359	2000	46.611	14.44744396	341.0378723
-71.5	-51.564	15.04	315	655.229	416.289	861	57.116	14.78347588	374.8889771
-70.5	-51.564	13.15	285.167	622.688	247.667	418	66.142	20.54120636	392.6990967
-69.5	-51.564	15.56	158.833	607.313	161.634	367	69.428	23.69093513	386.2383728
-74.5	-50.373	266.93	512.833	540.292	427.273	2164	60.755	12.20302963	278.6205139
-73.5	-50.373	108.13	353.333	562.875	1127.405	3405	29.841	14.35677052	314.4966431
-72.5	-50.373	31.43	296.333	761.104	568.539	1756	61.505	25.55801201	418.8746643
-71.5	-50.373	13.61	275	655.229	500.653	1080	65.597	26.75129128	476.8866882
-70.5	-50.373	11.79	207.833	622.688	340.328	775	74.516	22.04994202	503.4150391
-69.5	-50.373	13.93	198.167	607.313	171.078	549	83.211	20.19462204	514.8027954
-68.5	-50.373	16.74	134.333	448.188	96.374	463	87.676	22.06239319	502.4994507
-74.5	-49.21	252.75	512.833	547.905	383.44	1567	65.613	8.876086235	275.4307251
-73.5	-49.21	110.05	353.333	497.929	1054.021	3435	36.699	12.14703465	320.0220642
-72.5	-49.21	39.53	296.333	589.905	931.375	1961	48.015	20.98670387	388.9425964
-71.5	-49.21	16.23	275	582.929	768.218	1447	61.56	27.47363091	454.5921631

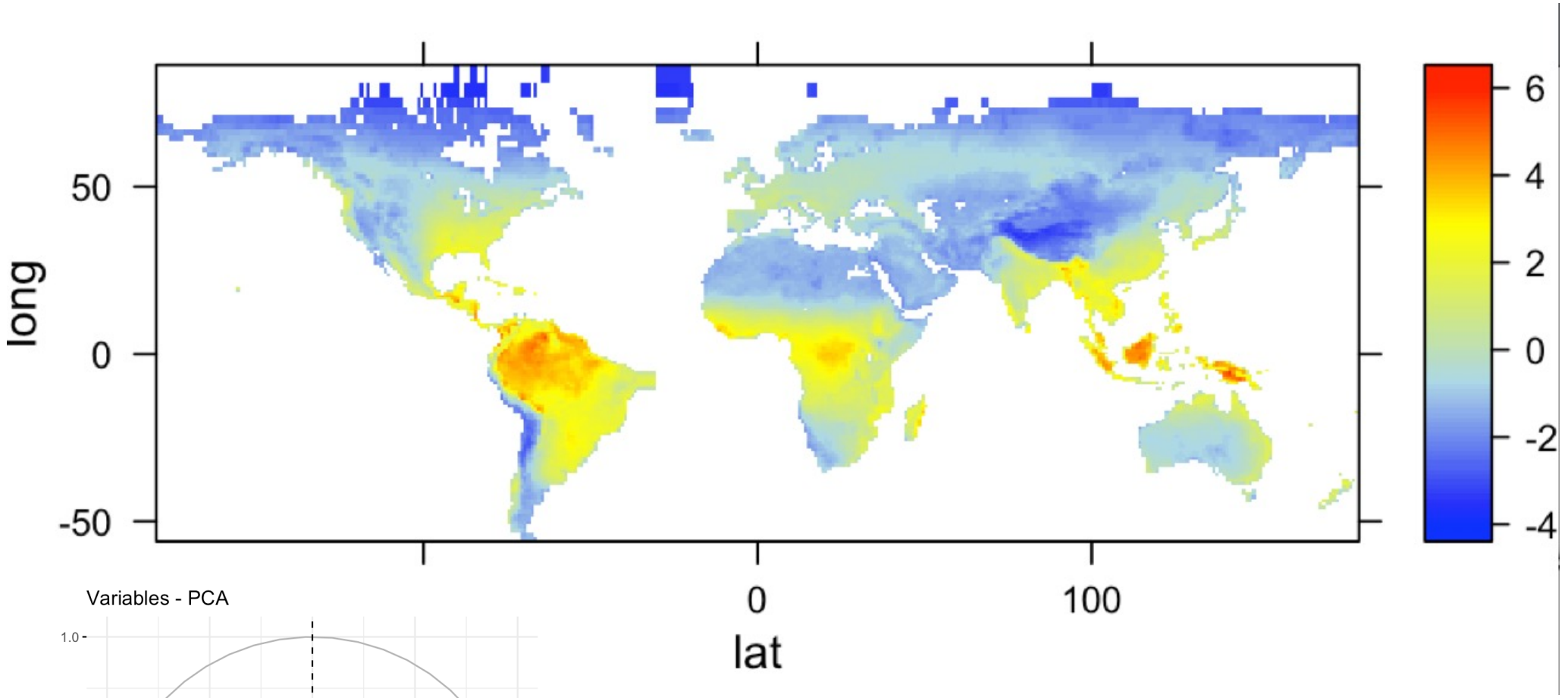
1) Latitude (Lat) and Longitude (Long) at the centre of geographic cell.
2) Average precipitation (last 40 years; avg_prec)
3) Average actual evapotranspiration (avg_ET, a proxy of productivity)
4) Average vegetation index (avg_VI)
5) Mean altitude (avg_Alt)
6) Maximum altitude minus minimum altitude (altitudinal range; range_Alt)
7) Average temperature (avg_temp)
8) Seasonal temperature (annual range in temperature; seas_temp)
9) Seasonal precipitation (annual range in precipitation; seas_prec)



Eigenvalue contribution – the traditional scree plot

eigenvector structure

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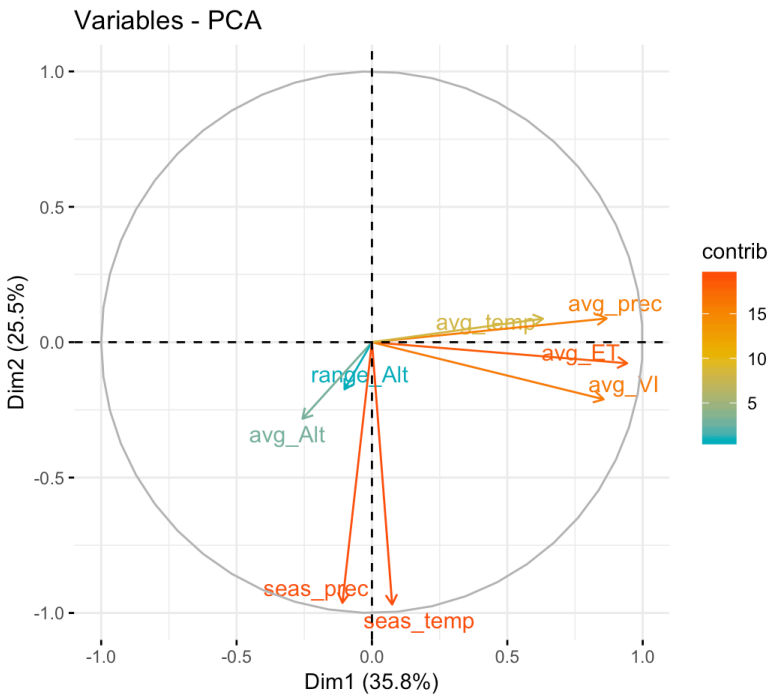
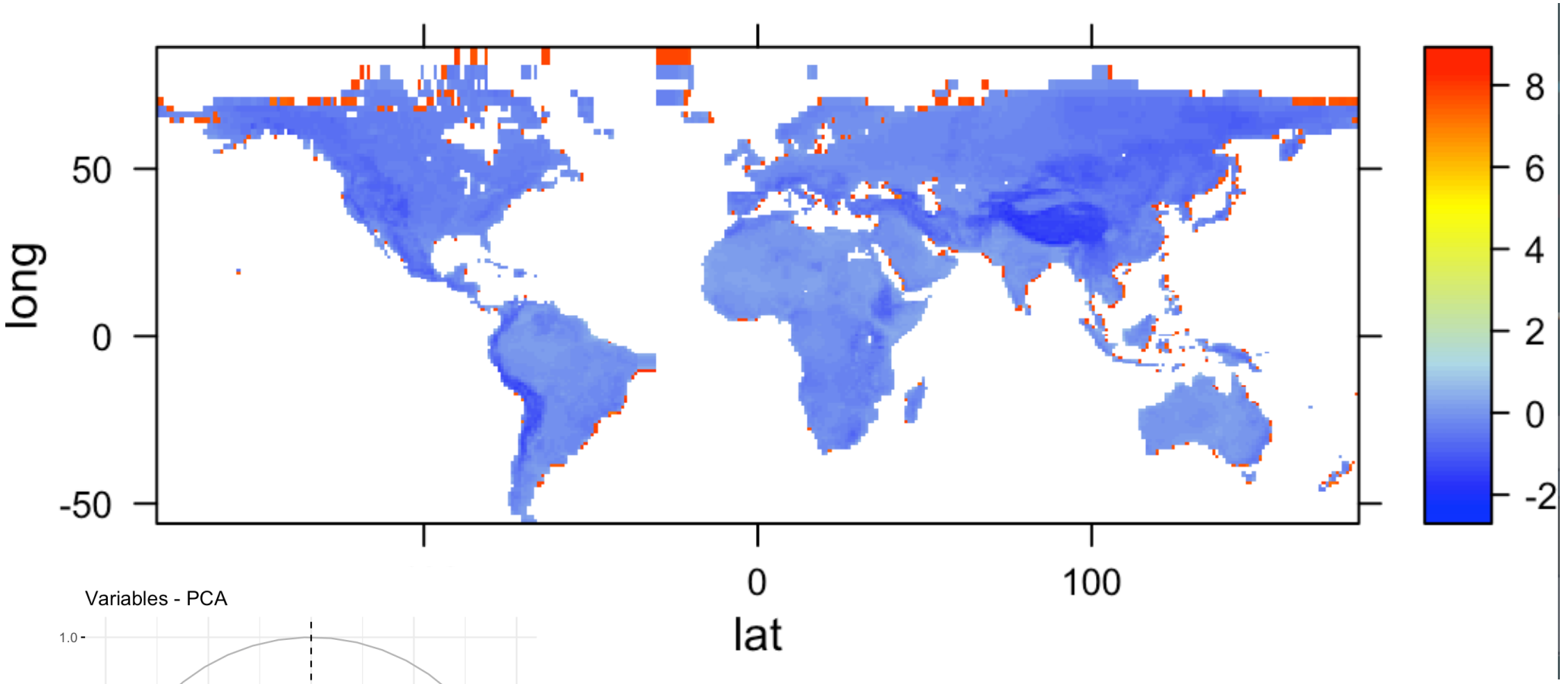
0
100
lat
6
4
2
0
-2
-4


Variables - PCA
Dim2 (25.5%)
Dim1 (35.8%)
1.0
0.5
0.0
-0.5
-1.0
avg_temp
avg_prec
avg_ET
avg_VI
range_Alt
avg_Alt
seas_prec
seas_temp
contrib
15
10
5

Map of PC-1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lat
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0
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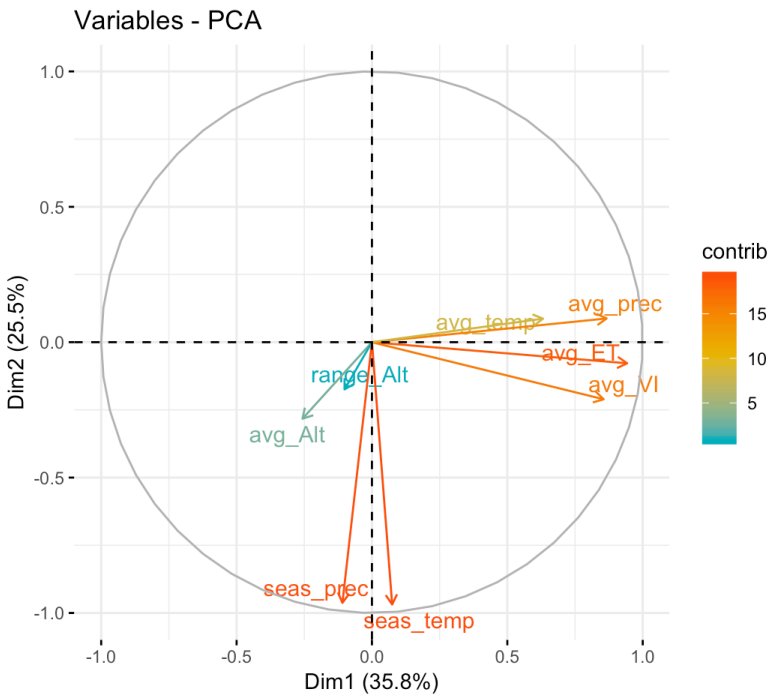
Variables - PCA
Dim2 (25.5%)
Dim1 (35.8%)
1.0
0.5
0.0
-0.5
-1.0
avg_prec
avg_temp
avg_ET
avg_VI
range_Alt
avg_Alt
seas_prec
seas_temp
contrib
15
10
5

Map of PC-2