Ordination

- **Principal component analysis (PCA)**
- **Factor analysis (FA)**
- **Correspondence analysis (CA)**
- **Principal coordinate analysis (PCoA) or multidimensional scaling (MDS)**
- **Non-metric multidimensional scaling (NMDS)**
- **Redundancy analysis (RDA)**
- **Canonical correspondence analysis (CCA)**
- **Generalized Joint Attribute Modeling (GJAM)**

History of ordination methods

- In 1930, Ramensky began to use informal ordination techniques for vegetation. Such informal and largely subjective methods became widespread in the early 1950's (Whittaker 1967).
- In 1951, Curtis and McIntosh (1951) developed the 'continuum index', which later lead to conceptual links between species responses to gradients and multivariate methods. Shortly thereafter, Goodall (1954) introduced the term 'ordination' in an ecological context for Principal Components Analysis.
- Bray and Curtis (1957) developed polar ordination, which became the first widely-used ordination technique in ecology.
- Austin (1968) used canonical correlation to assess plant-environment relationships in what may have been the first example of multivariate direct gradient analysis in ecology.
- In 1973, Hill introduced correspondence analysis, a technique originating in the 1930's, to ecologists. Correspondence analysis gradually supplanted polar ordination, which today has few practitioners.
- Fasham (1977) and Prentice (1977) independently discovered and demonstrated the utility of Kruskal's (1964) nonmetric multidimensional scaling, originally intended as a psychometric technique, for community ecology.
- Hill (1979) corrected some of the flaws of Correspondence Analysis and thereby created Detrended Correspondence Analysis, which is the most widely used indirect gradient analysis technique today. The software to implement Detrended Correspondence Analysis, DECORANA, became the backbone of many later software packages.
- Gauch's (1982) book "Multivariate Analysis in Community Ecology" described ordination in non-technical terms to the average practitioner, and allowed ordination techniques to enter the mainstream.
- Fuzzy set theory, introduced to ecologists by Roberts (1986), is a promising approach with ties to polar ordination, but has yet to gain many adherents.
- Ter Braak (1986) ushered in the biggest modern revolution in ordination methods with Canonical Correspondence Analysis. This technique coupled Correspondence Analysis with regression methodologies, and provides for hypothesis testing.
- Ter Braak and Prentice (1988) developed a theoretical unification of ordination techniques, hence placing gradient analysis on a firm theoretical foundation.

Principal Component Analysis (PCA)

Invented by Pearson (1901) and Hotelling (1933)

Use in ecology by Goodall (1954) under the name “factor analysis” (“principal factor analysis” is a synonym of PCA).

Principal component analysis

Principal component analysis (PCA) is a technique that is useful for the compression and classification of data. The purpose is to **reduce the dimensionality of a data set** (sample) by finding a new set of variables, smaller than the original set of variables, that nonetheless retains most of the sample's information.

By information we mean the variation present in the sample, given by the correlations between the original variables. The new variables, called principal components (PCs), are uncorrelated, and are ordered by the fraction of the total information each retains.

Example

In this example wildlife (moose) population density was measured over time (once a year) in three areas.

Year	Area 1	Area 2	Area 3
1	11.3	14.1	6.9
2	10.4	14	11.2
3	9.9	13	8.7
4	8.2	11.4	3.3
5	10.1	11.9	8.7
6	10.7	13.8	12.5
7	11	14.9	8.9
8	7.1	8.5	3.7
9	14.7	14.5	12.1
10	5.4	9	4.1
11	7.3	7.6	5.6
12	10.2	10.9	7.3
13	6.1	9.9	6.8
14	9.7	13.2	6.6
15	8.1	9.4	4
16	11.3	11.8	4.9
17	8.8	11.5	8.8
18	9.4	11.6	5.7
19	7.5	11.4	4.9
20	8.8	10.7	7.2
21	7.5	11.1	7
22	9.1	13.2	8.9
23	6.8	9.8	7.6

https://timgsa.baidu.com/timg?image&quality=80&size=b9999_10000&sec=1491476303003&di=f903f1e5bc129bcf ff1201fa4fdeb8b8&imgtype=0&src=http%3A%2F%2Fwww.bigthings.ca%2Fscotia%2Fpictures%2Fmoose1.jpg

From Laverty's presentation "Techniques for studying correlation and covariance structure"

Habitats

Year	Area 1	Area 2	Area 3
1	11.3	14.1	6.9
2	10.4	14	11.2
3	9.9	13	8.7
4	8.2	11.4	3.3
5	10.1	11.9	8.7
6	10.7	13.8	12.5
7	11	14.9	8.9
8	7.1	8.5	3.7
9	14.7	14.5	12.1
10	5.4	9	4.1
11	7.3	7.6	5.6
12	10.2	10.9	7.3
13	6.1	9.9	6.8
14	9.7	13.2	6.6
15	8.1	9.4	4
16	11.3	11.8	4.9
17	8.8	11.5	8.8
18	9.4	11.6	5.7
19	7.5	11.4	4.9
20	8.8	10.7	7.2
21	7.5	11.1	7
22	9.1	13.2	8.9
23	6.8	9.8	7.6

From Laverty's presentation "Techniques for studying correlation and covariance structure"

The Sample Statistics

$$\vec{\bar{x}} = \begin{bmatrix} 9.10 \\ 11.62 \\ 7.19 \end{bmatrix}$$

```
A = A[, c(2:4)] # The covariance matrix
apply(A, 2, mean) # mean
```

$$S = \begin{bmatrix} 4.297 & 3.307 & 3.295 \\ & 4.015 & 3.527 \\ & & 6.566 \end{bmatrix}$$

```
# variance-covariance matrix
S = var(A)
```

$$R = \begin{bmatrix} 1 & .796 & .620 \\ & 1 & .687 \\ & & 1 \end{bmatrix}$$

```
cor(A) # correlation matrix
```

```
A = read.table(header = T, text = "
Year Area1 Area2 Area3
1 11.3 14.1 6.9
2 10.4 14 11.2
3 9.9 13 8.7
4 8.2 11.4 3.3
5 10.1 11.9 8.7
6 10.7 13.8 12.5
7 11 14.9 8.9
8 7.1 8.5 3.7
9 14.7 14.5 12.1
10 5.4 9 4.1
11 7.3 7.6 5.6
12 10.2 10.9 7.3
13 6.1 9.9 6.8
14 9.7 13.2 6.6
15 8.1 9.4 4
16 11.3 11.8 4.9
17 8.8 11.5 8.8
18 9.4 11.6 5.7
19 7.5 11.4 4.9
20 8.8 10.7 7.2
21 7.5 11.1 7
22 9.1 13.2 8.9
23 6.8 9.8 7.6 ")
```

From Laverty's presentation "Techniques for studying correlation and covariance structure"

Eigenvalues and eigenvectors eigen(S)

$$S=\begin{bmatrix} 4.297 & 3.307 & 3.295 \\ & 4.015 & 3.527 \\ & & 6.566 \end{bmatrix}$$

The eigenvalues of S

$$\lambda_1 = 11.85974, \quad \lambda_2 = 2.204232, \quad \lambda_3 = 0.814249$$

The eigenvectors of S

$$a_1=\begin{bmatrix} 0.522 \\ 0.523 \\ 0.674 \end{bmatrix} \quad a_2=\begin{bmatrix} -0.582 \\ -0.359 \\ 0.730 \end{bmatrix} \quad a_3=\begin{bmatrix} 0.624 \\ -0.773 \\ 0.117 \end{bmatrix}$$

The principal components

$$C_1 = 0.522X_1 + 0.523X_2 + 0.674X_3$$

$$C_2 = -0.582X_1 - 0.359X_2 + 0.730X_3$$

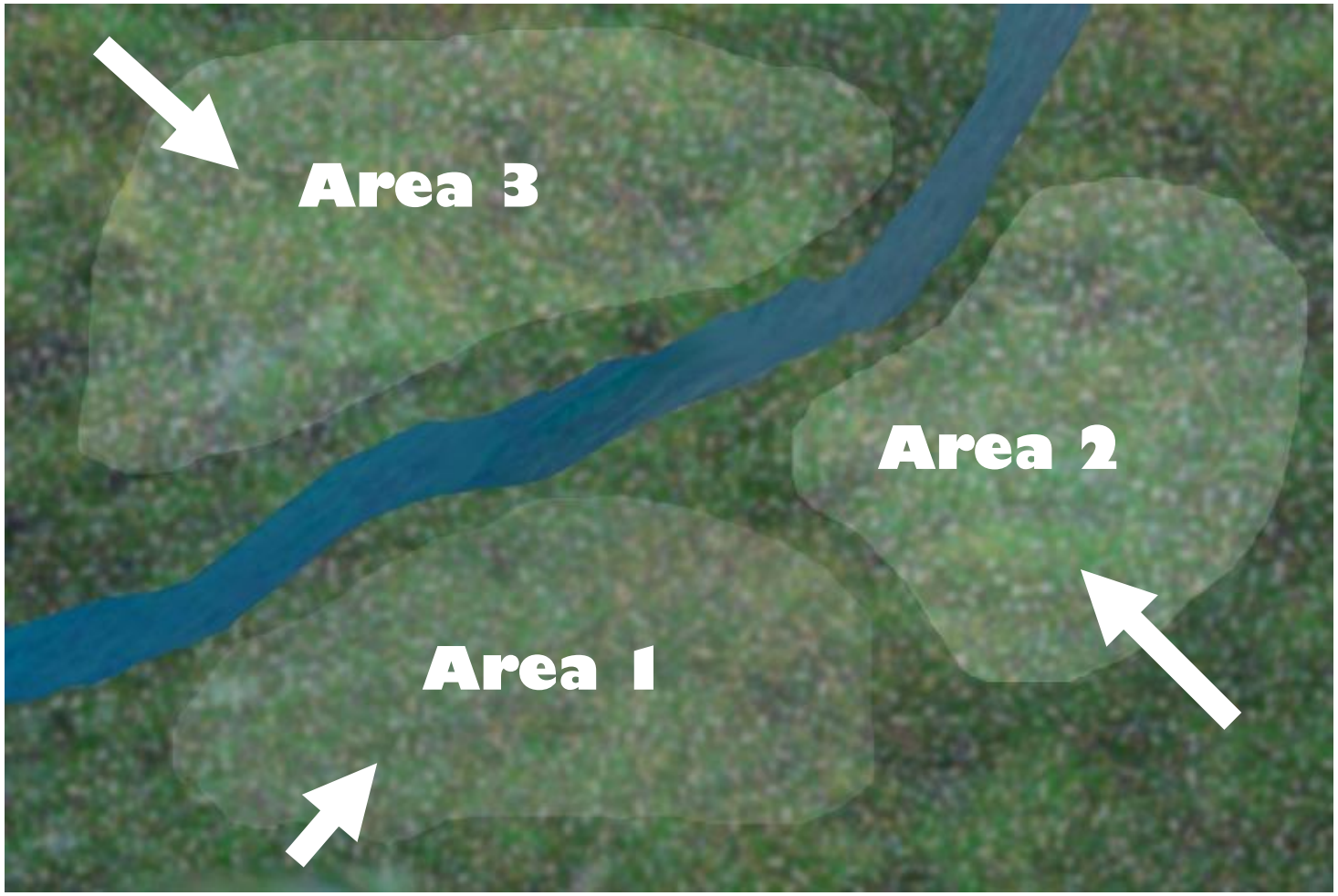
$$C_3 = 0.624X_1 - 0.733X_2 + 0.117X_3$$

	Comp.1	Comp.2	Comp.3
[1,]	-2.2489	2.3813	-0.5841
[2,]	-4.6230	-1.3164	-0.5654
[3,]	-2.1549	-0.1418	-0.3964
[4,]	3.2071	2.2356	-0.8506
[5,]	-1.6840	-0.4203	0.5787
[6,]	-5.5508	-2.1624	-0.0718
[7,]	-3.8578	1.0343	-1.1559
[8,]	5.0289	0.2627	0.7520
[9,]	-7.7363	0.7082	1.8344
[10,]	5.3857	-0.8389	-0.6477
[11,]	4.1154	-1.3306	1.7945
[12,]	-0.2701	0.3006	1.2504
[13,]	2.7307	-2.0790	-0.5914
[14,]	-0.7405	1.3462	-0.9211
[15,]	3.8339	0.9487	0.7149
[16,]	0.3013	3.0153	0.9601
[17,]	-0.8633	-1.3932	0.0890
[18,]	0.8592	1.2541	0.0235
[19,]	2.4949	0.6607	-1.1001
[20,]	0.6329	-0.5127	0.5204
[21,]	1.2373	-0.9796	-0.6227
[22,]	-1.9765	-0.6814	-1.0264
[23,]	1.8786	-2.2914	0.0159

Corrected from Laverty's presentation "Techniques for studying correlation and covariance structure"

Example 1/3

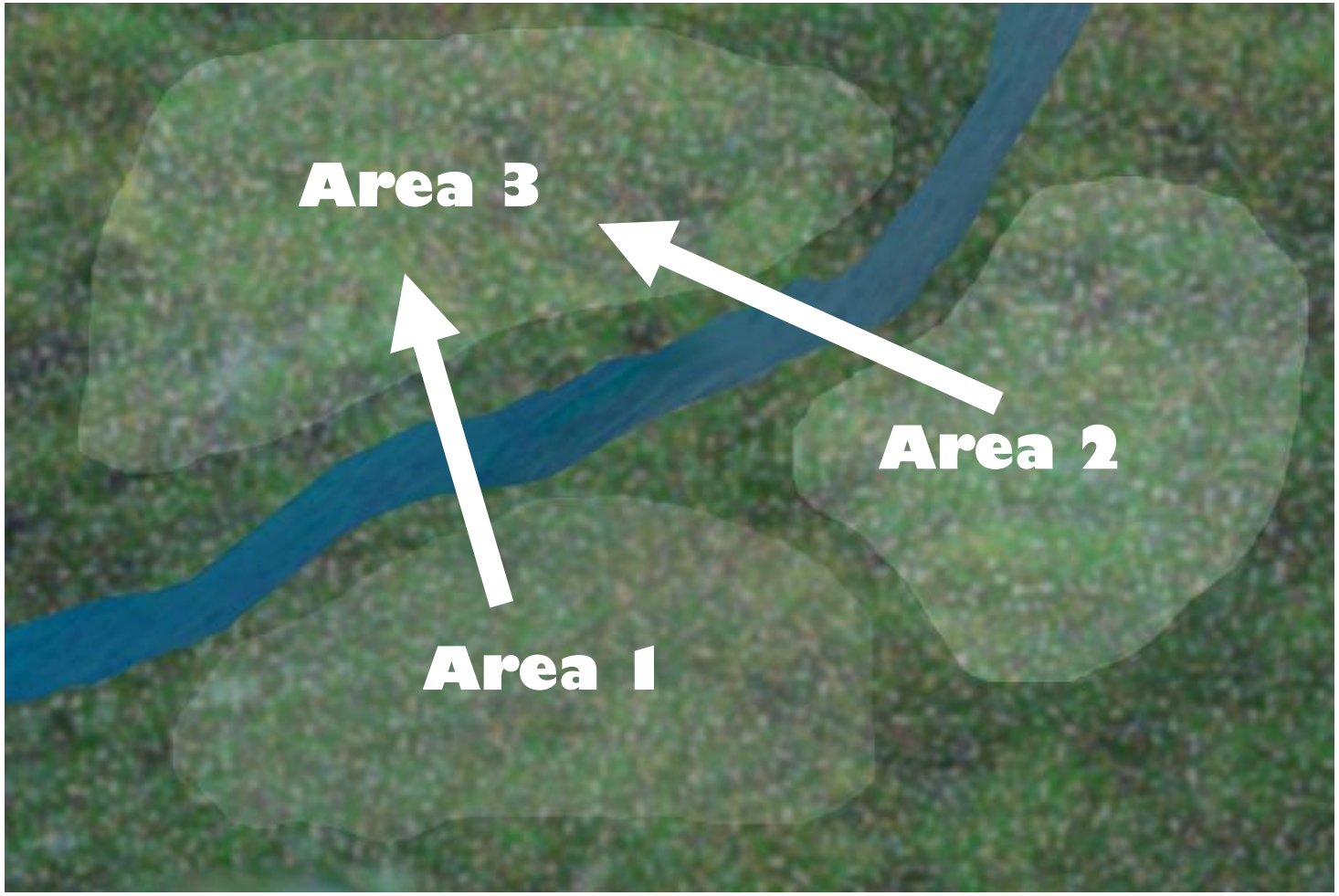
$$C_1 = 0.522X_1 + 0.523X_2 + 0.674X_3$$



From Laverty's presentation "Techniques for studying correlation and covariance structure"

Example 2/3

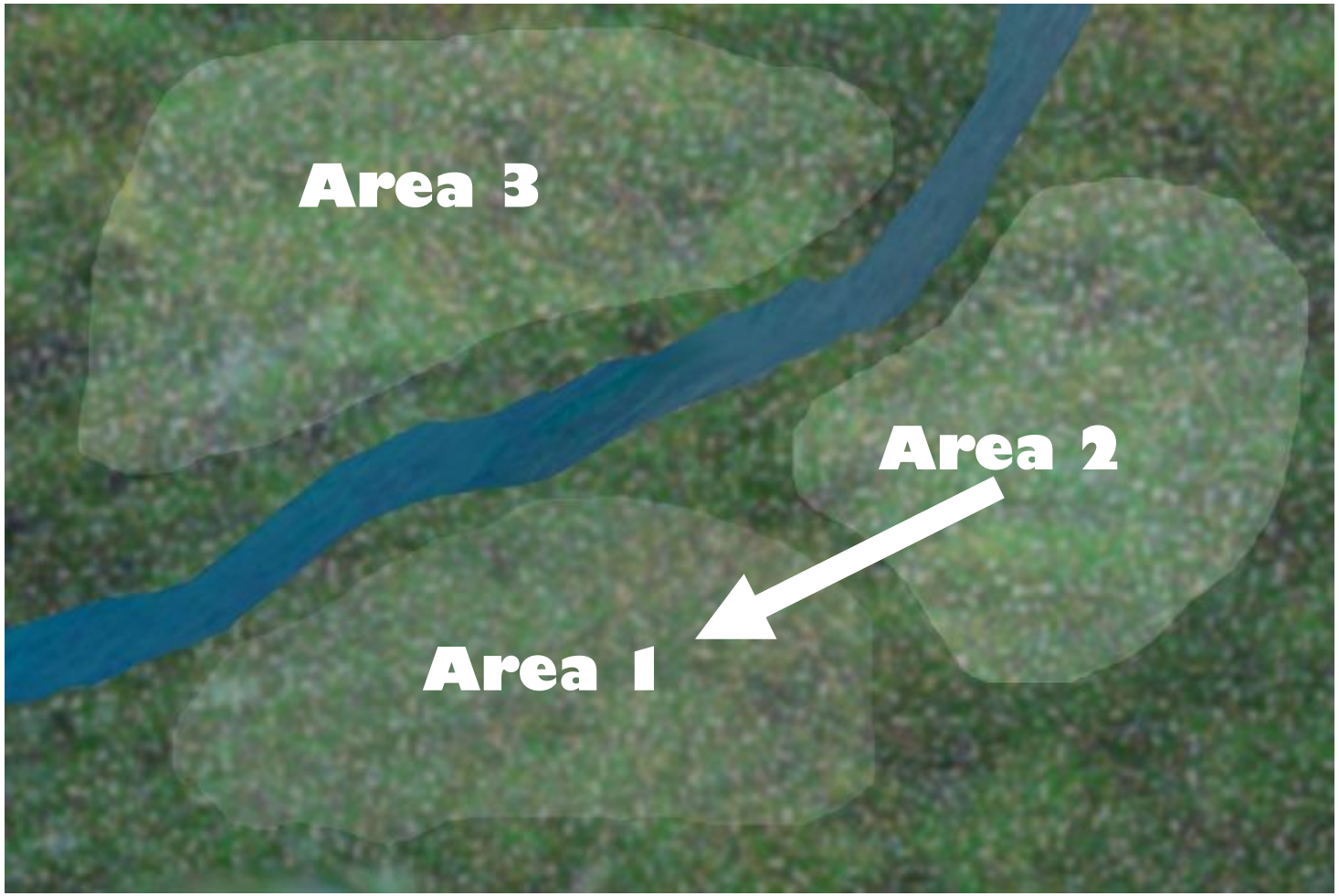
$$C_2 = - 0.582X_1 - 0.359X_2 + 0.730X_3$$



Corrected from Laverty's presentation "Techniques for studying correlation and covariance structure"

Example 3/3

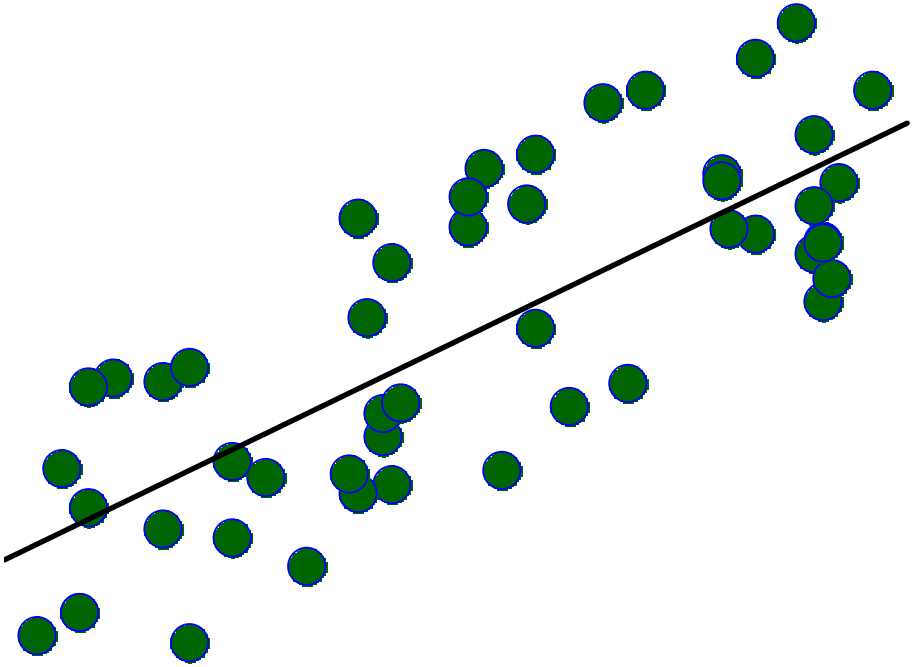
$$C_3 = .624x_1 - .733x_2 + .117x_3$$



From Laverty's presentation "Techniques for studying correlation and covariance structure"

Principal Component Analysis

- Given m points in a n dimensional space, for large n, how does one project on to a 1 dimensional space?
- Choose a line that fits the data so the points are spread out well along the line.

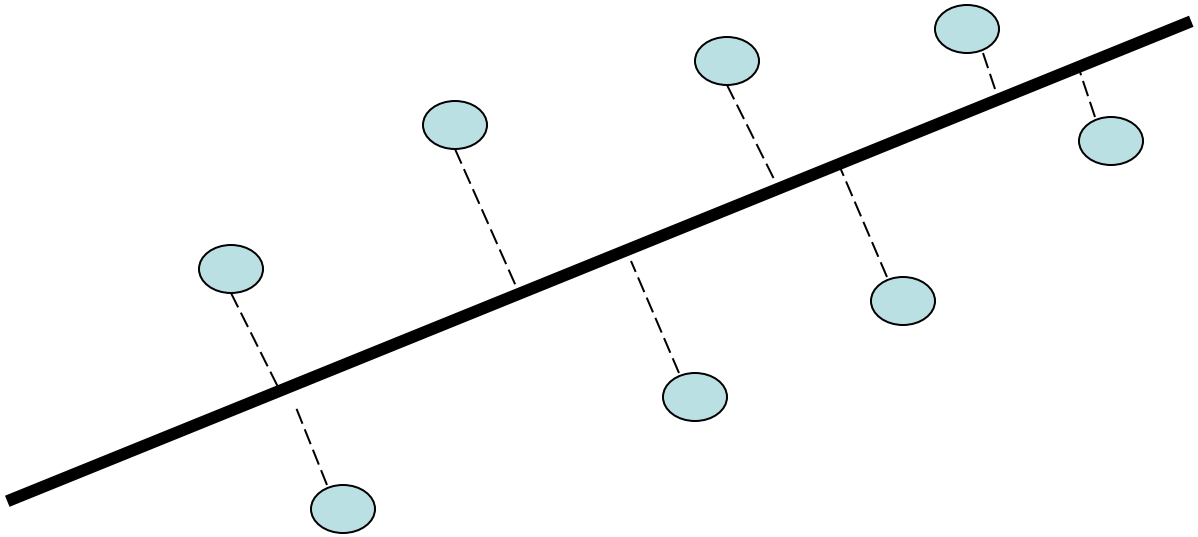


```
X = sample(1:100, 50, rep = TRUE)
# Y = X + rnorm(50, 0, 20)
Y = jitter(X, factor = 1, amount = 40)

plot(X, Y, pch = 21, cex = 3, col = "blue",
      bg = "darkgreen", lwd = 1,
      axes = FALSE, xlab = "", ylab = "")
abline(lm(Y~X), lwd=3)
```

Principal Component Analysis

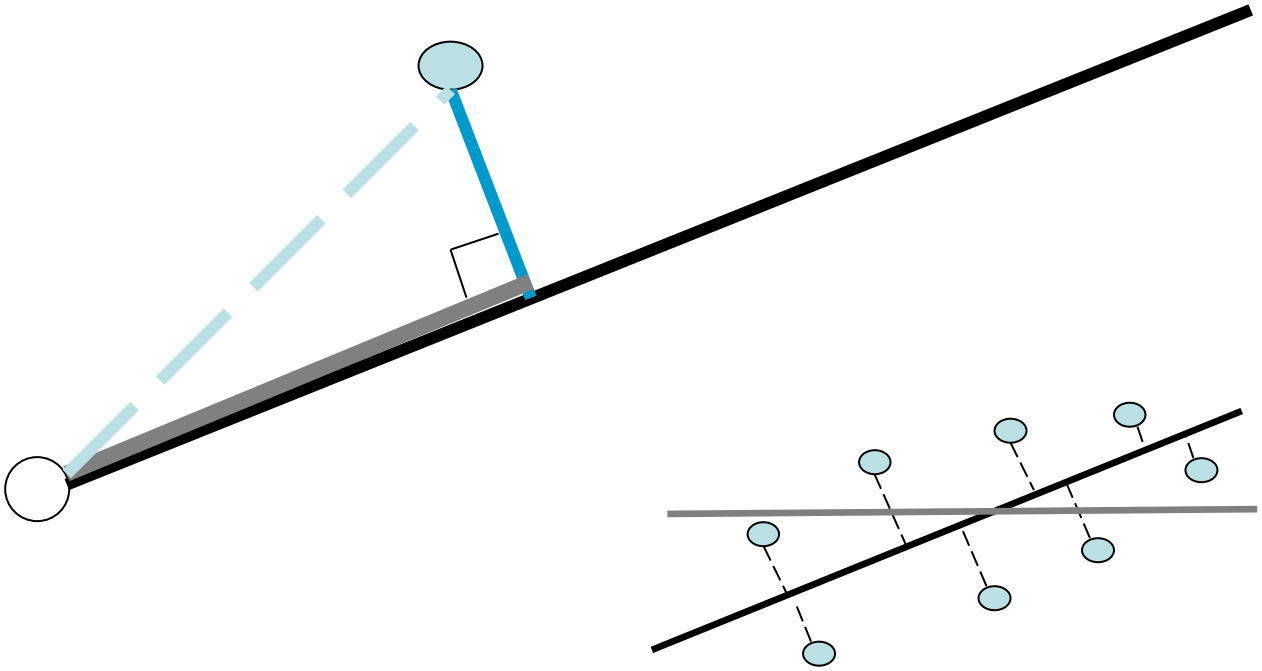
- Formally, minimize sum of squares of distances to the line.



- Why sum of squares? Because it allows fast minimization.

Principal Component Analysis

- For one data point and a line through point (0,0), minimizing sum of squares of distances to the line is the same as maximizing the sum of squares of the projections on that line (Pythagoras, long ago)



PCA: General methodology

From *k* original variables: $x_1,x_2,\ldots,x_k$:

Produce *k* new variables: $y_1,y_2,\ldots,y_k$:

$$y_1 = a_{11}x_1 + a_{12}x_2 + \ldots + a_{1k}x_k$$
$$y_2 = a_{21}x_1 + a_{22}x_2 + \ldots + a_{2k}x_k$$
$$\ldots$$
$$y_k = a_{k1}x_1 + a_{k2}x_2 + \ldots + a_{kk}x_k$$

y_k's are **Principal Components**

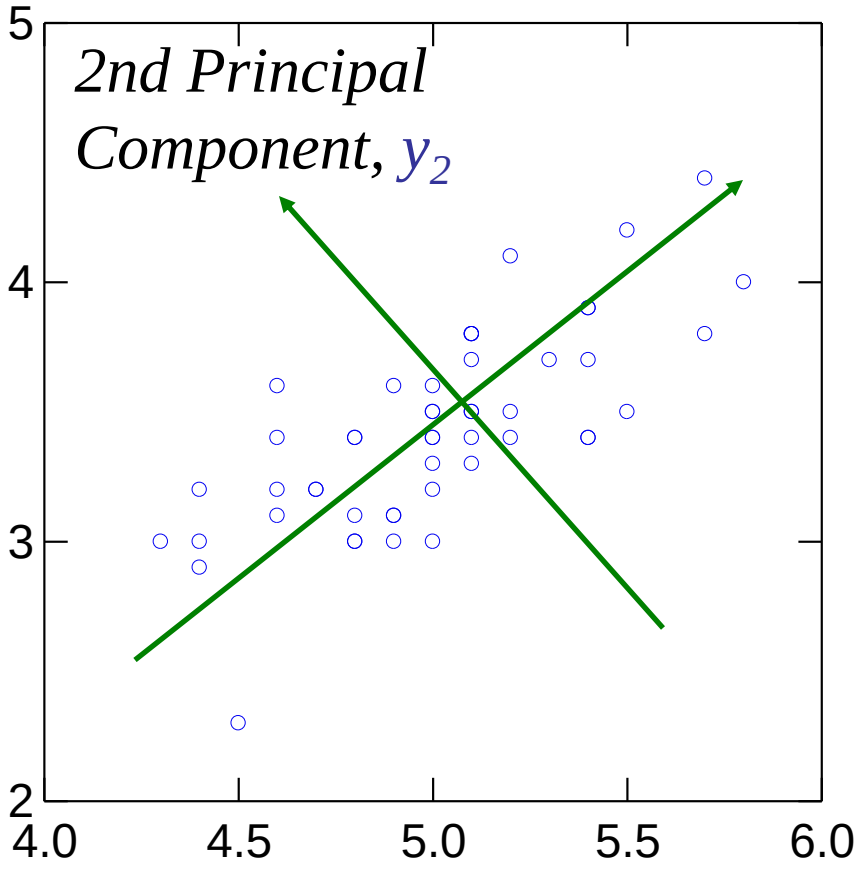
such that:

y_k's are uncorrelated (orthogonal)

y_1 explains as much as possible of original variance in data set

y_2 explains as much as possible of remaining variance

Graphical interpretation



Eigenvalues

Amount of **variance accounted for** by:

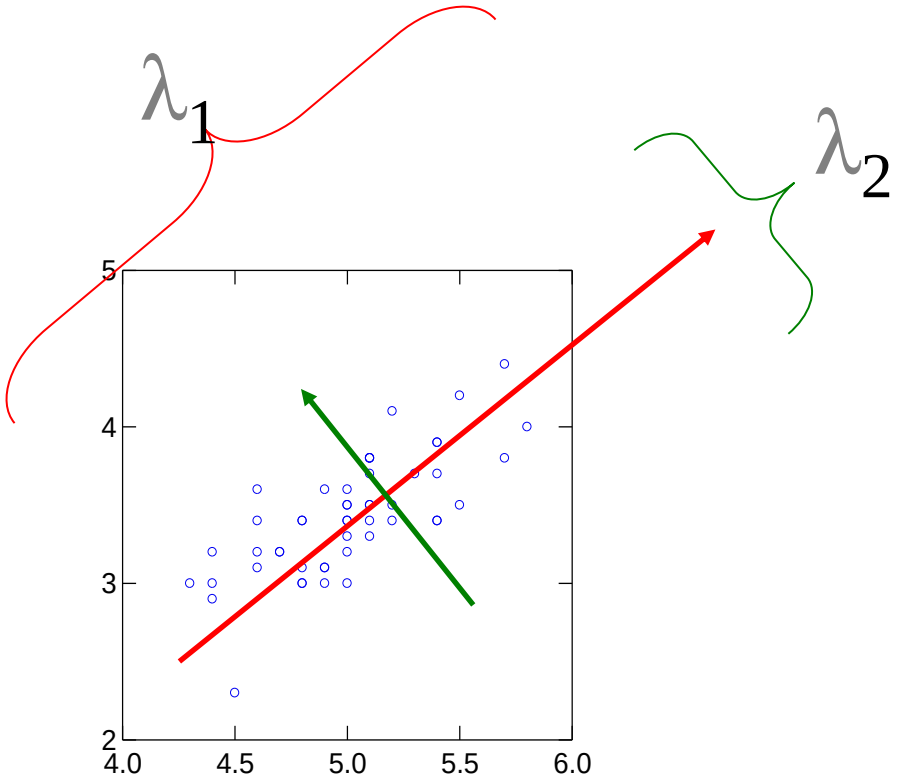
1st principal component, λ_1, 1st **eigenvalue**

2nd principal component, λ_2, 2nd **eigenvalue**

...

$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \geq \ldots$

Average $\lambda_j = 1$ if the matrix is standardized.



Eigenvectors

$\{a_{11},a_{12},...,a_{1k}\}$ is 1st **Eigenvector** of covariance matrix, and **coefficients** of first principal component

$\{a_{21},a_{22},...,a_{2k}\}$ is 2nd **Eigenvector** of covariance matrix, and **coefficients** of 2nd principal component

…

$\{a_{k1},a_{k2},...,a_{kk}\}$ is *k*th **Eigenvector** of covariance matrix, and **coefficients** of *k*th principal component

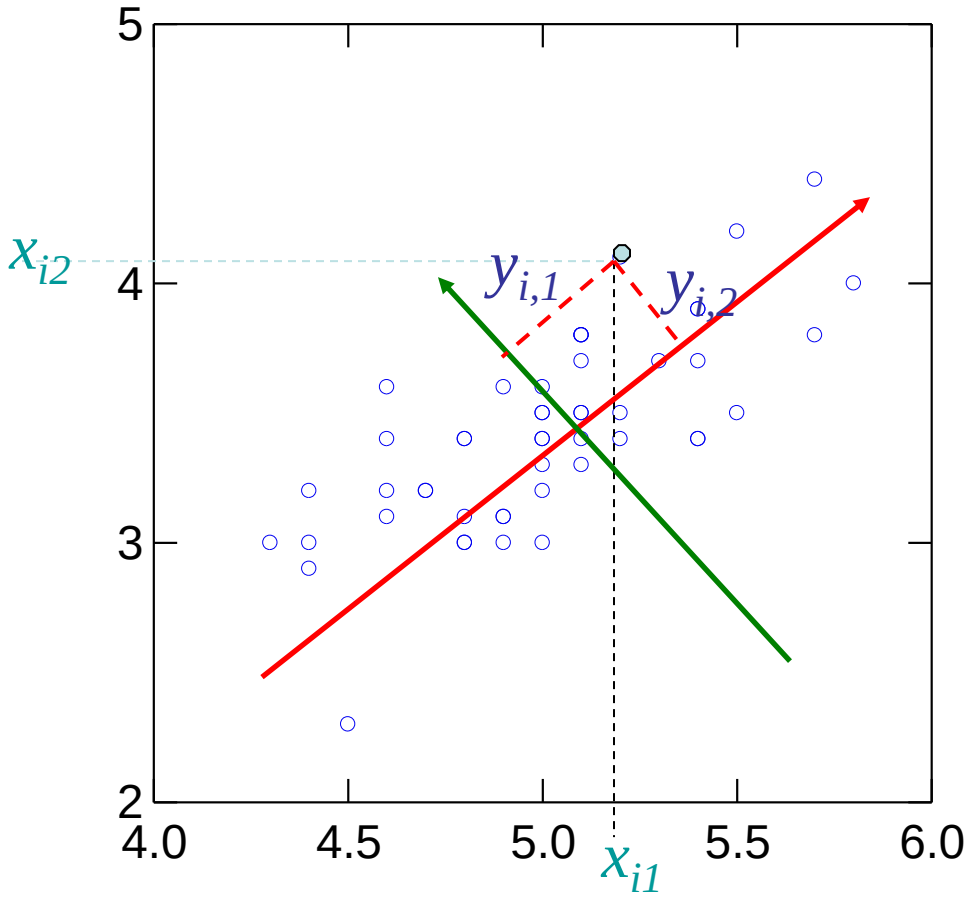
PCA: Terminology

- *j*th **principal component** is linear combination of all variables
- **coefficients**, a_{jk}, are elements of eigenvectors and relate original variables (standardized if using correlation matrix) to components
- **scores** are values of units on components (produced using coefficients)
- **amount of variance accounted for** by component is given by eigenvalue, λ_j
- **proportion of variance accounted for** by component is given by $\lambda_j / \Sigma \lambda_j$
- **loading** of *k*th original variable on *j*th component is given by a_{jk}

  correlation between variable and component

Scores

Score of *i*th unit on *j*th principal component



R code: PCA

head(mtcars)

	mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
Mazda_RX4	21	6	160	110	3.9	2.62	16.46	0	1	4	4
Mazda_RX4_Wag	21	6	160	110	3.9	2.875	17.02	0	1	4	4
Datsun_710	22.8	4	108	93	3.85	2.32	18.61	1	1	4	1
Hornet_4_Drive	21.4	6	258	110	3.08	3.215	19.44	1	0	3	1
Hornet_Sportabout	18.7	8	360	175	3.15	3.44	17.02	0	0	3	2
Valiant	18.1	6	225	105	2.76	3.46	20.22	1	0	3	1

mpg	Miles/(US) gallon
cyl	Number of cylinders
disp	Displacement (cu.in.)
hp	Gross horsepower
drat	Rear axle ratio
wt	Weight (lb/1000)
qsec	1/4 mile time
vs	V/S
am	Transmission (0 = automatic, 1 = manual)
gear	Number of forward gears
carb	Number of carburetors

```
################ PCA ################
## vary by orders of magnitude, so scaling is appropriate
pca1 <- princomp(mtcars) # inappropriate

# use the correlation matrix NOT the covariance matrix
# =^= prcomp(ibis.pre, scale=TRUE)
pca2 <- princomp(mtcars, cor = TRUE)
```

R code: PCA

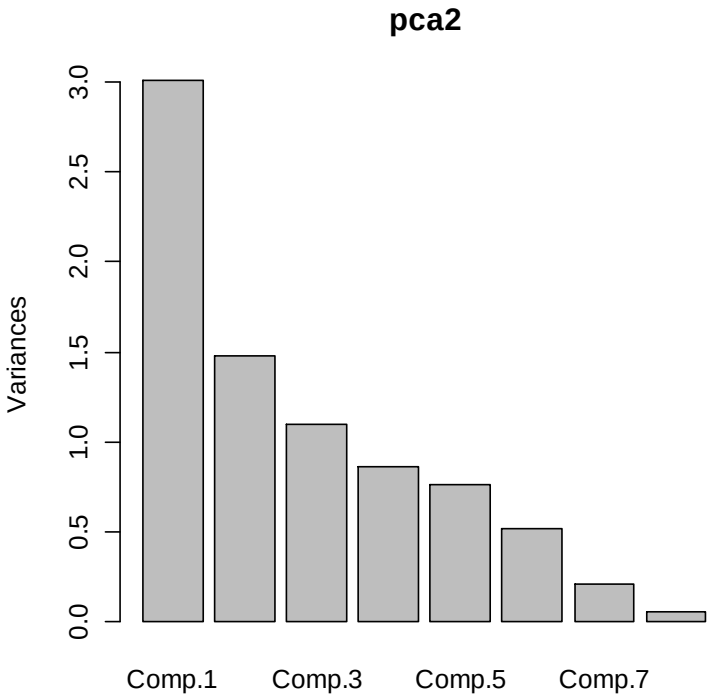
plot(pca2) ***# shows a scree plot***

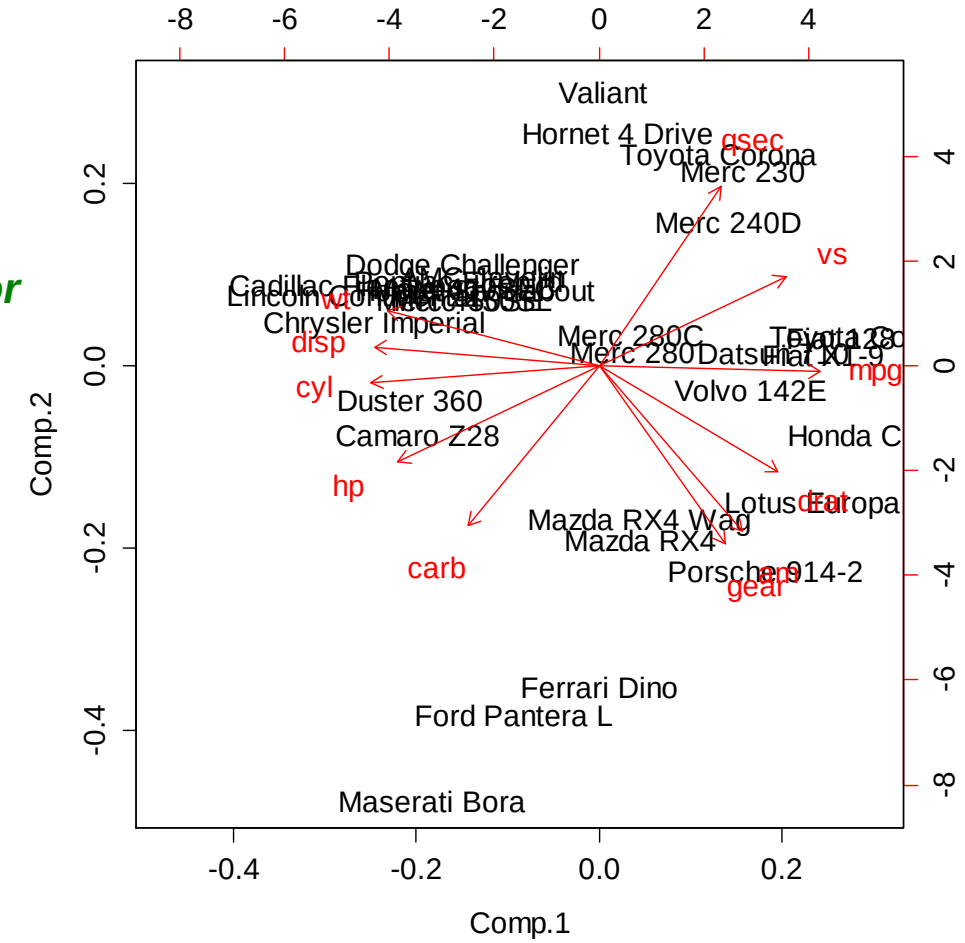
biplot(pca2)

summary(pca2)

pca2$loadings

pca2$scores ***# principal component vector***





R code: PCA

pca2$loadings # in R princomp(), the loadings are coefficients (eigenvectors)

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5	Comp.6	Comp.7	Comp.8	Comp.9	Comp.10	Comp.11
mpg	0.363		-0.226		-0.103	0.109	0.368	0.754	0.236	0.139	0.125
cyl	-0.374		-0.175			-0.169		0.231		-0.846	0.141
disp	-0.368			0.257	-0.394	0.336	0.214		0.198		-0.661
hp	-0.33	-0.249	0.14		-0.54			0.222	-0.576	0.248	0.256
drat	0.294	-0.275	0.161	0.855		-0.244				-0.101	
wt	-0.346	0.143	0.342	0.246		0.465			0.359		0.567
qsec	0.2	0.463	0.403		0.165	0.33		0.232	-0.528	-0.271	-0.181
vs	0.307	0.232	0.429	-0.215	-0.6	-0.194	-0.266		0.359	-0.159	
am	0.235	-0.429	-0.206			0.571	-0.587			-0.178	
gear	0.207	-0.462	0.29	-0.265		0.244	0.605	-0.336		-0.214	
carb	-0.214	-0.414	0.529	-0.127	0.361	-0.184	-0.175	0.396	0.171		-0.32

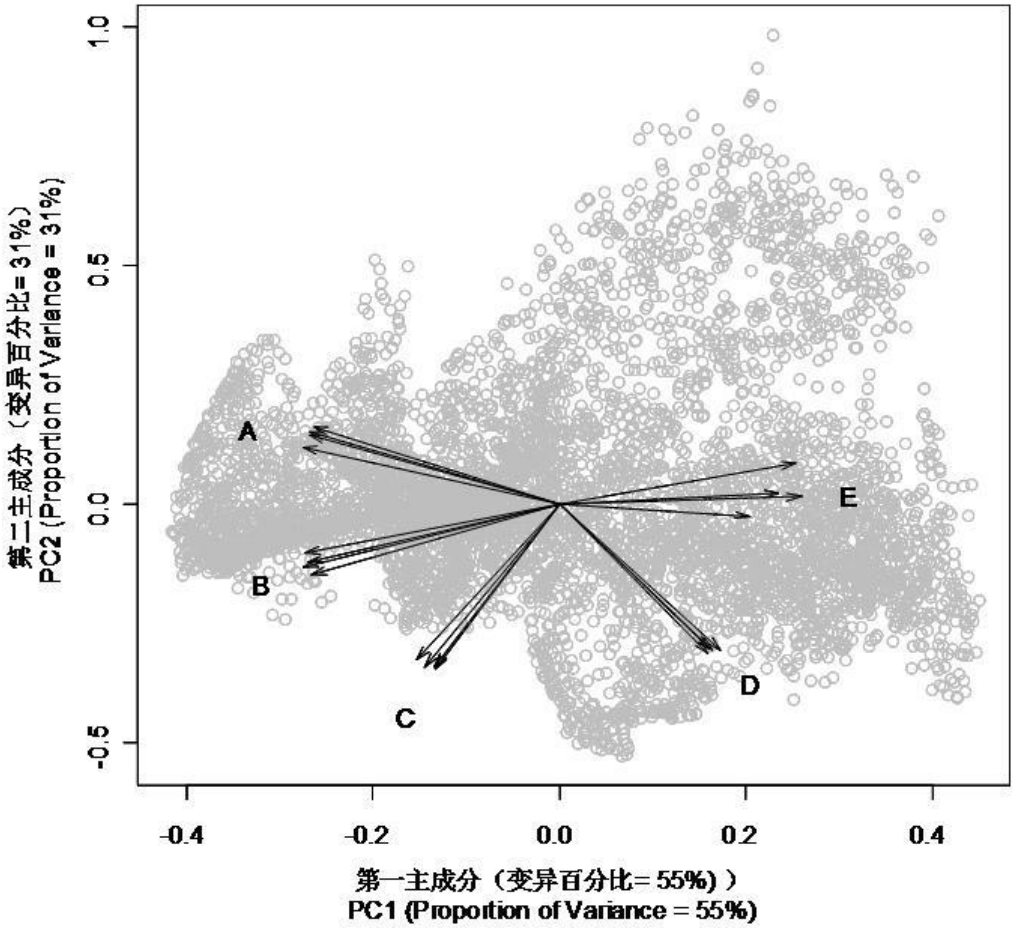
eigen(var(scale(mtcars))) [[2]] # coefficients, eigenvectors

R code: PCA

pca2$scores

	Comp.1	Comp.2	Comp.3	Comp.4	Comp.5
Mazda RX4	0.657213	-1.73545	-0.6012	0.115522	0.960653
Mazda RX4 Wag	0.629396	-1.55003	-0.38232	0.202307	1.032949
Datsun 710	2.779397	0.146457	-0.24124	-0.24914	-0.40514
Hornet 4 Drive	0.311771	2.363019	-0.13576	-0.51186	-0.558
Hornet Sportabout	-1.97449	0.754402	-1.1344	0.075653	-0.21084
Valiant	0.056138	2.786	0.163826	-0.99077	-0.21505
Duster 360	-3.00267	-0.33489	-0.36276	-0.05235	-0.34935
Merc 240D	2.055329	1.465181	0.943895	-0.1444	0.321718
Merc 230	2.287408	1.983527	1.797241	0.291807	0.339022
Merc 280	0.526381	0.162013	1.49277	0.067324	0.070738
Merc 280C	0.509205	0.323895	1.683585	0.095867	0.151185
Merc 450SE	-2.24781	0.683474	-0.37538	-0.13187	0.384669
Merc 450SL	-2.04782	0.683221	-0.48446	-0.21437	0.361302
Merc 450SLC	-2.14854	0.80174	-0.29511	-0.17814	0.439055
Cadillac Fleetwood	-3.89979	0.827948	0.647291	0.295154	0.049017
Lincoln Continental	-3.95412	0.733382	0.72061	0.411823	-0.00396
Chrysler Imperial	-3.59297	0.421135	0.548891	0.676317	-0.21136
Fiat 128	3.856284	0.296752	-0.42283	0.056074	-0.2235
Honda Civic	4.254033	-0.68841	-0.20684	1.186208	-0.09924
Toyota Corolla	4.234221	0.279288	-0.46626	0.186246	-0.22571

Example: study on climate change consequences to the crested ibis

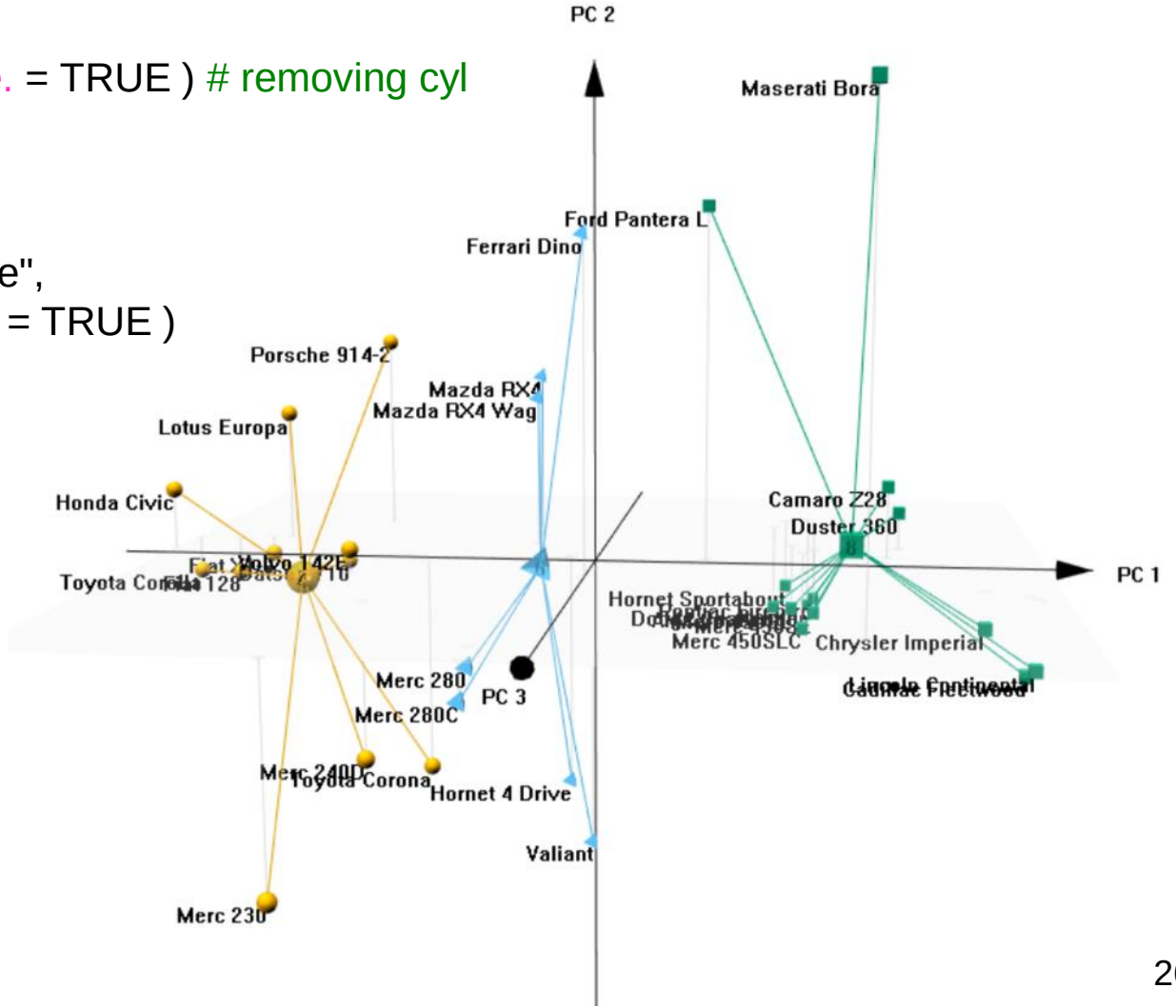


The loadings of 20 variables (five climate variables, i.e. annual total precipitation (A), annual minimum temperature (B), annual maximum temperature (C), seasonal variance of temperature (D), and seasonal variance of precipitation (E), at four time periods, i.e. present, 2020, 2050, and 2080 at the first and second principal components space. The grey circles are the scores of 5751 sites in Yang county at the first and second principal components space. (Zhai & Li 2012)

3D plot

```
library(pca3d)

data(mtcars)
pca <- prcomp( mtcars[,-2], scale. = TRUE ) # removing cyl
# using cyl as the three groups
pca3d( pca, group = mtcars[,2] )
pca3d( pca, group = mtcars[,2],
          fancy = TRUE, bg = "white",
          axes.color = "black", new = TRUE )
```



PCA: potential problems

- Lack of independence between variables
  - **No problem**
- Lack of normality
  - Normality desirable but not essential
- Not monotonous between any two variables
  - **Problem** (use correspondence analysis)
- Many zeroes in data matrix
  - **Problem** (use correspondence analysis)

Note

- The principal components are dependent on the units used to measure the original variables as well as on the range of values they assume.

- We **usually** standardize the data prior to using PCA.

Hourly records of sperm whale behaviour

- Variables:
  - Mean cluster size
  - Max. cluster size
  - Mean speed
  - Heading consistency
  - Fluke-up rate
  - Breach rate
  - Lobtail rate
  - Spyhop rate
  - Sidefluke rate
  - Coda rate
  - Creak rate
  - High click rate
- Data collected:
  - Off Galapagos Islands
  - 1985 and 1987
- Units:
  - hours spent following sperm whales
  - 440 hours

Whitehead, Hal and Weilgart, Linda. 1991. Patterns of Visually Observable Behaviour and Vocalizations in Groups of Female Sperm Whales. Behaviour 118 (3): 275-296

Principal Components

	Principal Components:			
	1	2	3	4
% of variance accounted for	31.09	13.41	12.08	10.52
Loadings:				
Mean cluster size	0.82	0.35	0.01	-0.14
Max. cluster size	0.83	0.24	0.17	-0.12
Mean speed	-0.38	0.30	0.44	-0.09
Heading consistency	-0.48	0.39	0.19	-0.04
Fluke-up rate	-0.65	-0.19	0.30	0.25
Breach rate	0.24	0.24	-0.13	0.74
Lobtail rate	0.29	0.30	-0.09	0.71
Spyhop rate	0.46	-0.60	-0.23	0.01
Sidefluke rate	0.49	-0.57	-0.20	0.07
Coda rate	0.68	-0.08	0.53	0.03
Creak rate	0.57	-0.11	0.70	0.02
High click rate	-0.41	-0.55	0.47	0.31

Whitehead, Hal and Weilgart, Linda. 1991. Patterns of Visually Observable Behaviour and Vocalizations in Groups of Female Sperm Whales. Behaviour 118 (3): 275-296

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High click rate	-0.41	-0.55	0.47	0.31
Principal Components meanings	"Socializing/ foraging"	"Directed movement"	"Vocal"	"Aerial"

Whitehead, Hal and Weilgart, Linda. 1991. Patterns of Visually Observable Behaviour and Vocalizations in Groups of Female Sperm Whales. Behaviour 118 (3): 275-296

Factor Analysis (FA)

Factor Analysis

- Data reduction tool
- Removes redundancy or duplication from a set of correlated variables
- Represents correlated variables with a smaller set of “derived” variables.
- Factors are formed that are relatively independent of one another.
- Two types of “variables”:
  - latent variables: factors
  - observed variables

Some applications of factor analysis

1. Identification of underlying factors:
   - clusters variables into homogeneous sets
   - creates new variables (i.e. factors)
   - allows us to gain insight to categories
2. Screening of variables:
   - identifies groupings to allow us to select one variable to represent many
   - useful in regression (recall collinearity)
3. Summary:
   - Allows us to describe many variables using a few factors
4. Clustering of objects:
   - Helps us to put objects (people) into categories depending on their factor scores

R code: Factor Analysis

```
# Exploratory Factor Analysis (Maximum Likelihood)
# extracting 3 factors, with varimax rotation
fit <- factanal(scale(mtcars), 3, rotation = "varimax")
print(fit, digits = 2, cutoff = .01, sort = TRUE)
```

Call:
factanal(x = scale(mtcars), factors = 3, rotation = "varimax")

Uniquenesses:

mpg	cyl	disp	hp	drat	wt	qsec	vs	am	gear	carb
0.13	0.06	0.09	0.13	0.29	0.06	0.05	0.22	0.21	0.12	0.16

Loadings:

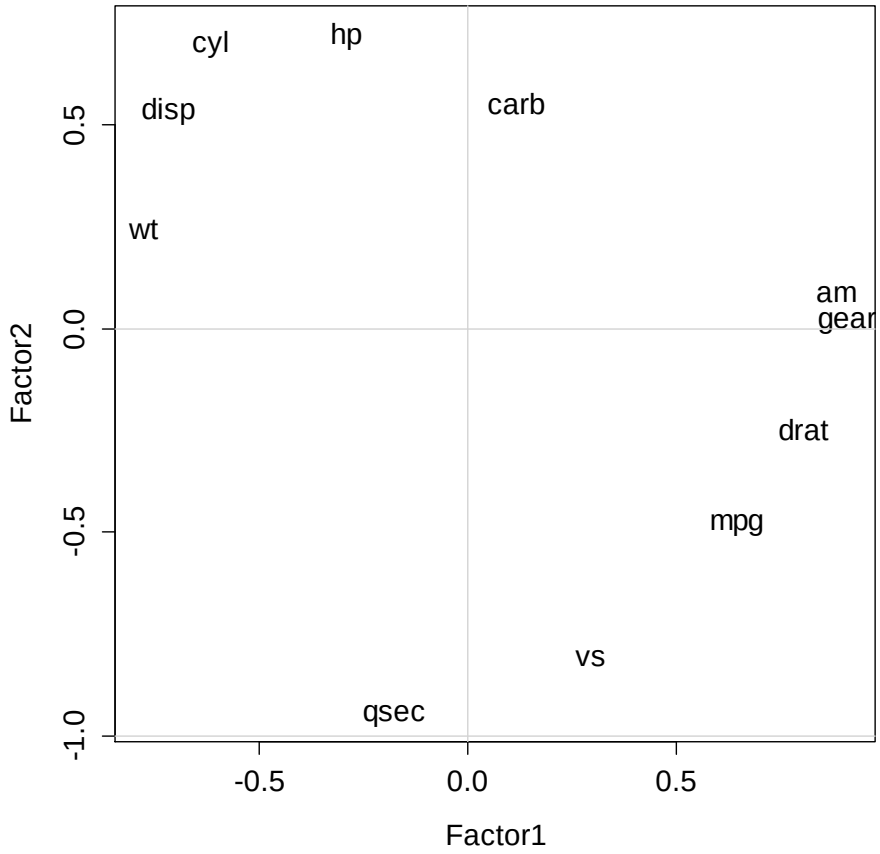
	Factor1	Factor2	Factor3
mpg	0.64	-0.48	-0.47
disp	-0.72	0.54	0.32
drat	0.8	-0.24	-0.07
wt	-0.78	0.25	0.52
am	0.88	0.09	-0.09
gear	0.91	0.02	0.22
cyl	-0.62	0.7	0.26
hp	-0.29	0.72	0.51
qsec	-0.18	-0.95	-0.15
vs	0.3	-0.8	-0.2
carb	0.11	0.56	0.72

	Factor1	Factor2	Factor3
SS loadings	4.38	3.52	1.58
Proportion Var	0.40	0.32	0.14
Cumulative Var	0.40	0.72	0.86

Test of the hypothesis that 3 factors are sufficient. The chi square statistic is 30.53 on 25 degrees of freedom. The p-value is 0.205

R: Result

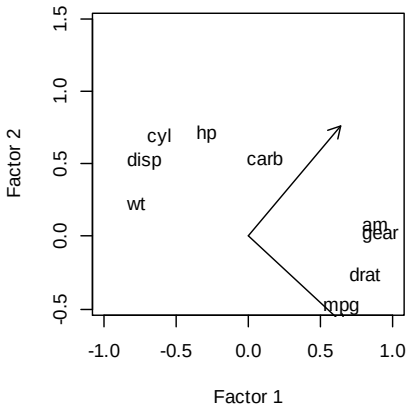
```
# plot factor 1 by factor 2
load <- fit$loadings[, 1:2]
plot(load, type = "n") # set up plot
text(load, labels = names(mtcars), cex = 1) # add variable names
abline(h = -1:1, v = -1:1, col = "lightgray", lty=1)
```

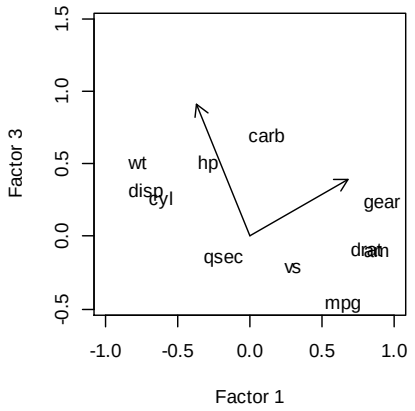


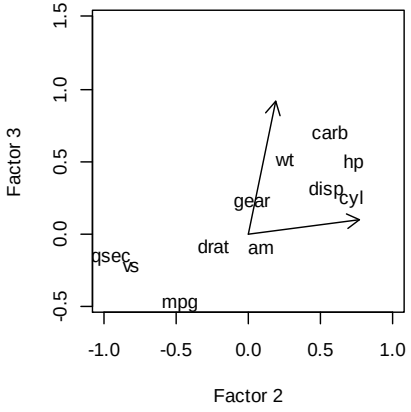
R code: Factor Analysis

```
library(MASS)
COV = cov(mtcars)
FA <- factanal(covmat = COV, factor = 3, rotation = “varimax")
load <- loadings(FA); rot <- FA$rot

#Pairs of factor loadings to plot
ind <- combn(1:3,2)
par(mfrow = c(2,2))
nms <- row.names(load)
#Loop over pairs of factors and draw each plot
for (i in 1:3){
  eqscplot(load[,ind[1,i]], load[,ind[2,i]], xlim = c(-1,1),
        ylim = c(-0.5,1.5), type = "n",
        xlab = paste("Factor", as.character(ind[1,i])),
        ylab = paste("Factor", as.character(ind[2,i])))
  text(load[,ind[1,i]],load[,ind[2,i]], labels = nms)
  arrows(c(0,0), c(0,0), rot[ind[,i], ind[,i]][,1],
           rot[ind[,i], ind[,i]][,2], length = 0.1)}
```

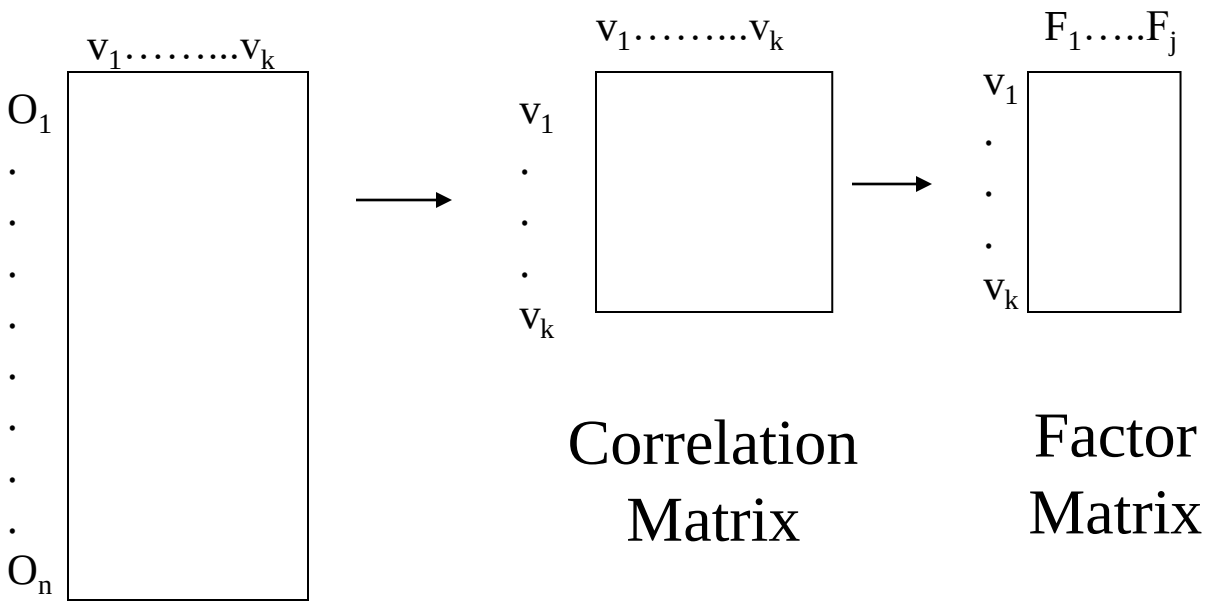






Data Matrix

- Factor analysis is **totally dependent** on correlations between variables.
- Factor analysis summarizes correlation structure



Choosing number of factors

- Intuitively: The number of uncorrelated constructs that are jointly measured by the X's.
- Only useful if number of factors is less than number of X's (recall "data reduction").

Use "principal components" to help decide

- number of factors is equivalent to number of variables
- each factor is a weighted combination of the input variables:

$$F_1 = a_{11}X_1 + a_{12}X_2 + \ldots.$$

Eigenvalues

- To select how many factors to use, consider *eigenvalues* from a principal components analysis
- Two interpretations:
  - eigenvalue ≅ equivalent number of variables which the factor represents
  - eigenvalue ≅ amount of variance in the data described by the factor.
- Rules to go by:
  - number of eigenvalues > 1
  - scree plot
  - % variance explained
  - comprehensibility
- Note: sum of eigenvalues is equal to the number of items

Steps in Factor Analysis

- Factor analysis usually proceeds in four steps:
  - 1: the correlation matrix for all variables is computed
  - 2: Factor extraction
  - 3: Factor rotation
  - 4: Make final decisions about the number of underlying factors

The Correlation Matrix

- **1: the correlation matrix**
  - Generate a correlation matrix for all variables
  - Identify variables not related to other variables
  - If the correlation between variables are small, it is unlikely that they share common factors (variables must be related to each other for the factor model to be appropriate).
  - Correlation coefficients greater than 0.3 in absolute value are indicative of acceptable correlations.
  - Examine visually the appropriateness of the factor model.

Factor Extraction

- **2nd Step: Factor extraction**
  - The primary objective of this stage is to determine the factors.
  - Initial decisions can be made here about the number of factors underlying a set of measured variables.
  - Estimates of initial factors are obtained using **Principal components analysis**.
  - The principal components analysis is the most commonly used extraction method . Other factor extraction methods include:
    - Maximum likelihood method
    - Principal axis factoring
    - Alpha method
    - Unweighted lease squares method
    - Generalized least square method
    - Image factoring.

Factor Extraction

- In principal components analysis, **linear combinations** of the observed variables are formed.
- The 1st principal component is the combination that accounts for the **largest amount of variance** in the sample (1st extracted factor).
- The 2nd principle component accounts for the next largest amount of variance and **is uncorrelated with the first** (2nd extracted factor).
- Successive components explain progressively smaller portions of the total sample variance, and all are uncorrelated with each other.

Factor Extraction

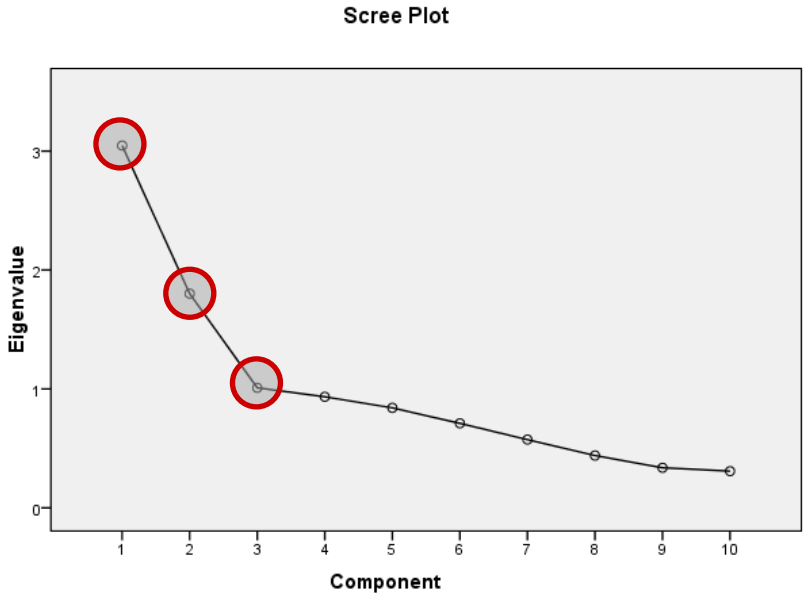
- To decide on how many factors we need to represent the data, we use 2 statistical criteria:
  - **Eigen Values,** and
  - The **Scree Plot**.

- The determination of the number of factors is usually done by considering only factors with Eigen values greater than 1.

- Factors with a variance less than 1 are no better than a single variable, since each variable is expected to have a variance of 1.

Factor Extraction

- The examination of the **Scree plot** provides a visual of the total variance associated with each factor.
- The steep slope shows the large factors.
- The gradual trailing off (scree) shows the rest of the factors usually lower than an Eigen value of 1.
- In choosing the number of factors, in addition to the statistical criteria, one should make initial decisions based on conceptual and theoretical grounds.
- At this stage, the decision about the number of factors is not final.



Factor Rotation

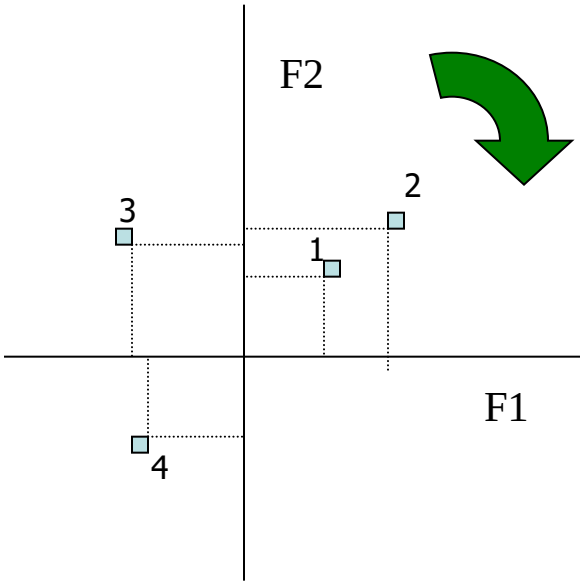
- **3rd Step: Factor rotation.**
- In this step, factors are rotated.

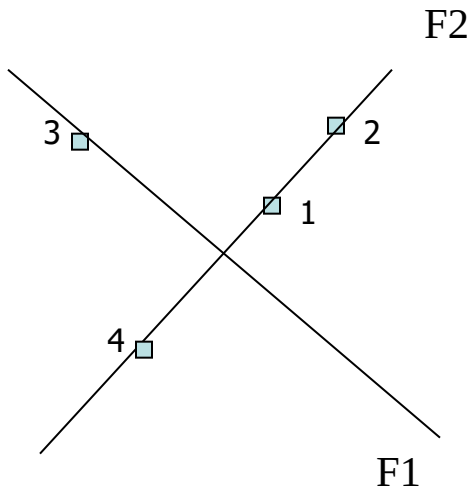
- Un-rotated factors are typically not very interpretable (most factors are correlated with may variables).

- Factors are rotated to make them more meaningful and easier to interpret (each variable is associated with a minimal number of factors).

- Different rotation methods may result in the identification of somewhat different factors.

Factor Rotation





	Factor 1	Factor 2
x1	0.5	0.5
x2	0.8	0.8
x3	-0.7	0.7
x4	-0.5	-0.5

	Factor 1	Factor 2
x1	0	0.6
x2	0	0.9
x3	-0.9	0
x4	0	-0.9

Factor Rotation

- Quartimax
  - Simplify rows – variable loads high on one factor, low on others
- Varimax
  - Simplify columns – clearer separation of factors – each factor has variables that either load high or load very low
- Equimax
  - Compromise between the two – rarely used

- The most popular rotational method is **Varimax rotations.**
- Varimax use orthogonal rotations yielding uncorrelated factors/components.
- Varimax attempts to minimize the number of variables that have high loadings on a factor. This enhances the interpretability of the factors.

Making Final Decisions

- 4th Step: Making final decisions
  - The final decision about the number of factors to choose is the number of factors for the rotated solution that is **most interpretable**.
  - To identify factors, group variables that have large loadings for the same factor.
  - Plots of loadings provide a visual for variable clusters.
  - Interpret factors according to the meaning of the variables

- This decision should be guided by:
  - A priori conceptual beliefs about the number of factors from past research or theory
  - Eigen values computed in step 2.
  - The relative interpretability of rotated solutions computed in step 3.

Assumptions

- Assumption underlying factor analysis include:
  - The measured variables are linearly related to the factors + errors.
  - The data should have a bivariate normal distribution for each pair of variables.
  - Observations are independent.
  - The factor analysis model assumes that variables are determined by common factors and unique factors. All unique factors are assumed to be **uncorrelated** with each other.

Factor Analysis (FA) vs. PCA

- PCA analyzes variance; FA analyzes covariance.
- PCA is to extract as much variance with the least amount of factors.
- FA is to explain as much of the correlations with a minimum number of factors.
- PCA gives a unique solution. If all components are retained, all variance is explained.
- FA can give multiple solutions depending on the method and the estimates of communality.

Factor Analysis vs. Cluster Analysis

- Both are data reduction techniques.
- Factor Analysis is to reduce original set of variables to smaller set of factors.
- Cluster Analysis is to form groups from the observations or records, thus reducing original number of elements to fewer groups.
- Factor Analysis can be seen as a clustering technique than is focused on the columns of data frame, rather than the rows.

Correspondence Analysis (CA)

Correspondence Analysis

- Also called Reciprocal Averaging (Hill 1973)
- Weighted averaging of site scores to yield species scores and vice versa
- Simultaneous ordination of both rows and columns of a matrix
- Used to examine relationship of species assemblages to site characteristics
- Sites typically span an environmental gradient

Using Chi-Square approach to measure correspondence between rows and columns

Observed					
	Sp1	Sp2	Sp3	Sp4	Plot total
Plot1	**6**	12	18	24	**60**
Plot2	5	10	15	20	50
Plot3	4	8	12	16	40
Plot4	3	6	9	12	30
Plot5	2	4	6	8	20
Species total	**20**	40	60	80	**200**
Expected					
	Sp1	Sp2	Sp3	Sp4	
Plot1	**6**	12	18	24	
Plot2	5	10	15	20	
Plot3	4	8	12	16	
Plot4	3	6	9	12	
Plot5	2	4	6	8	
Chi Square					
	Sp1	Sp2	Sp3	Sp4	
Plot1	**0**	0	0	0	
Plot2	0	0	0	0	
Plot3	0	0	0	0	
Plot4	0	0	0	0	
Plot5	0	0	0	0	

6/60 = 20/200

= 20x60 / 200

= $(Exp-Obs)^2$ / Exp

Inertia = Chi Square / Grand Sum
= 0 / 200 = 0

In this dataset, rows and columns are not independent. Thus, the contents of each cell are predictable based on row total, column totals, and the grand total.

As rows and column deviate (more independent), Chi Square values (and inertia) grows

Observed					
	Sp1	Sp2	Sp3	Sp4	Plot total
Plot1	**6**	12	18	24	**60**
Plot2	5	10	15	20	50
Plot3	4	8	12	16	40
Plot4	3	6	9	12	30
Plot5	2	4	6	8	20
Species total	**20**	40	60	80	**200**
Expected					
	Sp1	Sp2	Sp3	Sp4	
Plot1	**6**	12	18	24	
Plot2	5	10	15	20	
Plot3	4	8	12	16	
Plot4	3	6	9	12	
Plot5	2	4	6	8	
Chi Square					
	Sp1	Sp2	Sp3	Sp4	
Plot1	**0**	0	0	0	
Plot2	0	0	0	0	
Plot3	0	0	0	0	
Plot4	0	0	0	0	
Plot5	0	0	0	0	

6/60 = 20/200

= 20x60 / 200

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In this dataset, rows and columns are not independent. Thus, the contents of each cell are predictable based on row total, column totals, and the grand total.

As rows and column deviate (more independent), Chi Square values (and inertia) grows

Observed					
	Sp1	Sp2	Sp3	Sp4	Plot total
Plot1	**6**	8	12	15	**41**
Plot2	5	2	20	7	34
Plot3	4	8	11	3	26
Plot4	3	6	8	5	22
Plot5	2	5	1	8	16
Species total	**20**	29	52	38	**139**
Expected					
	Sp1	Sp2	Sp3	Sp4	
Plot1	**5.899**	8.554	15.338	11.209	
Plot2	4.892	7.094	12.719	9.295	
Plot3	3.741	5.424	9.727	7.108	
Plot4	3.165	4.590	8.230	6.014	
Plot5	2.302	3.338	5.986	4.374	
Chi Square					
	Sp1	Sp2	Sp3	Sp4	
Plot1	**0.002**	0.036	0.726	1.282	
Plot2	0.002	3.657	4.167	0.567	
Plot3	0.018	1.223	0.167	2.374	
Plot4	0.009	0.433	0.006	0.171	
Plot5	0.040	0.827	4.153	3.006	
Sum					**22.867**

6/41 ~ 20/139

= 20x41 / 139

= $(Exp-Obs)^2$ / Exp

Inertia = Chi Square / Grand Sum
= 22.867 / 139 = 0.165

Total variance the CA will attempt to explain.

The chi square matrix describes all the variability in the dataset not explainable by row or column profiles (totals).

Correspondence Analysis

Chi-Sqr	sp1	sp2	sp3	sp4	Row totals
sam1	0.07877	0.124363	0.0806	0.232143	***0.515876***
sam2	0.501505	0.341336	0.256398	1.193828	***2.293067***
sam3	4.892877	0.300778	1.172794	1.028178	***7.394627***
sam4	3.462503	0.590862	0.791607	0.224873	***5.069845***
sam5	0.557292	0.005016	0.132378	0.473542	***1.168228***
Col totals	***9.492948***	***1.362354***	***2.433777***	***3.152565***	

Chi Sqr	Inertia
16.44164	0.08519

Look at where the variability is in the Chi Sqr matrix…

```
Partitioning of mean squared contingency coefficient:
              Inertia Proportion
Total         0.08519          1
Unconstrained 0.08519          1
…
Importance of components:
                          CA1    CA2      CA3
Eigenvalue             0.0748 0.0100 0.000414
Proportion Explained   0.8776 0.1176 0.004850
Cumulative Proportion 0.8776 0.9951 1.000000
…
Species scores
          CA1       CA2        CA3
sp1 -0.39331 -0.030492 -0.0008905
sp2  0.09946  0.141064  0.0219980
sp3  0.19632  0.007359 -0.0256591
sp4  0.29378 -0.197766  0.0262108

Site scores (weighted averages of species scores)
         CA1     CA2     CA3
sam1 -0.2405 -1.9357  3.4903
sam2  0.9471 -2.4310 -1.6574
sam3 -1.3920 -0.1065 -0.2535
sam4  0.8520  0.5769  0.1625
sam5 -0.7355  0.7884 -0.3974
```

CA does an eigenvalue decomposition to summarize this variability in fewer axes (components).

Species and sites that contribute most to the inertia have the largest magnitude CA1 scores.

Scores are centered and scaled to be directly comparable.

Correspondence Analysis

- Output
  - Row and column sums, total Chi Square
  - Species and sample scores that can be plotted in the same space. Interpretation is similar to sample scores and species weighted averages in NMDS.
  - # axes = n-1 for whichever dimension of the data matrix is lower (samples or species).
  - Eigenvalues – relative importance of each axis, interpreted as the percentage of total **inertia** explained.

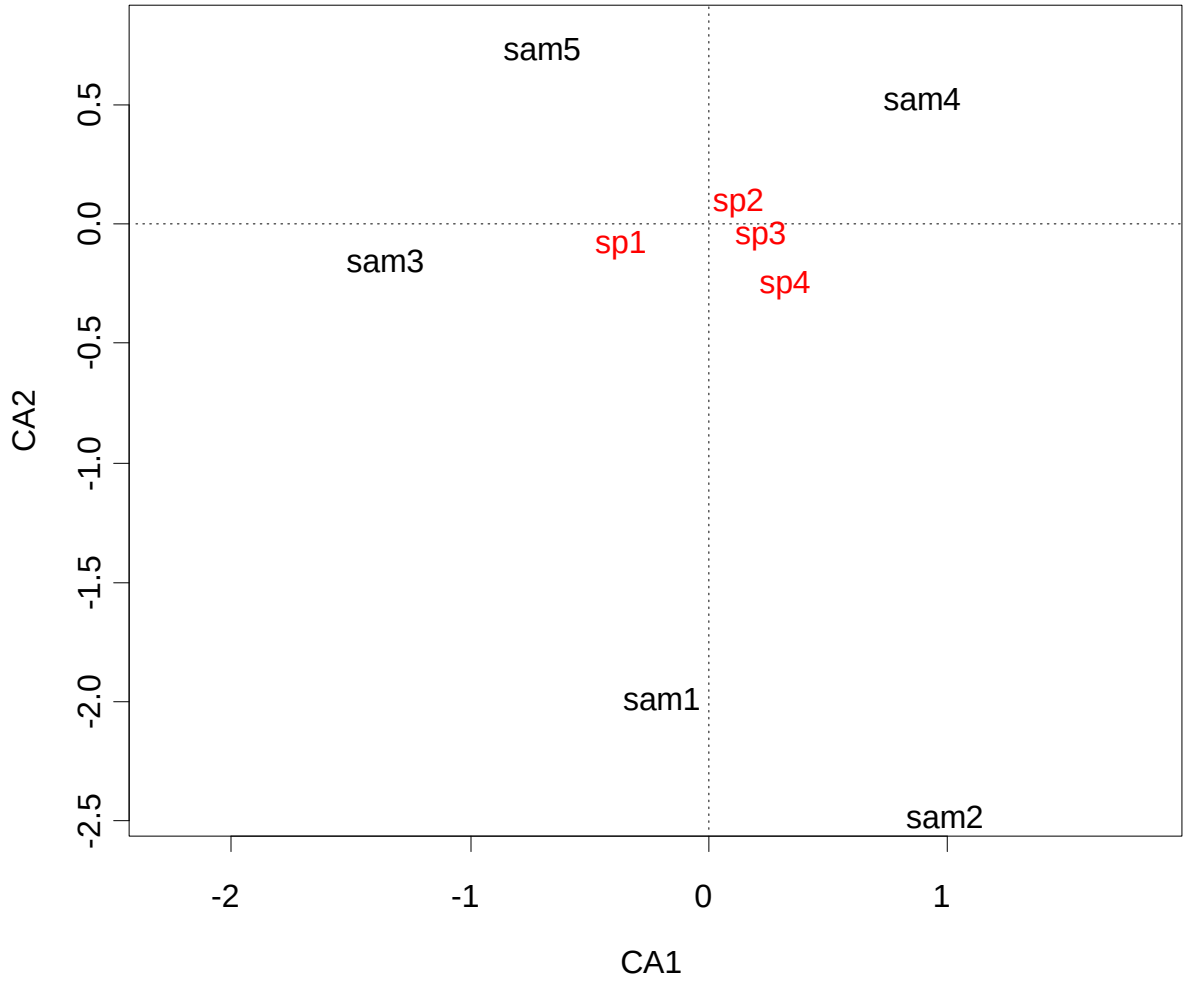
```
Partitioning of mean squared contingency coefficient:
              Inertia Proportion
Total           1.780          1
Unconstrained   1.780          1

Eigenvalues, and their contribution to the mean squared contingency coefficient

Importance of components:
                          CA1   CA2   CA3    CA4    CA5     CA6     CA7     CA8     CA9
Eigenvalue              0.850 0.530 0.252 0.0953 0.0303 0.01097 0.00638 0.00307 0.00179
Proportion Explained    0.478 0.298 0.142 0.0536 0.0170 0.00616 0.00358 0.00173 0.00101
Cumulative Proportion 0.478 0.775 0.917 0.9705 0.9875 0.99368 0.99727 0.99899 1.00000
```

0.85/1.780=0.478

Correspondence Analysis



Distances between species are two-dimensional approximations of their Chi-square distances. Distances between samples are also two-dimensional approximations of Chi-square distances. Distances between species and sites cannot be interpreted.

How does CA work?

- Site-species matrix
- Eigen analysis

  similar to PCA but differs in some details

  axes rotated through species and sample space with the goal of maximizing their correspondence
- Reciprocal averaging

  calculate species scores as weighted averages of the sites in which they occur

  calculate new site scores by weighted averaging of the species scores

Output of CA

- Yields principal axes and scores
  - scores for rows (sites) and columns (species)
  - 1st axis has the largest eigenvalue (and accounts for largest variance); maximizes association between rows and columns
  - subsequent axes account for residual variation and have smaller eigenvalues
  - rarely use more than 2-3 axes in CA

R code: Correspondence analysis

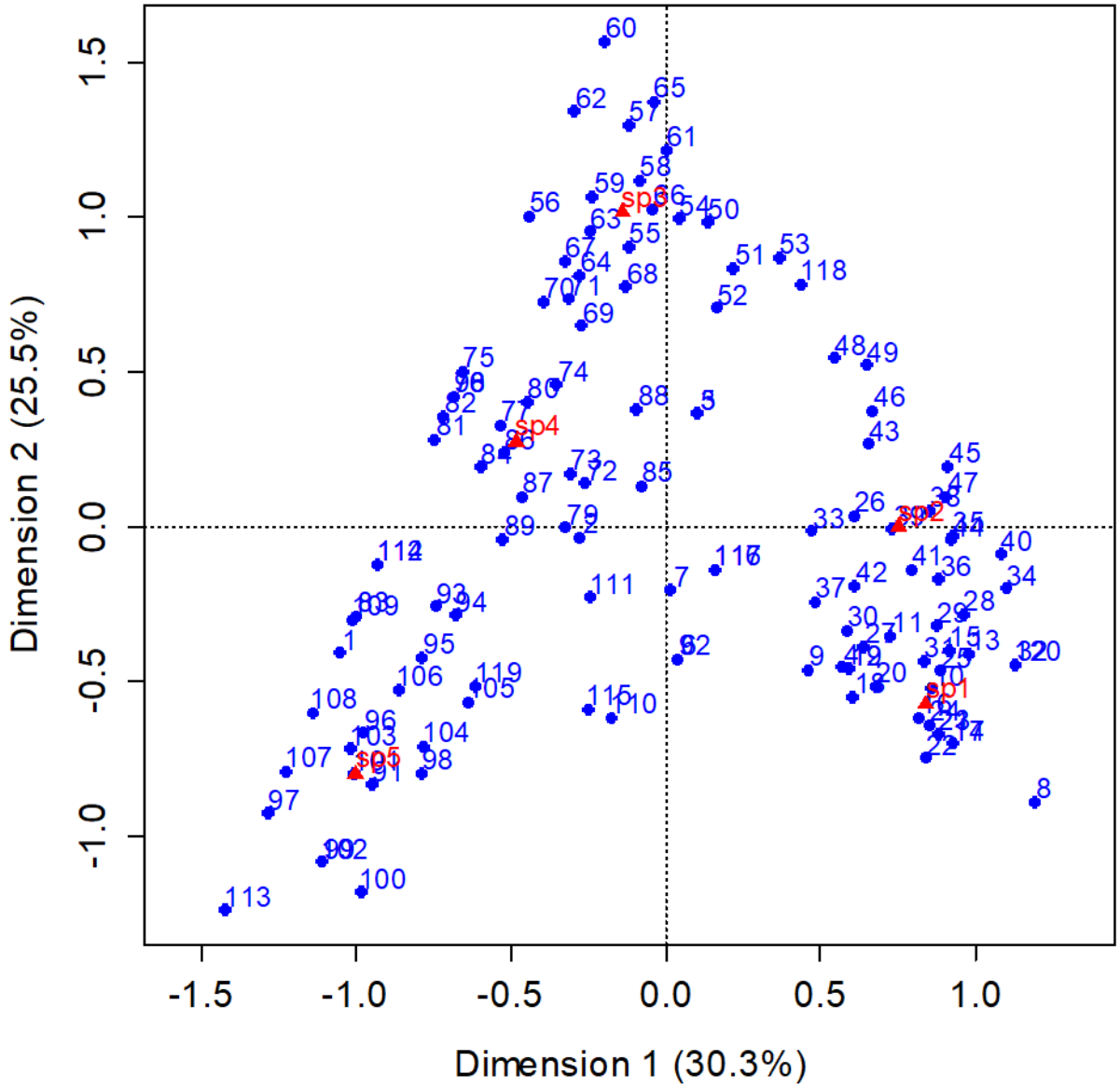
```
library(ca) # Package for Correspondence analysis
data(author); ca(author); plot(ca(author)) # One example

# Generate 5 species density data at 120 sites
sp1 = round(rnorm(120, 20, 7)); sp1 = abs(sp1)
sp2 = round(rnorm(120, 40, 7))
sp3 = round(rnorm(120, 60, 7))
sp4 = round(rnorm(120, 80, 7))
sp5 = round(rnorm(120, 100,7))
species = data.frame(sp1, sp2, sp3, sp4, sp5); species = species * 0
sp.1 = table(sp1)
sp.2 = table(sp2)
sp.3 = table(sp3)
sp.4 = table(sp4)
sp.5 = table(sp5); sp.5 = sp.5[1:(nrow(sp.5)-2)]
species$sp1[c(as.numeric(names(sp.1)))] = sp.1
species$sp2[c(as.numeric(names(sp.2)))] = sp.2
species$sp3[c(as.numeric(names(sp.3)))] = sp.3
species$sp4[c(as.numeric(names(sp.4)))] = sp.4
species$sp5[c(as.numeric(names(sp.5)))] = sp.5

#Generate a noise
random = matrix(sample(c(0,1),600, rep=T), nrow=120, ncol=5)
species = species + random
rownames(species) = c(1:120) #define row names
ca(species) #Correspondence analysis
plot(ca(species))
```

	sp1	sp2	sp3	sp4	sp5
1	0	0	0	1	1
2	1	0	1	1	1
3	1	0	1	1	0
4	2	0	0	1	0
5	1	0	1	1	0
6	1	1	0	1	1
7	2	0	1	1	1
8	2	0	0	0	0
9	5	0	1	1	1
10	4	1	0	1	0
11	5	0	1	1	0
12	6	1	1	1	1
13	5	1	1	0	0
14	6	0	0	1	0
15	4	0	1	0	0
16	8	1	1	0	1
17	6	0	0	1	0
18	7	0	1	1	1
19	6	1	1	1	1
20	5	1	1	0	1
21	5	0	0	1	0
22	10	1	0	1	1
23	5	0	0	1	0
24	9	1	1	0	1
25	8	1	1	1	0
26	2	2	1	1	0
27	3	4	0	1	1
28	4	2	1	0	0
29	3	3	0	1	0
30	3	2	1	0	1
31	3	5	0	0	1
32	4	4	0	0	0
33	1	5	1	1	1
34	2	7	0	0	0
35	2	4	1	0	0
36	2	5	0	1	0
37	1	4	0	1	1
38	0	7	0	1	0
39	1	12	1	1	1
40	1	9	0	0	0
41	0	8	0	0	1
42	1	6	0	1	1
43	1	6	2	1	0
44	1	9	0	1	0
45	0	7	1	0	0
46	1	3	2	0	0
47	1	5	1	0	0
48	1	3	3	0	0
49	0	2	1	0	0
50	0	3	6	1	0

Five species at 120 sites



Correspondence Analysis

- First axis always most informative
- Number of axes produced is set by the dimensionality of the data, not a user option
- Not distance based, data transformations typically more important
- Ordinates both samples and species directly

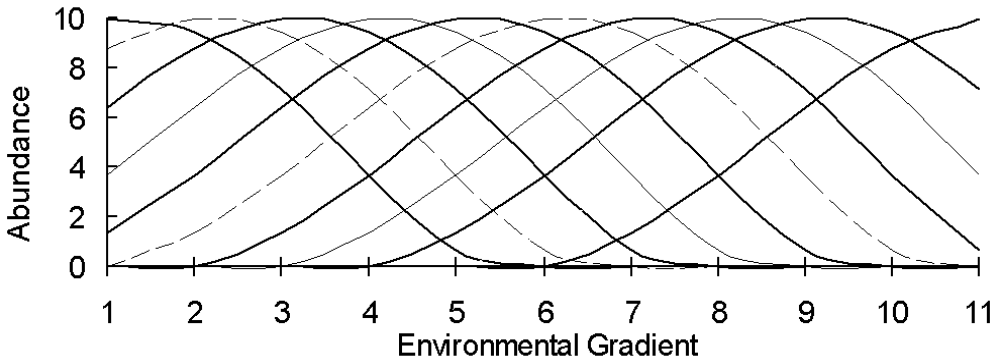
CA vs. PCA

- Both are eigenvector methods
- PCA uses Euclidean distance, while CA uses Chi-square distance
- Underlying assumption – species abundance distributions are Gaussian (normal and unimodal)
- CA orders the points correctly on the first axis
- Curvature and “tucking in” of the ends of the gradient in PCA results in failure to order points correctly (horseshoe effect)

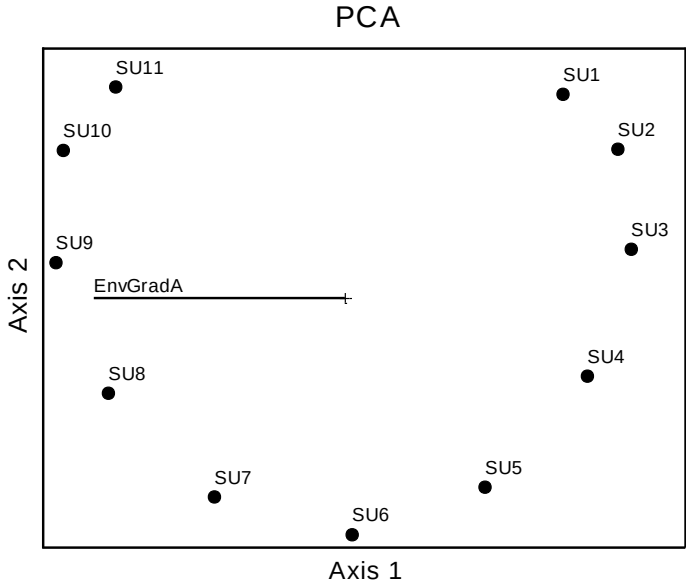
Advantage of CA

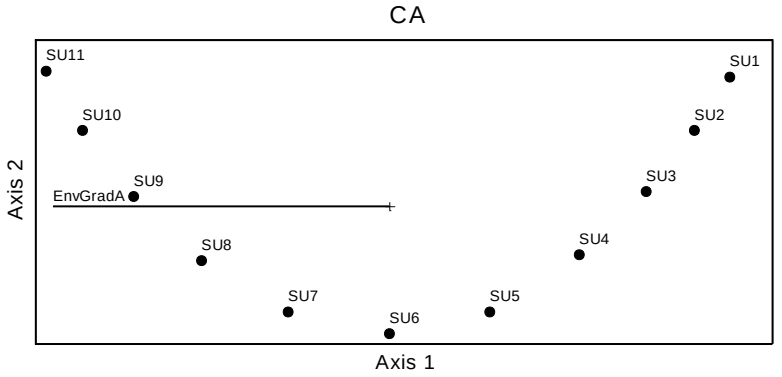
- Weaknesses of PCA:
  - Assumes species are linearly related with each other and/or gradients
  - **Samples are ordinated in species space**
  - Results in “horseshoe effect” where ends of ordination axes are distorted
- Correspondence analysis allows for non-linear unimodal relationships
  - Both samples and species handled similarly, axes do not explicitly represent species-space

Represent environmental gradient



A synthetic data set of eleven species with noiseless hump-shaped responses to an environmental gradient. The gradient was sampled at eleven points (sample units), numbered 1-11.

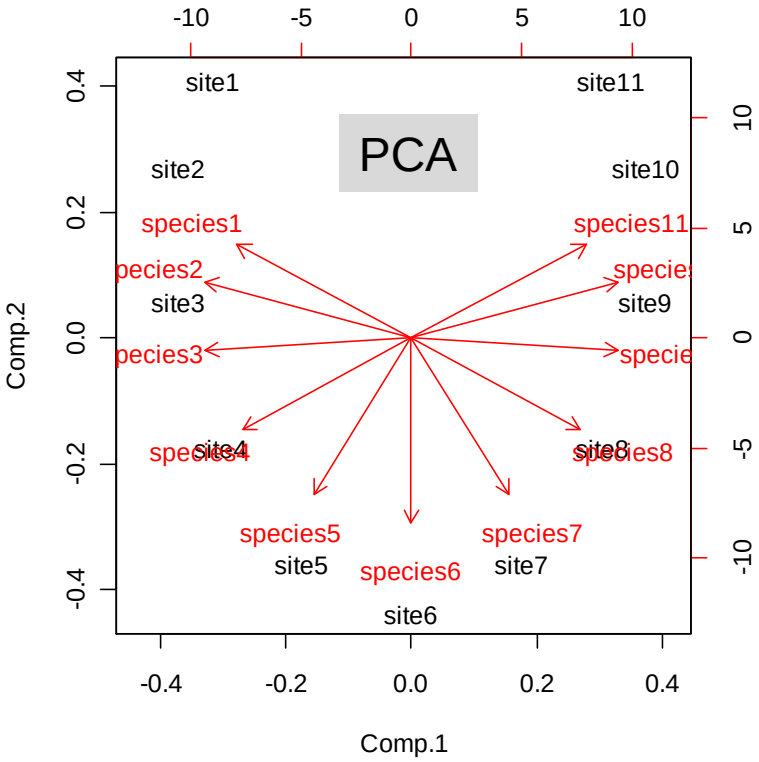


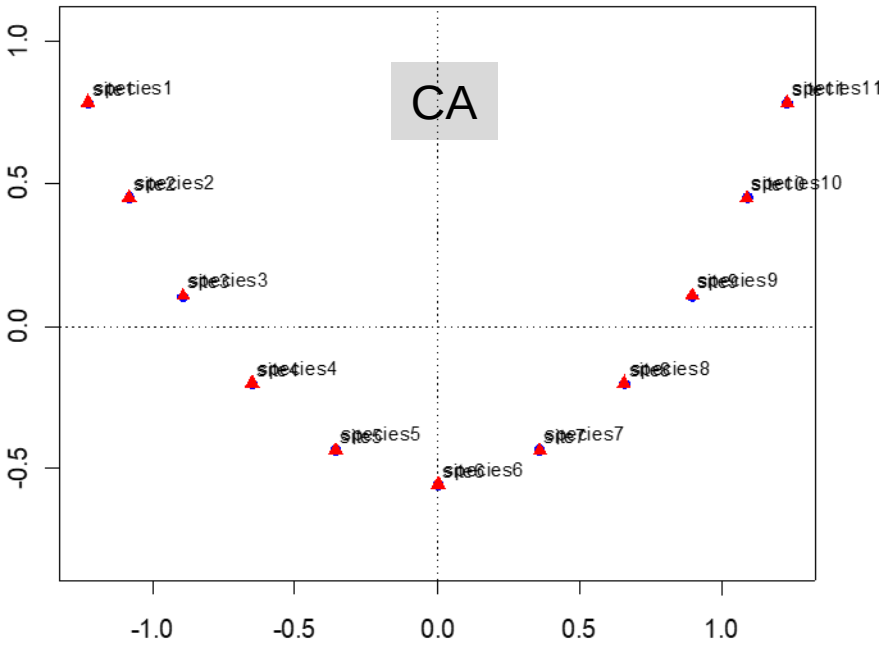


Comparison of PCA and CA of the data set shown in Figure 19.1. PCA curves the ends of the gradient in, while CA does not. The vectors indicate the correlations of the environmental gradient with the axis scores.

From: McCune, B. & J. B. Grace. 2002. *Analysis of Ecological Communities*. MjM Software Design, Gleneden Beach, Oregon http://www.pcord.com

Horseshoe effect






```
# horseshoe effect
species <- read.csv('D:/PCA species environment gradient.csv', header = T) # see following table for data
rownames(species) <- species$site
species <- species[,-1] #remove the first column (row names)
pca <- princomp(species)
biplot(pca)

library(ca) # Package for CA
ca(species) #Correspondence analysis
plot(ca(species))
```

site	species1	species2	species3	species4	species5	species6	species7	species8	species9	species10	species11
site1	10	8	6	4	2	0	0	0	0	0	0
site2	8	10	8	6	4	2	0	0	0	0	0
site3	6	8	10	8	6	4	2	0	0	0	0
site4	4	6	8	10	8	6	4	2	0	0	0
site5	2	4	6	8	10	8	6	4	2	0	0
site6	0	2	4	6	8	10	8	6	4	2	0
site7	0	0	2	4	6	8	10	8	6	4	2
site8	0	0	0	2	4	6	8	10	8	6	4
site9	0	0	0	0	2	4	6	8	10	8	6
site10	0	0	0	0	0	2	4	6	8	10	8
site11	0	0	0	0	0	0	2	4	6	8	10

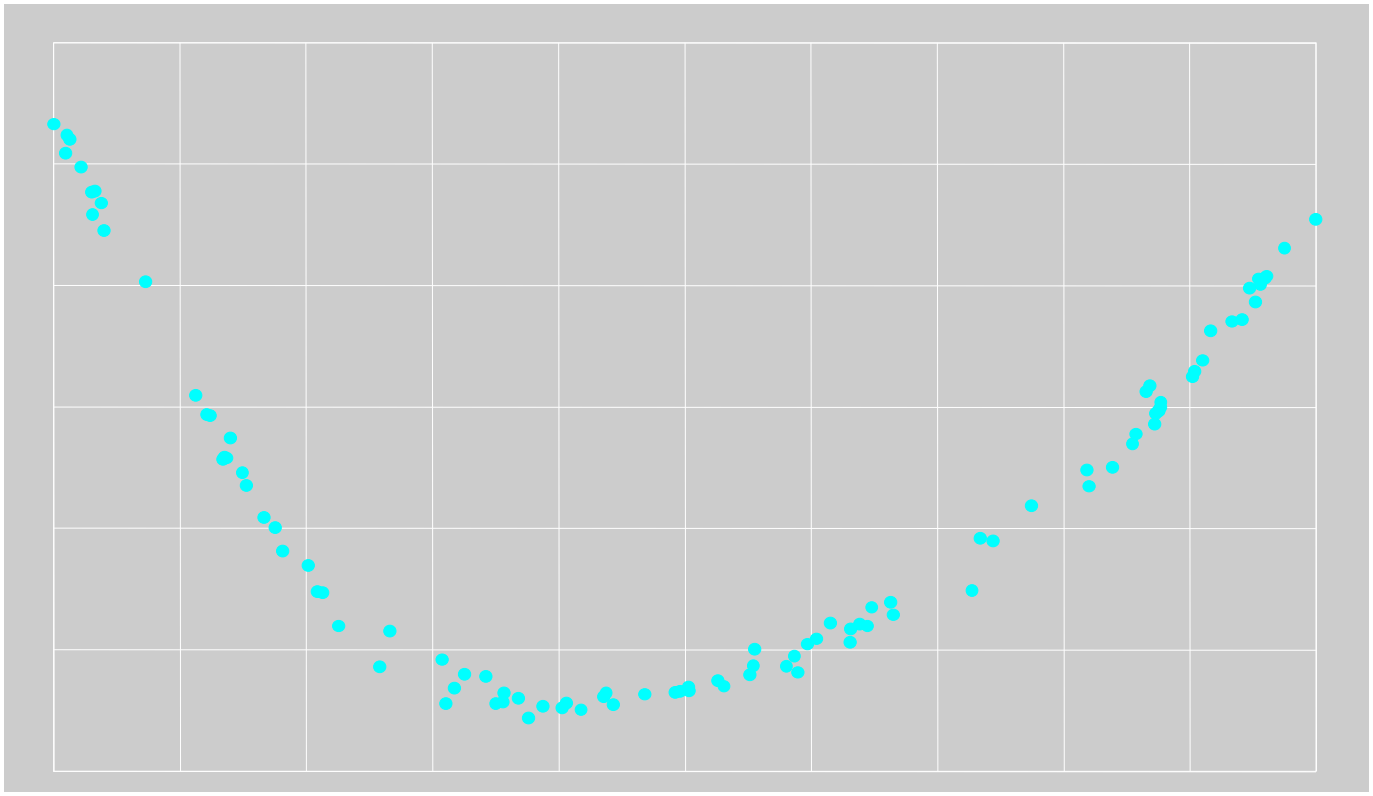
Problems with CA

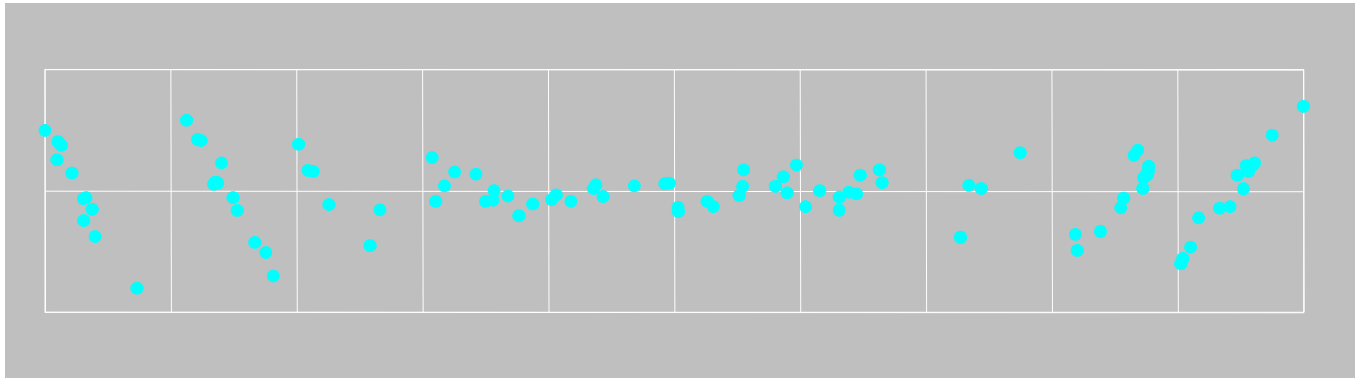
- The 1st CA axis is reliable, but 2nd and later axes are quadratic distortions of the first – produces the "arch effect"
- Distances compressed toward the ends of the axes and stretched in the middle
- Chi-square distance gives high weight to species with low abundance, which exaggerates distinctiveness of samples containing several rare species (Faith et al. 1987, Minchin 1987)

Detrended correspondence analysis (DCA)

- The “arch effect” of CA is unwanted; the ends of the axes in CA are also compressed
- Detrending (detrended correspondence analysis, DCA) deals with the arch by:
  - 5 segment smoothing of 1st axis. Divide into segments (weights of 1,2,3,2,1), center each at 0.
  - Rescaling of axis into “standard deviation” units of species turnover.
- Only first 4 axes are adjusted, the rest are discarded
- Assumptions
  - Same as for CA
  - DCA is not really an analysis. It is a post hoc modification of a CA

Detrended correspondence analysis (DCA)

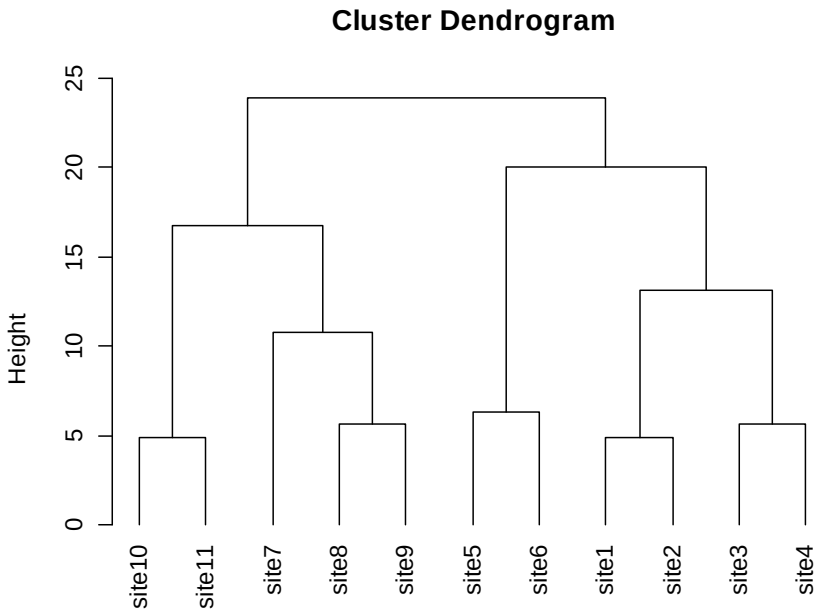




R code: Detrended correspondence analysis (DCA)

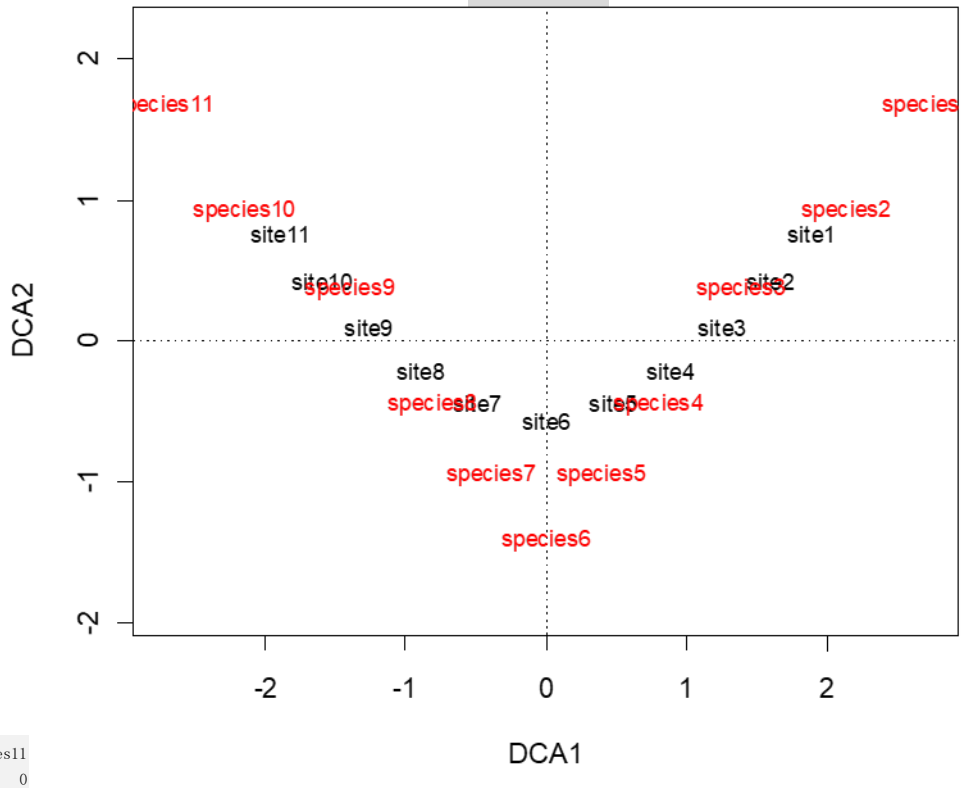
library(vegan); plot(decorana(species))

Cluster analysis



site	species1	species2	species3	species4	species5	species6	species7	species8	species9	species10	species11
site1	10	8	6	4	2	0	0	0	0	0	0
site2	8	10	8	6	4	2	0	0	0	0	0
site3	6	8	10	8	6	4	2	0	0	0	0
site4	4	6	8	10	8	6	4	2	0	0	0
site5	2	4	6	8	10	8	6	4	2	0	0
site6	0	2	4	6	8	10	8	6	4	2	0
site7	0	0	2	4	6	8	10	8	6	4	2
site8	0	0	0	2	4	6	8	10	8	6	4
site9	0	0	0	0	2	4	6	8	10	8	6
site10	0	0	0	0	0	2	4	6	8	10	8
site11	0	0	0	0	0	0	2	4	6	8	10

DCA



Assignment

General objectives: learn about PCA

- Develop a dataset to perform PCA
- Describe your data, e.g. X1, X2, X3, etc.
- Plot explained variance (by PCs), loadings and scores, explain the relationship between variables, between scores, and variable-score association.